

NEW ENGLAND
COMPLEX SYSTEMS
INSTITUTE
BOOK SERIES

Springer:
COMPLEXITY

Ali A. Minai
Dan Braha
Yaneer Bar-Yam
Editors

Unifying Themes in Complex Systems

VOLUME V

Proceedings
of the Fifth International Conference
on Complex Systems



Springer



NECSI

Unifying Themes in Complex Systems

Volume V

Springer Complexity

Springer Complexity is a publication program, cutting across all traditional disciplines of sciences as well as engineering, economics, medicine, psychology and computer sciences, which is aimed at researchers, students and practitioners working in the field of complex systems. Complex Systems are systems that comprise many interacting parts with the ability to generate a new quality of macroscopic collective behavior through self-organization, e.g., the spontaneous formation of temporal, spatial or functional structures. This recognition, that the collective behavior of the whole system cannot be simply inferred from the understanding of the behavior of the individual components, has led to various new concepts and sophisticated tools of complexity. The main concepts and tools – with sometimes overlapping contents and methodologies – are the theories of self-organization, complex systems, synergetics, dynamical systems, turbulence, catastrophes, instabilities, nonlinearity, stochastic processes, chaos, neural networks, cellular automata, adaptive systems, and genetic algorithms.

The topics treated within Springer Complexity are as diverse as lasers or fluids in physics, machine cutting phenomena of workpieces or electric circuits with feedback in engineering, growth of crystals or pattern formation in chemistry, morphogenesis in biology, brain function in neurology, behavior of stock exchange rates in economics, or the formation of public opinion in sociology. All these seemingly quite different kinds of structure formation have a number of important features and underlying structures in common. These deep structural similarities can be exploited to transfer analytical methods and understanding from one field to another. The Springer Complexity program therefore seeks to foster cross-fertilization between the disciplines and a dialogue between theoreticians and experimentalists for a deeper understanding of the general structure and behavior of complex systems.

The program consists of individual books, books series such as “Springer Series in Synergetics”, “Institute of Nonlinear Science”, “Physics of Neural Networks”, and “Understanding Complex Systems”, as well as various journals.



New England Complex Systems Institute

President

Yaneer Bar-Yam

New England Complex Systems Institute

238 Main Street Suite 319

Cambridge, MA 02142, USA

For over ten years, the New England Complex Systems Institute (NECSI) has been instrumental in the development of complex systems science and its applications. NECSI conducts research, education, knowledge dissemination, and community development around the world for the promotion of the study of complex systems and its application for the betterment of society.

NECSI was founded by faculty of New England area academic institutions in 1996 to further international research and understanding of complex systems. Complex-system science is a growing field that aims to understand how parts of a system give rise to the system's collective behaviors, and how it interacts with its environment. These questions can be studied in general, and they are also relevant to all traditional fields of science.

Social systems formed (in part) out of people, the brain formed out of neurons, molecules formed out of atoms, and the weather formed from air flows are all examples of complex systems. The field of complex systems intersects all traditional disciplines of physical, biological and social sciences, as well as engineering, management, and medicine. Advanced education in complex systems attracts professionals, as complex-systems science provides practical approaches to health care, social networks, ethnic violence, marketing, military conflict, education, systems engineering, international development and counter-terrorism.

The study of complex systems is about understanding indirect effects. Problems we find difficult to solve have causes and effects that are not obviously related. Pushing on a complex system "here" often has effects "over there" because the parts are interdependent. This has become more and more apparent in our efforts to solve societal problems or avoid ecological disasters caused by our own actions. The field of complex systems provides a number of sophisticated tools, some of them conceptual, helping us think about these systems; some of them analytical, for studying these systems in greater depth; and some of them computer-based, for describing, modeling or simulating them.

NECSI research develops basic concepts and formal approaches as well as their applications to real-world problems. Contributions of NECSI researchers include studies of networks, agent-based modeling, multiscale analysis and complexity, chaos and predictability, evolution, ecology, biodiversity, altruism, systems biology, cellular response, health care, systems engineering, negotiation, military conflict, ethnic violence, and international development.

NECSI uses many modes of education to further the investigation of complex systems. Throughout the year, classes, seminars, conferences and other programs assist students and professionals alike in their understanding of complex systems. Courses have been taught all over the world: Australia, Canada, China, Colombia, France, Italy, Japan, Korea, Portugal, Russia and many states of the U.S. NECSI also sponsors post-doctoral fellows, provides research resources, and hosts the International Conference on Complex Systems as well as discussion groups and web resources.



New England Complex Systems Institute
Book Series

Series Editor

Dan Braha

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The world around us is full of the wonderful interplay of relationships and emergent behaviors. The beautiful and mysterious way that atoms form biological and social systems inspires us to new efforts in science. As our society becomes more concerned with how people are connected to each other than how they work independently, so science has become interested in the nature of relationships and relatedness. Through relationships elements act together to become systems, and systems achieve function and purpose. The elements act together to become systems, and systems achieve function and purpose. The study of complex systems is remarkable in the closeness of basic ideas and practical implications. Advances in our understanding of complex systems give new opportunities for insight in science and improvement of society. This is manifest in the relevance to engineering, medicine, management and education. We devote this book series to the communication of recent advances and reviews of revolutionary ideas and their application to practical concerns.

Unifying Themes in Complex Systems V

*Proceedings of the
Fifth International Conference on Complex Systems*

**Edited by Ali Minai, Dan Braha
and Yaneer Bar-Yam**

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INTRODUCTION

The mysteries of highly complex systems that have puzzled scientists for years are finally beginning to unravel thanks to new analytical and simulation methods. Better understanding of concepts like complexity, emergence, evolution, adaptation and self-organization have shown that seemingly unrelated disciplines have more in common than we thought. These fundamental insights require interdisciplinary collaboration that usually does not occur between academic departments. This was the vision behind the first International Conference on Complex Systems in 1997: not just to present research, but to introduce new perspectives and foster collaborations that would yield research in the future.

As more and more scientists began to realize the importance of exploring the unifying principles that govern all complex systems, the 2004 ICCS attracted a diverse group of participants representing a wide variety of disciplines. Topics ranged from economics to ecology, from physics to psychology and from business to biology. Through pedagogical, breakout and poster sessions, conference attendees shared discoveries that were significant both to their particular field of interest, as well as to the general study of complex systems. These volumes contain the proceedings from that conference.

Even with the fifth ICCS, the science of complex systems is still in its infancy. In order for complex-systems science to fulfill its potential to provide a unifying framework for various disciplines, it is essential to provide a standard set of conventions to facilitate communication. This is another valuable function of the conference: it allowed an opportunity to develop a common foundation and language for the study of complex systems.

These efforts have produced a variety of new analytic and simulation techniques that have proven invaluable in the study of physical, biological and social systems. New methods of statistical analysis led to better understanding of polymer formation and complex fluid dynamics; further development of these methods has deepened our understanding of patterns and networks. The application of simulation techniques such as agent-based models, cellular automata and Monte Carlo calculations to complex systems has increased our ability to understand and even predict behavior of systems which once seemed completely unpredictable.

The concepts and tools of complex systems are of interest not only to scientists, but also to corporate managers, doctors, political scientists and policy makers. The same rules that govern neural networks apply to social or corporate networks, and professionals have started to realize how valuable these concepts are to their individual fields. The International Conferences on Complex Systems have provided the opportunity for professionals to learn the basics of complex systems and share their real-world experience in applying these concepts.

ORGANIZATION

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Helen Harte - NECSI

Ali Minai - University of Cincinnati

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Len Troncale - California State Polytechnic University
Chris Wiggins - Columbia University
Marlene Williamson
David Wolpert - NASA Ames Research Center

CONFERENCE PROGRAMME

SUNDAY, May 16

9:00AM–5:00PM PEDAGOGICAL SESSIONS

EVE MITLETON-KELLY – Pedagogical Sessions

- ANDREW WUENSCHÉ – *Studying discrete dynamical networks with DDLab*
- URI WILENSKY – *Modeling complex systems*
- JOHN PETER WIKSWO – *From physics to medicine*
- LEV LEVITIN – *Entropy and information*

URI WILENSKY – Pedagogical Sessions

- GREG CHAITIN – *Mathematics*
- PHILIP BALL – *History of social modeling*
- BILL HILLIER – *Urban space syntax*
- STEPHEN WOLFRAM – *New science*

EVENING RECEPTION

Stephen Heuser (*The Boston Globe*) and Tom Siegfried (*The Dallas Morning News*)

- ALVIN AND HEIDI TOFFLER – *The Future*

MONDAY, May 17

8:50AM–9:00AM CONFERENCE WELCOME

- YANEER BAR-YAM – **Conference Welcome**

9:00AM–10:30AM EMERGENCE

JOHN STERMAN – Emergence

- STEVEN STROGATZ – *Synchrony*
- ALAN GUTH – *Inflationary universe*

11:00AM–12:30PM NETWORKS

IRVING EPSTEIN – Networks

- GENE STANLEY – *Networks and Liquid Water*
- LEON COOPER – *Neural networks in vision*

1:30PM–2:50PM NETWORKS**IRVING EPSTEIN – Networks**

- NEO MARTINEZ – *Food Webs*
- RICARD SOLE – *Complex networks*

3:20PM–4:50PM ROBOTS**ALI MINAI – Robots**

- STEFANO NOLFI – *Evolving Swarm-Bots*
- WEI-MIN SHEN – *Self-Reconfigurable Robots and Digital Hormones*

6:00PM–9:00PM EVENING PARALLEL SESSIONS**ROGER HURWITZ – Social Systems**

- DUNCAN A. ROBERTSON – *A Dynamic Model of Inter-Firm Competition*
- KAZUYUKI IKKO TAKAHASHI – *An application of percolation theory on political science*
- CESAR E. GARCIA-DIAZ – *Market Partitioning Under Varying Resource Landscapes*
- CHRISTOPHER NEWMAN – *Revolution by Osmosis: A Case Study of West Florida, Texas, California and Hawaii*
- MAKINEN SAKU – *System dynamics approach to evolution and process of corporate political action*
- BRIAN LONSWAY – *A Self-Organizing Neural System For Urban Design*
- SORIN BAICULESCU – *Mathematical models of stochastic level that may be used within the complex system of ferry-boat sea navigation*
- DAVID SYLVAN – *Organized All the Way Down: The Local Complexity of “Thick” Social Systems*
- VLADISLAV KOVCHEGOV – *A model of communications as random walk on the semantic tree*
- B. COHEN – *Modelling the Enterprise and its Actors as Triply-Articulated Anticipatory Systems*
- DADANG SUBARNA – *Validation and Verification of Money Market Forecasting with a Non-Linear Method (USD vs IDR Currency Case)*
- CARLOS PARRA – *Evolutionary Dynamics of Knowledge*
- ANDREAS KEMPER – *Network Externalities in Corporate Financial Management*
- PASCAL MOSSAY – *Economic Geography and Rational Expectations*

CEFN HOILE – Concepts, Formalisms, Methods and Tools

- DANIEL JOSHUA STEINBOCK – *Self-Modeling Networks*
- ELIZAVETA PACHEPSKY – *A conceptual framework for mechanisms of self-organization*
- PABLO SANCHEZ-MORENO – *Information Planes for Complex Systems*
- TED BACH – *Using SIMP, a Laboratory for Cellular Automata and Lattice-Gas Experiments*
- WILLIAM SULIS – *Archetypal Dynamical Systems*
- LEN TRONCALE – *Is Artificial “Systems” Research Possible?*
- DAVID H. WOLPERT – *Metrics for sets of more than two points*
- DAVID H. WOLPERT – *Self-dissimilarity as a high dimensional complexity measure*
- HIDESHI ISHIDA – *Linearly time-dependent information on invariant set*
- SETH TISUE – *NetLogo: A Simple Environment for Modeling Complexity*
- RICARDO NIEVA – *An ANC Analytical Payoff Function for 3-Agent Multistage-Network Games with Endogenous Coalitions and Communication Structures*

HIROKI SAYAMA – Evolution and Ecology

- STEVEN S. ANDREWS – *Simulated niche partitioning by bacteria*
- ARIEL CINTRON-ARIAS – *Rumors on Complex Attractors*
- JACOB BEAL – *Predictive Modelling for Fisheries Management in the Colombian Amazon*
- DONNA K. FISHER – *Complexities of River Basin Management, The Case of the Pitimbu River in Brazil.*
- MBABAZI DISMAS – *Trophic structure of the fish communities in the Kyoga Basin lakes (East Africa) based on stable Nitrogen and Carbon isotopes.*
- GUY HOELZER – *A new model for exploring emergent phenomena in spatially explicit ecology and evolution*
- YUN ZHOU – *An approach to holistic ecological risk assessment: Food web responses to a warmed climate as a case study*
- TOLIBJON E. BURIYEV – *Bifurcation Study of Self-Oscillatory and Chaos Regimes in Predator-Prey Systems.*

- MICHAEL HAUHS – *A new type of models for managed ecosystems*
- RICARDO AZEVEDO – *The Simplicity of Metazoan Cell Lineages*
- PAN-JUN KIM – *Spatio-temporal Dynamics in the Origin of Genetic Information*
- JORGE DE BARROS PIRES – *Cognitus*
- THOMAS HILLS – *Animal foraging and the evolution of goal-directed cognition*

ALI MINAI – Learning / Neural, Psychological and Psycho-Social Systems

- BROCK DUBBELS – *Teaching Complex Systems in the Classroom with Video Games*
- OREN ZUCKERMAN – *Hands-on modeling and simulation of systems concepts*
- ARNO KLEIN – *Activity patterns in the brain: breaking up the problem into pieces*
- YUE JIAO – *Neuro-fuzzy modeling of human fatigue*
- IGOR YEVIN – *Controlling Chaos in the Brain and Structure of Music Tonality*
- PIETRO PANZARASA – *The Emergence of Collective Cognition in Social Systems*
- ADAM DOBBERFUHL – *Environmental Complexity Influences Visual Acuity in Cichlid Fishes*
- BURTON VOORHEES – *Cognitive Illusions and the Evolution of Science*
- MIHNEA MOLDOVEANU – *The Economics of Cognition. I. Algorithmic Information-Theoretic Explanation of Cognitive Biases and Fallacies*
- MIHNEA MOLDOVEANU – *The Economics of Cognition II. Fundamental Cognitive Choices that Shape Adaptation to Complexity*
- OLGA MITINA – *The use of fractal dimension calculation algorithm to determine the nature of autobiography memoirs.*
- MICHAEL D. FISCHER – *Indigenous Knowledge Systems: Emergent order and the internal regulation of shared symbolic systems*
- JENNIFER GOLBECK – *Complex Systems Analysis on the Semantic Web*

Networks

- ANDRE X. C. N. VALENTE – *2-Peak and 3-Peak Optimal Complex Networks*
- JOAO RODRIGUES – *Network dimension and the topology of life*
- MAZIAR NEKOVEE – *Rumor-like information dissemination in complex computer networks*
- JUKKA-PEKKA ONNELA – *Studies in correlation based financial networks*
- JEVIN WEST – *Comparing the dynamics of stomatal networks to the problem-solving dynamics of cellular computers*
- NATHAN EAGLE – *Genetically Modified Network Topologies*
- MARKUS BREDE – *Interaction networks of agents that exploit resources*
- BYUNGNAM KAHNG – *Avalanche dynamics on complex networks*
- WILLIAM SULIS – *Phase Transitions in Random Graphical Dynamical Systems*
- YONG-YEOL AHN – *Extremely clustered network*
- M.V. SIMKIN – *Theory of Aces: Fame by chance or merit?*

Physical Systems

- THOMAS PORTEGYS – *A Robust Game of Life*
- NATALIA A. BRYKSINA – *Fractal Statistics of Oscillatory Zoning Patterns in Calcite: A Qualitative and Quantitative Comparison of Modeled Zoning Patterns*
- MICHAEL BUKATIN – *“Russian Troika” as the New Spatio-Temporal Paradigm*
- EUGENIO DEGROOTE – *Fire Safety on Flame Spreading Over Liquid Fuels*
- MIKA LATVA-KOKKO – *Capillary rise and fluid-solid contact angle in Lattice Boltzmann simulations*
- S. POPESCU – *Physical basis of the self-organization at critically concept*
- HAI LIN – *$1/f$ Random Fields, Scaling Properties and Local Averages*
- KONSTANTIN L KOUPISOV – *Short Time Quantum Revivals in Chaotic Quantum Systems.*

- PRAGYA SHUKLA – *Level Statistics of Complex Systems*
- YONGTAO GUAN – *Spatial self-organization in interacting particle systems with cyclic local dynamics*

9:00PM–10:00PM INITIAL POSTER SESSION

Systems Biology

- DOLOMATOV M. YU. – *Features of Equilibrium Thermodynamics: Complex Systems with Chaos of Chemical Constitutions and Allocation of Organic Matter in the Universe*
- MITRA SHOJANIA – *The effect of minus ends on the microtubule steady state*
- SIMONETTA FILIPPI – *Complex Dynamics of the Cardiac Rhythms*
- VAL BYKOSKI – *Emergence of Genome: Generalization and Use of Environmental Information by Cell*
- JOSEPH G. HIRSCHBERG – *Fluorescence Imaging for Complex Dynamic Interactions of Organelles in Living Cells*
- LEN TRONCALE – *Systems Pathology as Systems Biology*
- RENHUA LI – *Modeling pleiotropic genetic systems in mice*
- JIYONG PARK – *Computational study on mechanical properties of self-assembled peptide filaments*
- MICHAEL L. BLINOV – *Modeling combinatorial complexity of signal transduction systems*

Networks and Structural Themes

- ATIN DAS – *From Bibliometrics to Webometrics: A Case Study*
- MANUEL MIDDENDORF – *Classification of Biological Networks Via Walks and Words*
- ERIK VOLZ – *Random graphs with clustering and arbitrary degree distribution*

Socio-economic Systems

- DAVID SAAKIAN – *Inter-hierarchic resonance in complex systems: search of anti-resonance situation.*
- VLADISLAV KOVCHegov – *The inhomogeneous product-potential social systems*

- PIERPAOLO ANDRIANI – *Power Law Phenomena in Organizations*
- VLADISLAV KOVCHegov – *The dynamic of product potential social systems and representation theory*
- ATIN DAS – *What Does Composite Index Of NYSE Represent In The Long Run?*
- HYUNG SAM PARK – *Evolution of Organizational Rationality in Social Complexity: Interorganizational Networks in Environmental Biotechnology Industry*
- HIROYUKI MASUDA – *Integrated Model of Emergency Evacuation of People after a Big Earthquake at the Busy Quarter near a Major Junction Station in Suburban Tokyo*
- JAMES K. HAZY – *Simulating Agent Intelligence as Local Network Dynamics and Emergent Organizational Outcomes*
- XIANG SAN LIANG – *Evolution of Money Distribution in a Simple Economic Model*
- DMITRY CHISTILIN – *To the wave nature of the economy cycle*
- INGAR MALMGREN – *The Complex Economics of Innovation, – Implications for the Shipping Industry*
- MARCIA ESTEVES AGOSTINHO – *The Building-Block Advantage*
- PAUL LANG – *An Essay on SFEcon's "Perfect Markets Model"*
- M.V. SIMKIN – *Stochastic modeling of citation slips*
- PIERPAOLO ANDRIANI – *Modelling diffusion of innovation using Cellular Neural Network approach*
- ALEX YAHJA – *A Model of Biological Attacks on a Realistic Population*
- CARLOS PARRA – *Evolutionary Dynamics of Knowledge*

Engineering Systems

- ALEX J. RYAN – *Hybrid Complex Adaptive Engineered Systems: A Case Study in Defence*
- MARK S. VOSS – *Cellular Automata + GMDH = Emergent Programming: A New Methodology for Hardware Intelligence*
- VLADISLAV KOVCHegov – *The Linguistic Models of Industrial and Insurance Companies*
- KATHARINE MULLEN – *Human-Technology Integration*

- SUMATHI SEETHARAMAN – *Self-Organized Scheduling of Node Activity in Large-Scale Wireless Sensor Networks*
- KAMPAN SAINI – *Artificial Neural NetworkBased Offline Hand written character recognition for Postal Services*
- REZA MEHRABANI – *Statistical Modeling of Creep Strength of Austenitic Stainless Steels*
- REZA MEHRABANI – *Statistical Modeling of Austenite Formation in Steels*
- GUSTAVO A. SANTANA TORRELLAS – *A Framework for Security Model Innovation using Knowledge Engineering*

Evolution and Ecology / Population Change

- DAVID SAAKIAN – *Exact error threshold for Eigen model with general fitness and degradation rate functions.*
- MARGARETA SEGERSTAHL – *Coupling sexual reproduction and complex multicellularity*
- LEN TRONCALE – *Using Systems Isomorphies to Explore the Feasibility of Giant Planet, Wetlab, Origins of Life Simulations*

Nonlinear Dynamics and Pattern Formation

- BURTON VOORHEES – *Emergence of Cellular Automata Rules Through Fluctuation Enhancement*
- CHIH-HAO HSIEH – *Regime shifts or red noise?*

Physical Systems, Quantum and Classical

- BHARAT KHUSHALANI – *Vortex Analogue of Molecules*
- JONATHAN VOS POST – *Imaginary Mass, Force, Acceleration, and Momentum*
- JONGJIN LEE – *Slow relaxations of randomly packed ball bearings*
- ALESSANDRO PLUCHINO – *Glassy dynamics hindering synchronization in a Hamiltonian system*

Learning / Neural, Psychological and Psycho-social Systems

- MIHNEA MOLDOVEANU – *The Economics of Cognition. III. A Weak Axiom of Revealed Cognitive Preference*

- CHRISTOPHER NEWMAN – *An Analysis of the Complexity of the System Everything Developed from and Raised from Heaven and Earth is in its Proper Place of Form Mind Boxing*
- S. HAGBERG – *Human interaction and nonlinear oscillators*
- TETSUJI EMURA – *A Coupled Oscillator Model for Emergent Cognitive Process*
- ROSEMARY WILLIAMS WRAY – *Towards More Generative Evaluation, Research and Assessment (ERA) in Education*
- DONG-UK HWANG – *Multistability of Coupled Neuronal Nets with Multiple Synapses*
- LEN TRONCALE – *Science General Education As A Way to Attract More Students to Studying Complex Systems*

Concepts, Formalisms, Methods and Tools

- AXEL G. ROSSBERG – *A generic scheme for choosing models and characterizations of complex systems*
- SORIN BAICULESCU – *Mathematical Aspects in Complexity of Biological, Neuro-Physiological and Psychological Systems*
- RUSS ABBOTT – *Emergence and Entities*
- P. FRAUNDORF – *Net surprisals ala Tribus: correlations from reversible thermalization*
- DAVID H. WOLPERT – *Adaptive Metropolis Sampling with Product Distributions*
- MARK AVRUM GUBRUD – *Defining “nano” in terms of complexity*
- GILBERT G. CHEN – *On Simulated Time*
- ROBERT CLEWLEY – *Dominant-scale analysis for automatic reduction of high-dimensional ODE systems*

Other Complex Systems Topics

- GERARD S. LEMIRE – *Formating Complex Systems and Aspects of Cross-disciplinary Research*
- DANIEL POLANI – *Defining Emergent Descriptions by Information Preservation*

TUESDAY, May 18**9:00AM–12:20PM EVOLUTION****CHARLES GOODNIGHT – Evolution**

- STUART KAUFFMAN – *Understanding Genetic Regulatory Networks: the ensemble approach*
- ALAN PERELSON – *Immunological Evolution*
- MARTIN NOWAK – *Evolutionary systems*
- LISA MARIE MEFFERT – *Experiments on the escape from extinction: Lessons from the common housefly.*

2:00PM–5:00PM AFTERNOON BREAKOUT SESSIONS**CHRISTINA STOICA – Social Systems**

- DWIGHT READ – *Change in the Form of Evolution: Transition from Primate to Hominid Forms of Social Organization*
- ROBERT G. REYNOLDS – *The Role of Culture in the Emergence of Decision-Making Roles: An Example Using Cultural Algorithms*
- CLAUDIO CIOFFI-REVILLA – *A Canonical Theory of Origins and Development of Social Complexity*
- JUERGEN KLUEVER – *The emergence of social order by the communicative generation of social types*

Networks

- RICH COLBAUGH – *Analysis of Complex Netowkrs Using Limited Information*
- STEVE KRONE – *On the Evolution of Structure in Ecological Networks*
- NISHA MATHIAS – *Small Worlds – How and Why*
- YING-CHENG LAI – *Synchronization in complex networks*
- LJUPCO KOCAREV – *Synchronization in complex network topologies*
- VALENTIN ZHIGULIN – *Dynamical Motifs: Building Blocks of Complex Network Dynamics*
- ROBERT PRILL – *Modeling Network Motifs as Linear Dynamical Systems*
- GYORGY KORNISS – *Extreme Fluctuations in Small-Worlds with Relaxational Dynamics and Applications to Scalable Parallel Computing*

GUY HOELZER – Evolution and Ecology

- JUSTIN WERFEL – *The evolution of reproductive restraint through social communication*
- ERIK RAUCH – *Diversity is unevenly distributed within species*
- JOSH MITTELDORF – *Selection in Ecosystems*
- KEI TOKITA – *Diversity dynamics in large complex biological networks*
- MADHUR ANAND – *Quantification of Biocomplexity*
- DANIEL S. FISHER – *The rate of evolution: Is anything understood?*

2:00PM–5:00PM AFTERNOON EXTENDED TALK SESSIONS

LEN TRONCALE – Systems Biology

- BENJAMIN J DUBIN-THALER – *Cell Motility: How Cellular Machines Generate Precise Responses in a Complex Environment*
- KEITH AMONLIRDVIMAN – *Mathematical modeling of planar cell polarity to understand domineering non-autonomy*
- CRAIG VAN HORNE – *The Basal Ganglia as a Complex system as it Relates to Normal Movement and Movement Disorders.*
- MARKUS BREDE – *Random Evolution of Idiotypic Networks: Dynamics and Architecture*
- ERIC MJOLSNESS – *Network Dynamics for Systems Biology*
- JENNIFER HALLINAN – *Tunable Asynchrony in an Artificial Genome Model of a Genetic Regulatory Network*
- BEN GOERTZEL – *Integrative Artificial Intelligence as a Key Ingredient of Systems Biology*
- TAESIK LEE – *A Function-Based Approach to Systems Biology*
- CHEOL-MIN GHIM – *Assessing lethality in the genome-scale metabolic network of Escherichia coli*

WILLIAM SULIS – Concepts, Formalisms, Methods and Tools

- ABHIJNAN REJ – *Multiscale Coordination and Dynamical Similarity*
- ROBERT CLEWLEY – *Dominant-scale analysis for automatic reduction of high-dimensional ODE systems*
- NED J. CORRON – *Information Flow in Synchronization*

- DMITRY NERUKH – *Statistical complexity of protein folding: application of computational mechanics to molecular dynamics*
- PRITHA DAS – *Classification of Indian Songs in Context of Complexity Measure*
- MICHAEL BAYM – *An analytical demonstration of adaptation to the edge of chaos*
- STEVEN H. BERTZ – *The Complexity of Graphs and Digraphs*
- MANOJ GAMBHIR – *Possible Steps Toward a Theory of Organization*
- CLAIRE MARTINET-EDELIST – *An experimentation strategy directed by kinetic logic*

7:00PM–10:00PM EVENING BREAKOUT SESSIONS

JEFF CARES – Social Systems

- IRENE CONRAD – *Educational Reform at the Edge of Chaos*
- CARLOS E. MALDONADO – *Complexity and the Social Sciences*
- LOUISE K. COMFORT – *Modeling Complexity in Disaster Environments*
- NANCY HAYDEN – *Knowing Terrorism as a Complex Adaptive System*
- EDWARD P. MACKERROW – *Agent-Based Simulation of the Demand for Islamist Terrorist Organizations*
- MAJOR MARK T. CALHOUN – *Complexity and Army Transformation*
- ROGER HURWITZ – *Computing the Battle for Hearts and Minds: Lessons from the Vendee*

JOEL MACAUSLAN – Nonlinear Dynamics and Pattern Formation

- TEEMU LEPPANEN – *Morphological diversity and robustness of Turing structures*
- MARTA IBANES – *A gradient model for proximo-distal differentiation in vertebrate limbs*
- DANIEL COORE – *Towards a Universal Language for Amorphous Computing*
- A. BRAD MURRAY – *Pattern Formation from Emergent, Finite Amplitude Interactions: the Example of Sandy-Coastline Evolution*
- ELEENNA DUGUNDJI – *Socio-Dynamic Discrete Choice: Analytical Results for the Nested Logit Model*

- E. LOZNEANU – *Self-organized plasma blobs as possible precursors of life*
- YING ZHANG – *3D Substitution Model for Limb Growth and Pattern Formation*

7:00PM–10:00PM EVENING EXTENDED TALK SESSIONS

JEFF SCHANK – Learning / Neural, Psychological and Psycho-Social Systems

- THEA LUBA – *MediaMetro / Museocracy / SonicMetro: A New Complex Systems Model for Arts Education*
- WENJIE HU – *Dynamics of Innate Spatial-Temporal Learning Process: Data Driven Education Results Identify Universal Barriers to Learning*
- GOTTFRIED MAYER-KRESS – *Multiple Time-Scale Landscape Models of Motor Learning*
- ROBERT K. LOGAN – *The Emergence of Language and Culture out of the Complexity of Hominid Existence*
- BRIAN D. JOSEPHSON – *How we might be able to understand the brain*
- CHRISTIAN MACHENS – *A push-pull model of prefrontal cortex during a sequential discrimination task*
- KARL YOUNG – *Global MRI Diagnostic Tools Via Statistical Complexity Measures*
- CAROLINE YOON – *Emergent Mathematical Ideas from Complex Conceptual Systems*
- LIQIANG ZHU – *Impacts of homo- and hetero- synaptic plasticities on neuronal networks*

Evolution and Ecology

- MANUEL MENDOZA-GARCIA – *How Communities Evolve*
- HIROKI SAYAMA – *Self-Protection and Diversity in Self-Replicating Cellular Automata*
- KOJI OHNISHI – *Autopoietic learning–neural network-like biomachinogenesis via semeiogenesis: A unified theory on the cognitive genesis and evolution of biosystems*
- AXEL G. ROSSBERG – *Holling cycles in simulations of complex food webs*
- JOHN W. PEPPER – *Emergent segregation and over-mixing from symmetric movement rules*

- WILLIAM SILVERT – *Speciation through Bifurcation*
- ANATOLY BRILKOV – *Mathematical and Experimental Modeling of Biological Evolution by the Example of Recombinant Bacteria at Continuous Cultivation*
- MICHAEL LEVANDOWSKY – *Complexity Measures for Ecological Assemblages*
- HANNELORE BRANDT – *Indirect Reciprocity and the Evolution of Morals*

WEDNESDAY, May 19

9:00AM–12:20PM SOCIAL SYSTEMS

MIRIAM HELLER – Social Systems

- THEODORE BESTOR – *Tracking global sushi*
- THOMAS HOMER-DIXON – *Complexity of global systems*
- SCOTT E PAGE – *Diversity: Aggregation or Perspectives and Heuristics*
- STEVEN ALAN HASSAN – *Strategic Interaction Approach: Complex Systems and Undoing Cult Mind Control*

2:00PM–3:30PM AFTERNOON BREAKOUT SESSIONS

Special Session

- MAYA PACZUSKI – *Scale Free Networks of Earthquakes and Aftershocks*
- EVE MITLETON-KELLY – *An Integrated Methodology to Facilitate The Emergence of New Ways of Organising*

HELEN HARTE – Healthcare

- FRANK FUNDERBURK – *Organizational Culture from a Complex Dynamic Systems Perspective: Moving from Metaphor to Action in Healthcare*
- ANITA PATIL – *Modeling Safety Outcomes on Patient Care Units*
- SALIL H. PATEL – *Complex Medical Information Systems: A Social Context*

LISA MARIE MEFFERT – Origins

- BRUCE WEBER – *Complex Systems Dynamics and the Emergence of Life and Natural Selection*
- TERRENCE W. DEACON – *Minimal conditions for natural selection*

2:00PM–5:00PM AFTERNOON PARALLEL SESSIONS**SUI HUANG – Systems Biology**

- MUNEESH TEWARI – *Systematic Interactome Mapping and Genetic Perturbation Analysis of a C. elegans TGF- β signaling network*
- JOHANNES SCHUCHHARDT – *Peptide Binding Landscapes*
- WILLIAM SILVERT – *Complexity and Allometry*
- CRISTIAN I. CASTILLO-DAVIS – *Where the earth meets the sky: understanding cis-regulatory evolution through genomics*
- PAULI RAMO – *Evolution of Gene Regulatory Networks: Growth and Dynamics*
- VADIM KVITASH – *Games Systems Play*
- CHRIS WIGGINS – *Information-theoretic measures of biological network modularity*
- JEONG SEOP SIM – *Transcription Factor Binding Sites Prediction based on Sequence Similarity*
- JORGE DE BARROS PIRES – *Clothing Earth with Mind*
- HAO XIONG – *Sensitivity Analysis of Optimal Production of Biomass in Metabolic Networks*
- MOMIAO XIONG – *Generalized Circuit Analysis of Biological Networks*

3:30PM–5:00PM AFTERNOON PARALLEL SESSIONS**Social Systems**

- TAKESHI ARAI – *Estimation of the Functions Describing Transition Potentials of Land Use at Cells Applied to Cellular Automata Based Models of Land Use*
- SANTA LA ROCCA – *Strategy emergence. A journey through modernism, postmodernism, complexity and nonmodernism*
- PHILIP VOS FELLMAN – *The Nash Equilibrium Revisited: Chaos and Complexity Hidden in Simplicity*
- SERGE HAYWARD – *An Artificial Neural Network for Simulating the Complex Dynamics of Financial Assets Prices*
- BILL MACMILLAN – *Modeling spatial economics with an agent-based approach*
- BRIAN RUBINEAU – *Job Sex Segregation As A Complex System: Exploring a Simulation Approach*

FRED M. DISCENZO – **Engineering Systems**

- SARJOUN DOUMIT – *Cartography application for autonomous sensory agents*
- MARINA A. EPELMAN – *A fictitious play approach to large-scale complex systems optimization*
- BENJAMIN KOO – *Architecting Systems Under Uncertainty with Object-Process Networks*
- DANIEL D. FREY – *Effect Sparsity, Heirarchy, and Inheritance: How System Structure Affects Robust Design of Engineering Systems*
- JONATHAN R. A. MAIER – *Understanding the Complexity of Design*
- PELIN GUVEN – *Separation of Real World Mixed Acousting Signals by Using Frequency Domain Approach*

DAN COORE – **Nonlinear Dynamics and Pattern Formation**

- BHARAT KHUSHALANI – *Polyhedral Pattern Formation*
- ILAN HARRINGTON – *Design and robustness of delayed feedback controllers for discrete systems*
- SATISH T.S. BUKKAPATNAM – *Complex Nonlinear stochastic dynamics of precision grinding operations: Implications for health monitoring and control*
- REZA RASTEGAR – *Chaotic Dynamics of Cellular Learning Automata*
- DAVID GOMEZ MIGUEZ – *Directional grow in chemical and biological pattern formation systems*
- ANDREW WUENSCHÉ – *Self-reproduction by glider collisions*
- MADALENA DAMASIO COSTA – *Multiscale entropy analysis of complex physiologic time series: Information loss with aging and disease*

Evolution and Ecology

- CHIN-KUN HU – *Quantum Spin Systems as Models for Biological Evolution*
- JAVIER A. ALCAZAR – *A Multi Agent Based Approach to the Multi-Predator Multi-Prey Pursuit Domain*
- MARGARETA SEGERSTAHL – *Coupling sexual reproduction and complex multicellularity*

- DANIEL SOLOW – *Mathematical Models for Explaining the Emergence of Specialization in Performing Tasks*
- ERIK RAUCH – *Long-range interactions and evolutionary stability in predator-prey systems*

YING-CHENG LAI – Physical Systems

- PABLO I. HURTADO – *Escape from Metastable States in a Nonequilibrium Environment*
- WM. C. MCHARRIS – *Chaos as a Bridge between Determinism and Probability in Quantum Mechanics*
- PIERRE EVESQUE – *Efficient reduction of complexity and non ergodicity due to dissipation: the case of a single ball in a vibrating box*
- DAVID SAAKIAN – *Universality classes of complexity*
- RICHARD METZLER – *Information flow through a chaotic channel : prediction and postdiction at finite resolution*

6:15PM–7:45PM BANQUET

6:50PM–7:30PM Global Social Systems and the Prevention of Tragic Conflict and Human Suffering

- ROBERT S. MCNAMARA – *Interview: Lessons from Experience*

7:45PM–9:30PM BANQUET SESSION

- KEITH CAMPBELL – *Cloning Dolly*

THURSDAY, May 20

9:00AM–12:20PM ENGINEERING & INNOVATION

ERIC BONABEAU – Engineering & Innovation

- JERRY SUSSMAN – *Engineering complex systems*
- DOUGLAS O. NORMAN – *Complexity in the engineering of the Air and Space Operations Centers: Enterprise Engineering*
- BUD MISHRA – *VALIS or VANISH... (a survivor's guide to computational and systems biology?)*
- CARLISS BALDWIN – *Design rules*

2:00PM–5:00PM AFTERNOON BREAKOUT SESSIONS

DAVID H. WOLPERT – Collectives

- BILL MACREADY – *Experimental tests of product distribution theory*

- NEIL F. JOHNSON – *Network Engineering and Evolution Management: theory and practice*
- JEFF SHAMMA – *Multiagent Repeated Games and Convergence to Nash Equilibria*
- ILAN KROO – *Collectives, Optimization, and Distributed Design*
- STEFAN BIENIAWSKI – *Using Product Distributions for Distributed Optimization*

MARLENE WILLIAMSON – **Engineering Systems**

- DAVID ALDERSON – *The Role of Design in the Internet and Other Complex Engineering Systems*
- FRED M. DISCENZO – *Dynamic Reconfiguration of Complex Systems to Avoid Failure*
- DARIO MANCINI – *Design, development, management and social organization of new very large scientific plants. The case study of the GMT (Giant Modular Telescope)*
- CARLOS GERSHENSON – *Protocol Requirements for Self-organizing Artifacts: Towards an Ambient Intelligence*
- TAESIK LEE – *Fundamental Long-Term Stability Conditions for Design of Complex Systems: Equilibrium and Functional Periodicity*
- JORGE FINKE – *The Ecological Ideal Free Distribution and Resource Allocation in Distributed Computing and Control: Theory and Cross-Fertilization for Applications*

Networks / Systems Biology

- JANET WILES – *Mapping biology onto computation: modelling and analysis of artificial genetic regulatory networks*
- L. M. ROCHA – *Extraction and Semi-metric Analysis of Social and Biological Networks*
- ETAY ZIV – *Systematic identification of statistically significant network measures*
- ALI ZARRINPAR – *Optimization of Specificity in a Cellular Protein Interaction Network by Negative Selection*
- LAZAROS GALLOS – *Simulation of random walks and reaction-diffusion processes on scale-free networks*

- MARKUS BREDE – *Constructing Scale-Free Networks by a Matrix Stability Criterium*

ALLAN R. ROBINSON – Oceanography

- GLENN FLIERL – *Multiscale Physical Ocean Dynamical Processes*
- BRIAN ROTHSCCHILD – *Biological Patchiness in Interdisciplinary Ocean Dynamics*
- JAMES MCCARTHY – *Climate Processes and Ocean Event Dynamics*
- JAMES BELLINGHAM – *Systems Oceanography: Ocean Observing and Prediction Systems*
- PIERRE LERMUSIAUX – *ITR-Based Data Driven Systems for Ocean Science*
- IRA DYER – *The End-to-End Sonar System (Physical–Meteorological–Ocean Acoustics–Geoacoustics) for Naval Operations*

2:00PM–5:00PM AFTERNOON EXTENDED TALK SESSIONS

JUERGEN KLUEVER – Social Systems

- PHILIP V. FELLMAN – *Adaptation and Coevolution on an Emergent Global Competitive Landscape*
- MATT GROSSMANN – *Group Allegiance & Issue Salience in Factional Competition*
- DMITRI PUSHKIN – *Bank–mergers as scale–free coagulation*
- YURI MANSURY – *Power–Law Size Distribution in an Externality–Driven Model of City Systems*
- MERCEDES BLEDA-MAZA DE LIZANA – *Regional Innovation Systems and Complex Systems Theory: Towards a Common Agenda*
- FRANCESCA GINO – *Complementarity, frustration and complex organizations. A constraint satisfaction network model.*
- ALEX YAHJA – *A Model of Biological Attacks on a Realistic Population*
- UROOJ Q. AMJAD – *Self–organizing Social Networks: Issues with Hierarchy, Power Dynamics in Decision Making*

7:00PM–10:00PM EVENING BREAKOUT SESSIONS

CHRIS WIGGINS – Systems Biology

- J.R. SEMEIKS – *Biological information networks of genetic loci and the scientific literature*

- MACIEJ SWAT – *Bifurcation Analysis of Regulatory Modules in Cell Biology*
- SABRINA L. SPENCER – *An ordinary differential equation model for the multistep transformation to cancer*
- JONATHAN VOS POST – *The Evolution of Controllability in Enzyme System Dynamics*
- JESUS PANDO – *Multiscale Analysis of Protein Sequence Data*
- RENHUA LI – *Modeling pleiotropic genetic systems: Relating bone density and body size to genes*

MARKUS BREDE – **Agents**

- WILLIAM A. GRIFFIN – *Small n Evolving Structures: Dyadic Interaction between Intimates*
- JEFFREY SCHANK – *A Multi-Modeling Approach to the Study of Animal Behavior*
- MICHAEL E. ROBERTS – *Modeling Complex Foraging Behavior*
- BURTON W. ANDREWS – *Social Foraging Theory for Multiagent Decision-Making System Design*
- FELIX REED-TSOCHAS – *Navigating through Network Structures in Strategic Decision Space*
- ROBERT GHANEA-HERCOCK – *Security Agents and Network Immunology*

7:00PM–10:00PM EVENING EXTENDED TALK SESSIONS

MIKE KURAS – **Engineering Systems**

- KASIDIT LEOVIRIYAKIT – *Challenges and Complexity of Aerodynamic Wing Design*
- GIOVANNA DI MARZO SERUGENDO – *Trust as an Interaction Mechanism for Self-Organising Engineered Systems.*
- MARK KLEIN – *Handling Resource Oscillations Through Selective Misinformation*
- MASAHIRO KIMURA – *Modeling Share Dynamics by Extracting Competition Structure*
- TOMOHISA YAMASHITA – *Effective Information Sharing based on Mass User Support for Reduction of Traffic Congestion*

- DAVID L. GROSE – *Understanding and Managing Design as a Chaotic Process*
- NAGENDRA MARUPAKA – *Whisperers and Shouters: Random Wireless Sensor Networks with Asymmetric Two-Tier Connectivity*
- KAGAN TUMER – *Coordination in Large Collectives*

7:00PM–10:00PM EVENING PARALLEL SESSIONS

IRENE CONRAD – Social Systems

- SURESH SOOD – *Patterns of Negotiation – A new way of looking at marketplace B2B Negotiations*
- JOHN A. BROADBENT – *An evolutionary systems view of civilizational sustainability*
- JAMES K. HAZY – *Modeling Social Structure as Network Effects: Computational Evidence That Rewarding Learning Improves Performance*
- ROSANNA GARCIA – *An Exploration into the Uses of Agent-Based Modeling in Innovation/New Product Development Research*
- RICH COLBAUGH – *Explaining economic and social phenomenon: models with low cognition, interacting agents*
- CZESLAW MESJASZ – *Security as Property of Complex Social Systems*
- DAVID PETER STROH – *Using Systems Thinking to Facilitate Organizational Change*
- C. JASON WOODARD – *Individuals and Institutions in Strategic Network Formation*
- JEROEN STRUBEN – *Competition between vehicle propulsion technologies: critical thresholds for sustained adoption*
- JAMES K. HAZY – *Permeable Boundaries in Organizational Learning: Computational Modeling Explorations*
- CAMILO OLAYA – *The sociological theory of Crozier and Friedberg on organized action seen through a simulation model*

FRIDAY, May 21

9:00AM–5:00PM SPECIAL DAY ON SYSTEMS BIOLOGY

DON INGBER – Systems Biology

- STUART KIM – *Global discovery of conserved genetic modules*
- SUI HUANG

- ANDRE LEVCHENKO – *Cellular signaling and communication*
- HOWARD BERG – *E. coli, a swimming system*

TOM KNIGHT – Systems Biology

- JIM COLLINS
- JOHN DOYLE
- CASSANDRA L. SMITH – *Schizophrenia: A Complex and Multifactorial Disease*
- PHILIPPE CLUZEL – *Noise and information in biological systems*

Chapter 1

A Simple Approach to Multi-Predator Multi-Prey Pursuit Domain

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We present a different approach to a class of pursuit games: the Multi-Predator Multi-Prey domain. In the typical game, a group of predators tries to capture a group of prey, and all the agents have perfect knowledge of prey and predator positions. In our problem definition the prey-agent and the predator-agent have only local information provided by its vision range, each predator independently tries to capture a prey in a one-predator-one-prey-pair way. The predator-prey-pair capture is not known in advance and both predators and prey are moving in the environment. We show that simple greedy local predator rules are enough to capture all prey.

1 Introduction and Previous Work

This class of pursuit game has become a popular domain for the study of cooperative behavior in Distributed Artificial Intelligence (DAI). The pursuit domain was introduced by Brenda et. al. [Brenda 1986]. In his formulation, prey moves randomly, and predators can occupy the same position. In his work he made use of the center of gravity of the agents. Stephens and Merx [Stephens 1989], [Stephens 1990] experimented in a domain that did not allow two agents to occupy the same

position, predators alternated moves and prey moved randomly. Their successful way to capture prey made use of a centralized control mechanism. Korf [Korf 1992] introduced a simple solution to the pursuit domain. His simple algorithm made use of “attractive forces” between predator and prey, and “repulsive forces” between predators. In his approach predators had knowledge of the existence of all other predators and prey, then every single predator computes the “resultant force” to choose their next move. All the approaches mentioned above share, among other things, two important properties: (1) the predators had knowledge of the existence of all other predators and prey, and (2) The predator’s goal is to capture only “one” prey. L. E. Parker [Parker 2002] has studied a more complete problem, named “Cooperative Multi-Robot Observation of Multiple Moving Targets” or CMOMMT for short. In her domain the goal of the robots is to maximize the average number of targets that are being observed by at least one robot. The problem presented in Parker’s paper has the goal of maximizing the number of captured prey by predators. Observation or prey detection is not enough; predator needs to move in a greedy way to maximize the number of captured prey. We look at the multi-predator multi-prey domain, where the property (1) is dropped and replaced with limiting sensing capabilities by predators and prey. This assumption is made because property (1) is inconsistent with biological systems since no creature has infinite sensing range. We also extended the problem by having more than one prey, this assumption introduces the problem of predator-prey assignment.

2 Multi-Predator Multi-Prey Problem Description

The Predator-Prey pursuit domain has many different instantiations that can be used to illustrate different multi agent scenarios. The Multi-Predator Multi-Prey scenario used in the present paper has the following characteristics:

1. The “arena” or “world” is two-dimensional, bounded and continuous with a “square” shape.
2. We define prey has been “captured” when a predator is on top of a prey.
3. Predators can move linearly choosing any heading angle from 0 to 360 degrees.
4. Predators can overlap and occupy the same position.
5. There are n predators and m prey on the arena.
6. Each predator and prey have a 360 degree field of view observation of limited range.
7. Predators and prey will move simultaneously.
8. Prey movement will be predator evasive.
9. No predator communication.
10. Predators and prey will bounce off the walls using the reflexion angle law: angle of incidence is equal to angle of reflexion.
11. Predators can move faster than prey.
12. Prey can see farther than predators.

Goal: To capture as many prey as possible, i.e. if $m > n$ we can not capture more than n prey, and if $m \leq n$ we will capture all m -prey.

Measure of performance: The total time to intercept (TTI) and capture as many prey as possible.

3 The Approach

The way we propose to capture “all” prey is by asking predators to sweep the terrain by changing its heading direction. Predators will change its heading angle 90 degrees to their left every time they travel the maximum distance D in the terrain. The terminology used in this paragraph is precisely defined below when we define the “metrics” of the multi-predator multi-prey domain.

3.1. The Multi-Predator Multi-Prey Metric

We believe that the first step towards a solution to this domain is to define in numerical terms the characteristics listed in part 2. For this purpose we define:

- D = Diagonal distance across the arena.
- r = Robot (predator) radius, i.e. physical radius dimension.
- R = Robot (predator) vision radius, i.e. how far they can see.
- rp = Robot (prey) radius, i.e. physical radius dimension.
- Rp = Robot (prey) vision radius, i.e. how far they can see.
- v = Velocity (magnitude) of predators.
- vp = Velocity (magnitude) of prey.

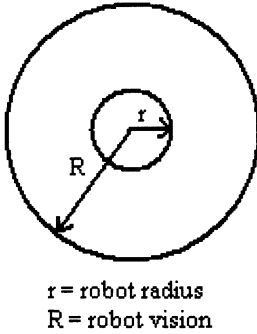


Figure 1. Robot representation.

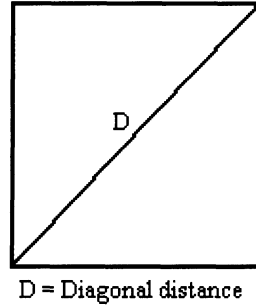


Figure 2. World representation.

Define the following ratios:

- $C1 = 2r/D$
- $C2 = 2R/D$
- $C3 = Rp/R$
- $C4 = D/v$
- $C5 = vp/v$

In this paper we consider homogeneous predators and homogeneous prey, i.e. the parameters r and v are the same for all predators, and rp and vp are the same for all prey. Therefore we will have same size predators with same magnitude velocity, and same size prey with same magnitude prey velocity.

Ratio's interpretation:

- $C1$ is a measure of the physical space used by the predator's dimension.
- $C2$ is a measure of the predator's vision coverage.
- $C3$ is the prey to predator vision ratio.
- $C4$ is the time unit, T , which takes a predator to travel the distance D .
- $C5$ is the prey to predator velocity ratio.

More formally, the used approach is to ask each predator to sweep the terrain changing its heading direction, by $-\pi/2$ radians, at every integer multiple of time $T=C4$.

In the rest of the paper we will consider that prey movement will always be evasive from predators, and that predators will either (a) sweep the terrain without changing its heading direction, or (b) sweep the terrain changing its heading direction, by minus 90 degrees, at every integer multiple of $C4$. Therefore the quantities $(D, C1, C2, C3, C4, C5, n, m)$ will perfectly define a homogeneous multi-predator multi-prey pursuit domain, and we will say that $(D, C1, C2, C3, C4, C5, n, m)$ will constitute the metrics of a particular pursuit domain.

3.2. Simulation of the Multi-Predator Multi-Prey domain.

To evaluate the effectiveness of predators capturing prey, we conducted several simulations where the Predators: (a) sweep the terrain without changing its heading direction, (b) sweep the terrain changing its heading direction, by minus 90 degrees, at every integer multiple of $C4$, or (c) sweep the terrain changing its heading direction, by minus 90 degrees, at every geometric multiple of $C4$, i.e. at q times $C4$, where q is the geometric series 0.5, 1, 2, 4, 8, etc. We call this sweeping strategy "spiral patterns". We are interested in the following question: How a change in $C5$ will affect the time to intercept prey (TTI)? Like in [Parker 2002] we will assume that $|C5| < 1$. This assumption allows predators an opportunity to capture prey, "if the prey could always move faster, then they could always evade the predators and the problem becomes trivially impossible for the predator team (i.e., assuming "intelligent prey")" [Parker 2002]. For predator evasion to take place, prey are privileged with a larger view range, i.e. $|C3| > 1$. Predator sweep as described above in (a), it is being used as a baseline for comparison with cases (b) and (c). In the following computer simulations prey will move "linearly evasively", i.e. prey try to avoid detection by nearby predators and if prey did not see a predator within its vision range, it will move linearly along its current heading direction. At the beginning of

each experiment, predators and prey are randomly positioned and oriented in the “world”.

We ran several simulations for the three cases: (a) Predators sweep the terrain without changing its heading direction “Simple sweep”, (b) Predator sweep the terrain changing its heading direction, by minus 90 degrees, at every integer multiple of $C4$ “Smart sweep” and (c) Predators sweep the terrain in “spiral patterns”. The idea behind the second and third approaches is to apply a simple local rule that will produce a “good” emergent behavior. In the context presented in [Hackwood 1991] SWARM Intelligence will emerge, in [Hackwood 1991] Swarm intelligence is defined as “a property of systems of non-intelligent robots exhibiting collectively intelligent behavior”. The results will show that strategy (b) “predators sweep the terrain changing its heading direction, by minus 90 degrees, at every integer multiple of $C4$ ”, gives an “intelligent collective behavior” as defined by Hackwood. In some other contexts the second approach, (b) strategy, is referred as emerging complex behaviors from the bottom up. In the following simulations predators are represented by squares, and prey are represented by triangles.

One run of the simulations is shown in figure 3, where we have 10 predators and 4 prey that have been captured in $TTI = 4.395 T$ time units. The “metrics” for figure 3 was $(80\sqrt{2}, 0.02, 0.1, 1.2, 0.5, 0.9, 10, 4)$

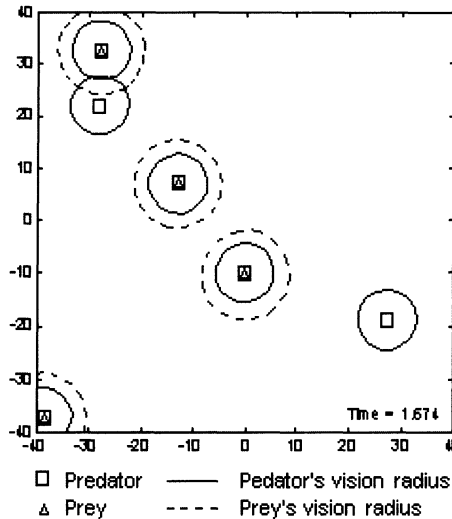


Figure 3. Simulation explanation.

4. Results

The following results were obtained using the following metrics: ($80\sqrt{2}$, 0.02, 0.1, 1.2, 0.5, C5, 10, 4)

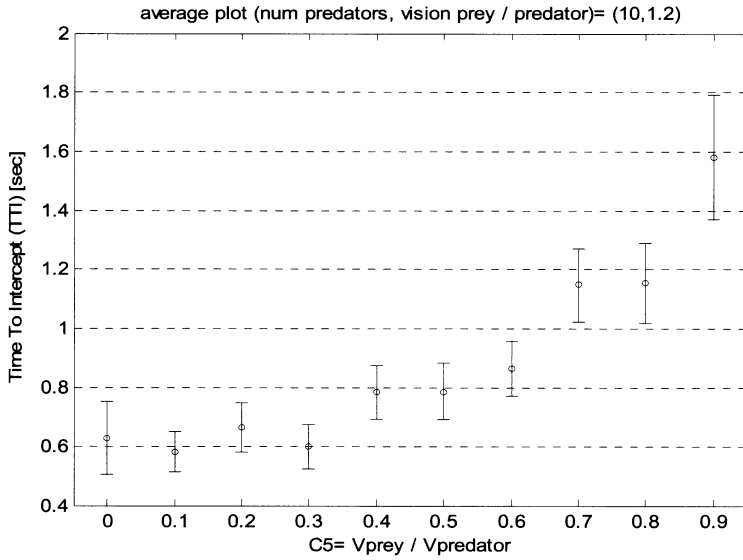


Figure. 4. “Simple sweep”.

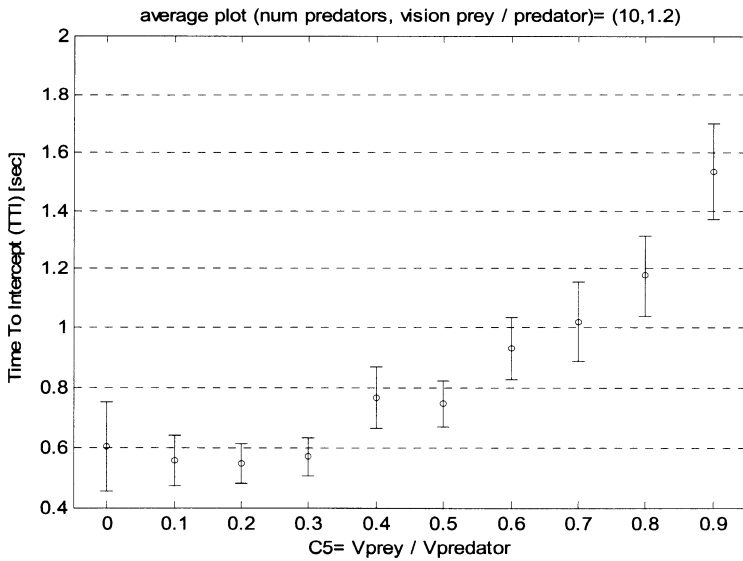


Figure. 5. “Smart sweep”.

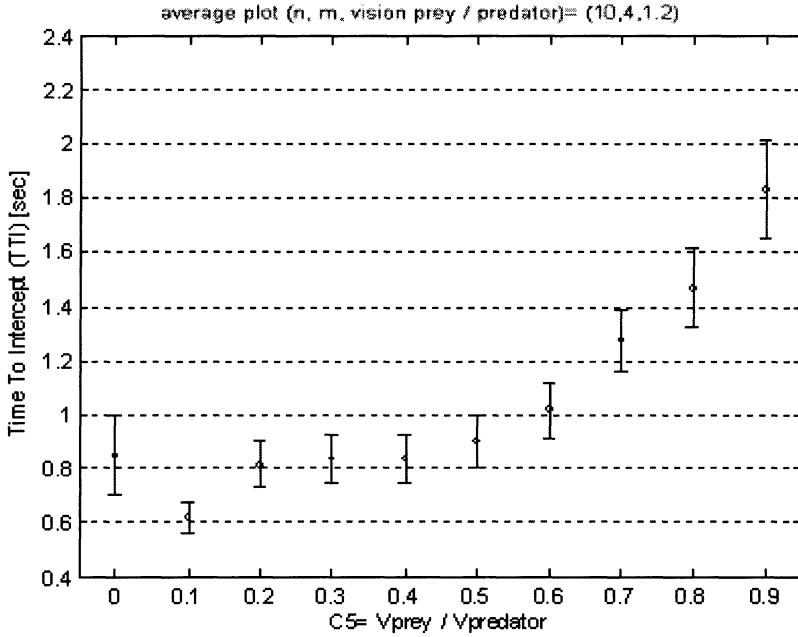


Figure. 6 “Spiral sweep”.

Every vertical line on each plot represents 100 runs of the domain with mean and plus/minus one standard deviation. We can see from figures 4, 5 and 6 that the “smart sweep” performed better on average, i.e. smallest *TTI*, than the “simple sweep” and the “spiral sweep”. The intuition will tell us that searching in a new direction every time we had travel the maximum distance *D* of the terrain could result in less time to capture all prey.

5 Conclusions and future work

The presented domain has a highly dynamic environment. We assumed that no prior knowledge of the terrain was given and the main question to be answered is: using reactive predators, can we come up with “intelligent” ways to minimize the time to intercept “all” prey? A reactive predator is such that the decision of action or behavior in the terrain will take almost no computational time. Therefore its actions will be like “reflexes”.

The area of multi agent and multi robot systems is experiencing an explosive research interest. Of particular interest are the systems composed of multiple autonomous mobile robots exhibiting collective behavior. Behavioral-based approaches have been used to implement formation control [Balch 1998]. We believe that a predator

formation will not reduce the time to intercept prey in the presented domain. It seems that forming clusters will not be a good searching strategy; on the other hand, a “predator spreading” strategy seems to be closer to a better search. We have introduced a “simple” attempt to solve real time problems of the multi-predator multi-prey pursuit domain. This constitutes a basic step towards more advance and fast ways to implement algorithms that can be use in real terrains. As yet, few applications of collective robotics have been reported, and supporting theory is still in its formative stages.

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Chapter 2

Simulated niche partitioning by bacteria

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1. Introduction

A central problem in ecology concerns the number of species that inhabit a given environment. A myriad of factors are involved, including speciation and extinction rates, geographic factors, seasonal cycles, food web stability, and a significant amount of random chance. The reductionist approach, taken here, is to reduce the system to its bare essentials and to then pose the question: is the biological community predictable for a simple given physical environment?

Our simplified system is a chemostat, which is a well stirred tank of bacterial growth medium that has been inoculated with a population of live bacteria. The culture is grown continually by adding fresh medium at a constant rate while simultaneously removing spent medium to maintain a constant volume. This model eliminates a tremendous amount of the complexity in natural environments: spatial issues are not relevant because the system is well mixed, diurnal and seasonal influences are removed, bacteria reproduce asexually so genetic recombination can be largely ignored, and an inoculating bacterial community can be selected in which there is no predation or parasitism. To simplify things even more, we investigate the chemostat model system with computer simulations so that every aspect is completely controlled and measurable. Clearly, the resulting toy system is no longer an accurate portrayal of natural ecology, although we believe that many of the essential factors are retained.

Continuous culture of bacteria often leads to competitive exclusion, meaning that one genotype outcompetes all others [1]. The resulting monoculture may evolve over time [2-4], sometimes with specific genomic changes that are the same in parallel experiments [5-7]. Evolution in a chemostat often proceeds with punctuated equilibria, in which periods of evolutionary stasis are periodically interrupted when faster growing mutants arise spontaneously and rapidly outcompete the resident population [8, 9]. A few experiments have also shown the stable coexistence of phenotypically distinct bacterial populations, a situation called niche partitioning [10, 11]. For example, a glucose limited continuous culture that was started with a single clone of *Escherichia coli* bacteria became polymorphic by generation number 773 with three populations that had different patterns of uptake and secretion of the metabolites acetate and glycerol [10].

Partly inspired by this experimental finding of coexistence, this work explores two simulated systems with niche partitioning, focusing on the steady-state result that is approached after many generations. We investigate ways in which the environment and the cellular design affect the co-existence of distinct populations.

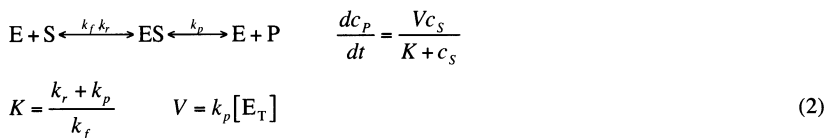
2. Description of the model

The model system consists of a simulated chemostat populated with simulated bacteria. Bacterial growth dynamics are treated using a population balance method, in which the entire community of bacteria are subdivided into a collection of phenotypes. Within each phenotype, all individuals are completely identical, without individuality that could arise from cell age, history of the cell surroundings, or stochastics. As a typical chemostat experiment has a bacterial population with around 10^8 to 10^{11} individuals, this use of average bacterial properties is appropriate for a study of the long term behavior of a bacterial community. While it does not affect the results presented here, the population balance method is not always good for studies of dynamics; for example, it does not include the stochastic effects that lead to punctuated equilibria. An alternate method, called a cell ensemble method, simulates each bacterium individually so as to capture bacterial individuality, but at a high computational cost for large populations [12].

Simulated bacteria are defined with a few arrangements of a biochemical functional module (Figure 1). This module reduces a bacterial metabolic pathway to a sequence of simple chemical reactions for substrate import, metabolism, and export of product. This is, of course, a gross simplification of a highly complex and interconnected biological network. Import and export processes, which also account for diffusion to and from the cell surface, are treated using passive transport, leading to linear kinetics and reaction rate constants that are equal for both transport directions:

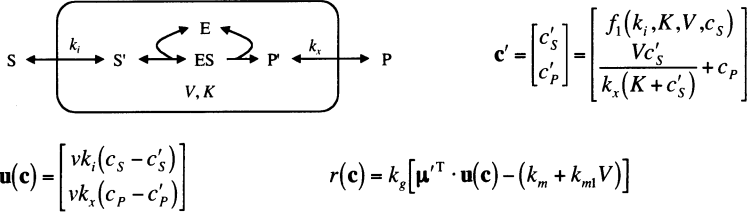
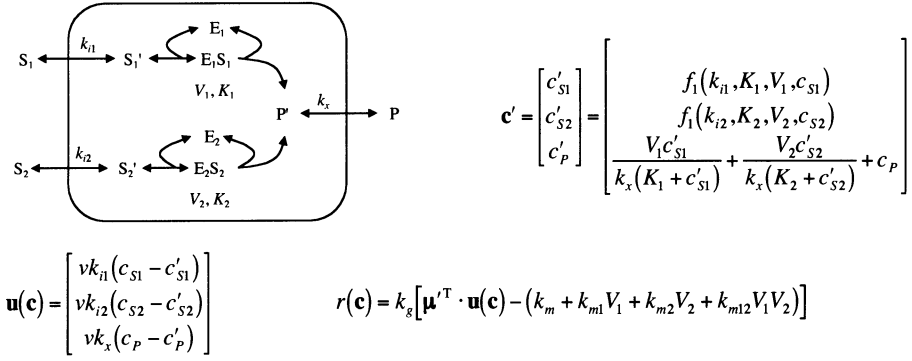
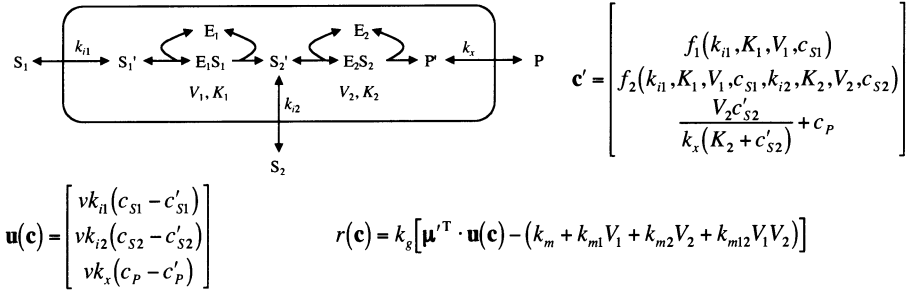


S denotes a substrate, P is a product, c_S and c_P are substrate and product concentrations in the bioreactor external to the cells, a prime symbol denotes chemicals or concentrations inside the cell, and k_i and k_x are import and export rate constants. Simplified metabolism is treated with a single-step conversion of substrate to product using Michaelis-Menten kinetics, which has the quasi-steady-state solution:



E denotes an enzyme, $[E_T]$ is the total concentration of the enzyme, k_f , k_r , and k_p are the forward, reverse, and product reaction rates respectively, K is the Michaelis-Menten constant, and V is the maximum reaction velocity (these latter symbols are typically shown as K_M and V_{max} , respectively, although the notation is abbreviated here to reduce clutter). Using these fundamental reactions for import, export, and metabolism, the quasi-steady-state solutions to the internal chemical concentrations were solved for the model metabolic networks, shown in Figure 1 as the column vector c' . While these solutions cannot capture transient behavior accurately, this work focuses on the long term behavior of the communities where they are appropriate.

The metabolic maximum reaction velocity V , or velocities V_1 and V_2 , are essentially the only parameters that differentiate one phenotype from another within the networks. These parameters are allowed to evolve while the reaction rate constants are fixed, acting as biochemical constraints on evolution. In biological terms, we are assuming that the metabolic enzymes are constitutively expressed but that mutations can affect their expression levels, given by $[E_T]$. The

Network I**Network II****Network III****Required functions**

$$f_1(k_i, K, V, c_S) \equiv \frac{1}{2k_i} \left[-V + k_i c_S - k_i K + \sqrt{(V - k_i c_S + k_i K)^2 + 4k_i^2 K c_S} \right]$$

$$f_2(k_{i1}, K_1, V_1, c_{S1}, k_{i2}, K_2, V_2, c_{S2}) \equiv \frac{1}{2k_{i2}} \left[V_2 - f_1(k_{i1}, K_1, V_1, c_{S1}) - k_{i2} c_{S2} + k_{i2} K_2 \right]$$

$$+ \frac{1}{2k_{i2}} \sqrt{(V_2 - f_1(k_{i1}, K_1, V_1, c_{S1}) - k_{i2} c_{S2} + k_{i2} K_2)^2 + 4k_{i2} K_2 (k_{i2} c_{S2} + f_1(k_{i1}, K_1, V_1, c_{S1}))}$$

Figure 1. Biochemical networks and the corresponding equations for steady-state metabolism and growth. Variables that are not described in the text: v is the volume of a bacterium; k_m , k_{m1} , k_{m2} , and k_{m12} are Taylor series expansion coefficients for the maintenance energy; and $f_1(\dots)$ and $f_2(\dots)$ are steady-state solutions for c_s' in Network I and c_{s2}' in Network III, respectively.

one exception is that the import/export rate constant k_{i2} in Network III, described below and in Figure 1, is also a phenotypic parameter that is allowed to evolve. These parameters were chosen to represent the phenotype using the biological rationalization that enzyme expression levels are likely to evolve more quickly than enzyme kinetics. Also, preliminary simulations showed that if other parameters are allowed to evolve, they typically shift towards either the smallest or the largest values permitted, regardless of the chemical environment, leading to less interesting results.

The chemical environment of the medium is affected by: *i*) inflow to the chemostat and *ii*) nutrient uptake and waste excretion by bacteria:

$$\frac{\partial \mathbf{c}}{\partial t} = D(\mathbf{c}^* - \mathbf{c}) - \sum_p X_p \mathbf{u}_p(\mathbf{c}) \quad (3)$$

$\mathbf{c}$ is the vector of chemical concentrations in the chemostat, $\mathbf{c}^*$ is the chemical concentrations in the chemostat feed tube, D is the chemostat dilution rate, which is the ratio of the flow rate to the chemostat volume, X_p is the number density of bacteria with phenotype p , and $\mathbf{u}_p(\mathbf{c})$ is the uptake function which expresses the net rate of chemical uptake by a bacterium of phenotype p (Figure 1). Waste excretion is expressed with a negative uptake rate.

The other differential equation that defines the model quantifies the change of bacterial populations over time, where the processes are: *i*) loss of bacteria from the system due to chemostat flow, *ii*) net bacterial reproduction, and *iii*) transitions from one phenotype to another:

$$\frac{\partial X_p}{\partial t} = -DX_p + X_p r_p(\mathbf{c}) + \sum_{p'} (X_{p'} T_{pp'} - X_p T_{p'p}) \quad (4)$$

$r_p(\mathbf{c})$, called the growth function, is the net reproduction rate per individual of phenotype p , where this includes both cell division and natural cell death. $T_{pp'}$ is a matrix for the transition rate of phenotype p' to phenotype p . While this transition rate formalism could account for cell cycle effects, in which the phenotype changes over a cell's lifetime, it is assumed here that a cell's phenotype is invariant. This allows the matrix $T_{pp'}$ to be interpreted as the phenotype mutation rate, making the value of the summation term in eq. 4 much smaller than those of the first two terms, for most situations. For convenience, phenotype transitions are only permitted between neighboring phenotypes in the simulations, allowing the transition rate to be expressed as a diffusion coefficient.

The growth function used for the three networks is proportional to the free energy released by metabolism, less the maintenance energy of a cell:

$$r_p(\mathbf{c}) = k_g [\boldsymbol{\mu}'^T \cdot \mathbf{u}(\mathbf{c}) - k_{m,p}] \quad (5)$$

k_g is the cell yield for a unit amount of available energy, $\boldsymbol{\mu}'$ is a column vector of chemical potentials inside the cell, $\boldsymbol{\mu}'^T$ is its transpose, and $k_{m,p}$ is the maintenance energy for phenotype p . Following the usual definition [13] and assuming ideal solutions, the chemical potential of species i is

$$\mu_i = \mu_i^\circ + RT \ln \frac{c_i}{c_i^\circ} \quad (6)$$

μ_i° is the standard chemical potential of chemical i at the standard concentration c_i° , and RT is the thermodynamic temperature. The former term of eq. 6 represents both the enthalpy and the entropy of the chemical at the standard concentration while the latter term represents the entropic change that arises from a change in the concentration. As shown in Figure 1, the maintenance energies are treated using a simple Taylor series expansion of the function $k_{m,p}$ in terms of the phenotype parameters, which is truncated after the linear terms. The constant term of the series represents the maintenance energy for all cell processes except metabolism, terms proportional to V , V_1 , or V_2 represent the energy used to synthesize the respective metabolic enzymes, and terms proportional to V_1V_2 represent interactions between metabolic pathways. Interactions can arise biologically from the sharing of enzymes by multiple pathways or the cross-inhibition of separate pathways.

There are several reasons for choosing these uptake and growth functions rather than one of the commonly used empirical functions [14, 15]. They are based on a physical model, allowing a direct and intuitive correspondence between mathematical parameters and physical properties. Also, they obey all physical constraints including mass conservation of chemicals and a free energy decrease for forward reactions (assuming a positive maintenance energy). With certain parameter choices, the Network I equations can be simplified to either the Monod or the Westerhoff growth function, which have been shown to accurately represent biological data [15, 16]. Finally, as shown below, these models produce interesting results because the metabolic maximum reaction velocities evolve toward finite values, rather than toward the ends of permitted parameter ranges. However, the parameter choices that are required to make this last point true are different from those that make the equations agree with experimental data on bacterial growth rates [15]. Differences arise primarily from the inability of these simulated bacteria to adapt to varying nutrient concentrations. Because of the discrepancy, quantitative values are only given for Network I and they are presented to give a sense of scale, rather than as biological predictions.

3. Results

3.1 Network I

The first network is composed of a single metabolic module that simply converts substrate to product. It was chosen to demonstrate the basic results of our uptake and growth functions in the population balance method, as well as simple evolution. It also forms a basis for comparison, both with Networks II and III which reduce to Network I in certain limits, and with experimental data [14-16].

The temporal growth dynamics of Network I are best illustrated with simulated batch growth, in which the growth medium is relatively rich at the beginning and is not refreshed (Figure 2A). Following the standard pattern, the bacterial population size grows exponentially until the nutrients are largely depleted, it levels off to form a stationary phase, and then it decreases during a long so-called death phase due to starvation. The stationary phase in the simulation is relatively short when compared to experimental results because these simulated bacteria have a maintenance energy cost that is independent of the environment, whereas real bacteria can adapt to low nutrient conditions.

Continuous growth is investigated by allowing a population to equilibrate in a chemostat at each of several dilution rates (Figure 2B), recording the population density and chemical

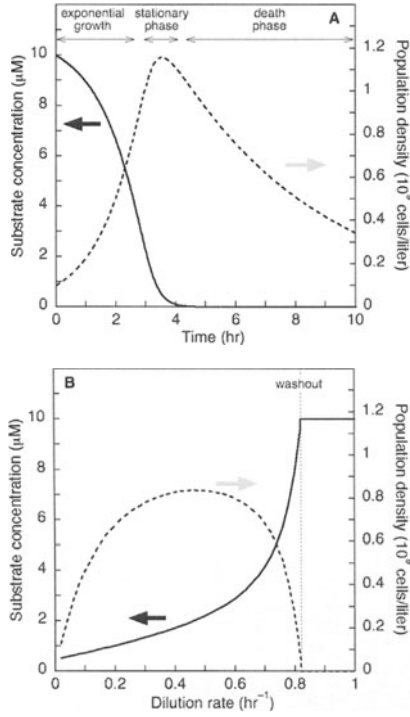


Figure 2. Simulated bacterial growth dynamics for Network I over time during batch growth (A) and at steady-state as a function of the dilution rate (B). Solid lines show the concentration of substrate (left axis) and dashed lines show the bacterial population density (right axis). Parameters: $k_i = k_r = 1000 \text{ s}^{-1}$, $K = 0.5 \text{ } \mu\text{M}$, $k_g = 5 \times 10^7 \text{ cells/J}$, $k_{m1} = 5 \times 10^{-16} \text{ J } \mu\text{M}^{-1} \text{ cell}^{-1}$, $k_m = 10^{-13} \text{ J s}^{-1} \text{ cell}^{-1}$, $RT = 0.0026 \text{ J/}\mu\text{mol}$, $V = 2000 \text{ } \mu\text{M s}^{-1}$, $v = 10^{-6} \text{ l}$, $\mu_s^o = 3 \text{ J } \mu\text{mol}^{-1}$, and $\mu_p^o = 0$. For (A), $c_s(0) = 10 \text{ } \mu\text{M}$, $c_p(0) = 0$, and $X(0) = 10^{-8} \text{ cells}$. For (B), $c_s^+ = 10 \text{ } \mu\text{M}$ and $c_p^+ = 0$.

concentrations at each steady state. At steady-state and with a negligible mutation rate, eq. 4 has two solutions:

$$\begin{aligned} r_p(\mathbf{c}) &= D \\ X_p &= 0 \end{aligned} \quad (7)$$

The former solution applies to the portion of Figure 2B where the dilution rate is less than about 0.82 hr^{-1} ; since the dilution rate is equal to the growth rate, the solid line in the figure also relates the growth rate to the substrate concentration. The simulation result was confirmed to be identical to the analytical result given in Figure 1. When the dilution rate exceeds the bacterial growth rate at the feed chemical concentrations, the bacteria cannot grow fast enough to replace those that are washed out of the system, leading to a state called washout in which the latter

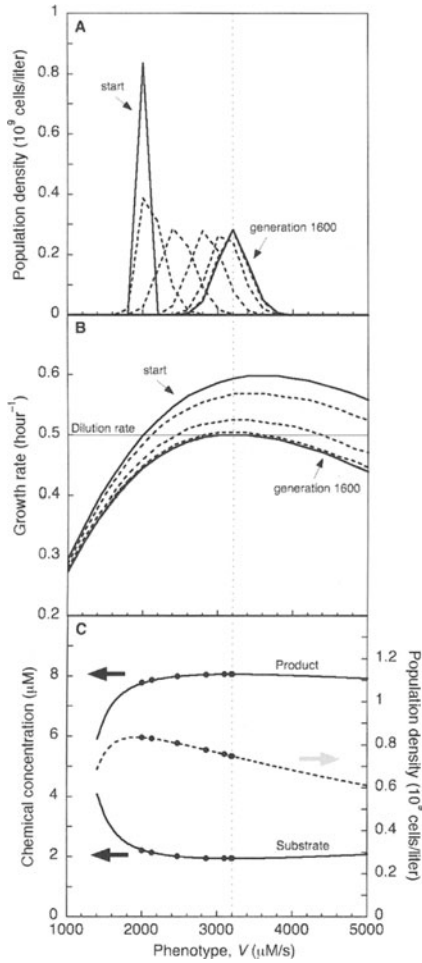


Figure 3. Evolutionary dynamics for Network I over 1600 generations. (A) Population density as a function of the phenotype, where the phenotype is classified into $200 \mu\text{M/s}$ wide bins. Curves are shown for generation 0 (solid line), 50, 100, 200, 400, 800, and 1600 (solid line). (B) Growth functions for the same time points. (C) Chemical concentrations and total population density for the same time points (dots) shown on lines generated with equivalent simulations that started with $V=1400 \mu\text{M/s}$ or $5000 \mu\text{M/s}$. Parameters are the same as in Figure 2, with the following additions: $D = 0.5 \text{ hr}^{-1}$, phenotype diffusion rate $= 0.02 \mu\text{M}^2 \text{ s}^{-3}$.

solution of eq. 7 applies. These simulated curves are in qualitative agreement with experimental results [14].

When the bacterial phenotype that was used to generate Figure 2 is left in a chemostat for many generations, the metabolic maximum reaction velocity, V , evolves to a larger value (Figure 3A). The numerical procedure is that 21 phenotypes were defined with V values ranging from 1000 to 5000 $\mu\text{M/s}$. The virtual chemostat was inoculated with cells with phenotype $V = 1400$

$\mu\text{M/s}$, the mutation rate was set to zero until the population size and extracellular chemical concentrations had stabilized (curves marked “start” in Figure 3), and then mutations were allowed again while the results shown in the figure were recorded. Because mutation is only possible between neighboring phenotypes, it is quantified with a diffusion coefficient, listed in the Figure 2 caption. This evolution can be understood by considering the growth rate as a function of the phenotype (Figure 3B). In Figure 3B, the initial population is localized to the intersection of the growth rate function and the horizontal line that marks the dilution rate (eq. 7). Mutational diffusion leads to populations with larger and smaller phenotype values; those with larger values are seen to have a faster growth rate than the others, so they multiply, take up more nutrient and thereby decrease the growth rate for all phenotypes, and the other bacteria starve. This process leads to an evolutionary drift of the phenotype that continues until no other phenotype has a faster growth rate. In the language of evolutionary game theory, the resulting phenotype is an evolutionarily stable strategy because the culture cannot be invaded by any other phenotype [17].

The same optimization is shown in a different way in Figure 3C. Here, it is seen that evolution results in the phenotype that minimizes the concentration of substrate in the medium and maximizes the concentration of waste (because of the stoichiometry of Network I, these are dependent parameters). However, evolution neither maximizes nor minimizes the population density. The lines in Figure 3C were produced with evolution simulations that are identical to the one shown in panels A and B, but starting with $V = 1400 \mu\text{M/s}$ or $V = 5000 \mu\text{M/s}$. In both cases, evolution resulted in phenotypic drift towards the vertical line shown in the figure at $V = 3204 \mu\text{M/s}$.

Another phenomenon seen in Figure 3A is the spreading of the population distribution from the initial monoculture to a broader profile. This arises from a combination of mutational diffusion away from the center of the peak and a constant loss of the slower growing phenotypes at the edges of the distribution due to their slower growth rates.

3.2 Network II

The situation is more interesting with Network II, which has two parallel metabolic modules that consume different substrates from the medium but excrete the same waste product. In the simulation, the two substrates are added to the medium at the same rate, but are assigned slightly different standard chemical potentials to avoid artifacts that might arise with a perfectly symmetric system. This network represents real bacteria that are grown with multiple nutrients where it is found that all substrates are consumed simultaneously [18]. However, it is not clear if every bacterium consumes all substrates or if the population becomes phenotypically heterogeneous with different individuals specializing on different substrates.

The evolutionary dynamics of this network were found to be similar to those of Network I in that evolution proceeds with a monotonic phenotypic drift towards a steady-state population distribution (data not shown). These final distributions were recorded as a function of the chemostat dilution rate (Figure 4), using dilution rates that were increased in steps that were separated by long delays to allow the population to achieve steady-state before continuing. At low dilution rates, the bacterial community spontaneously partitions itself into two stable co-existing phenotypes, each of which specializes on metabolism of one of the two nutrients (Figure 4A). At higher dilution rates, there is a rapid transition from a pair of specialist phenotypes to a single generalist phenotype that metabolizes both nutrients (Figures 4C and D). At the transition (Figure 4B), there is a range of dilution rates about 0.03 units wide where there are three co-existing populations, including both specialist phenotypes and the generalist phenotype.

Using a dilution rate that is decreased rather than increased, exactly the same simulation results are found except quite close to the transition, which is shifted by about 0.07 units towards a lower dilution rate, indicating the presence of hysteresis. This niche partitioning bistability occurs despite the fact that every steady-state population was confirmed to be an evolutionarily stable strategy (for all phenotypes p , either $r_p(c) < D$ or $X_p > 0$). It has not been investigated analytically.

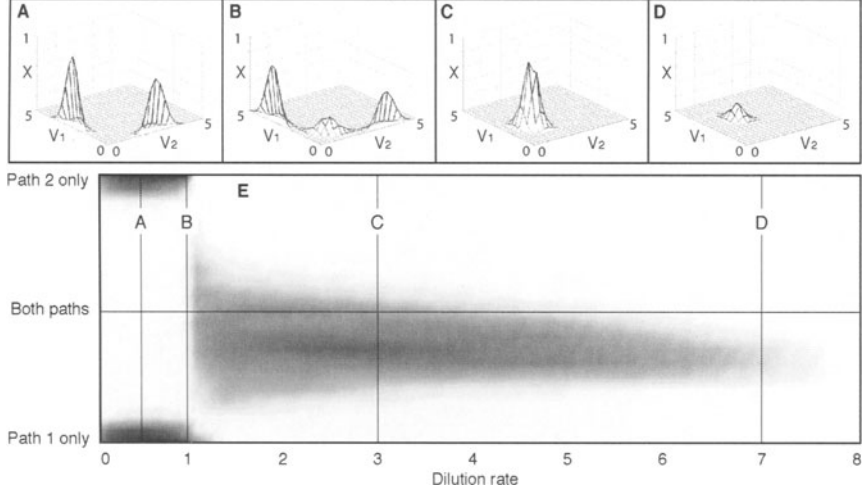


Figure 4. Steady-state population distributions across phenotypes for Network II as a function of the dilution rate. (A-D) Population densities in terms of the two phenotype parameters showing (A) stable coexisting specialist populations, (B) specialist and generalist populations, and (C and D) a single generalist population. (E) Population distribution as a function of the dilution rate, where dark regions represent high population density and light regions represent low population density. The vertical axis corresponds linearly to the angle between the phenotype parameters V_1 and V_2 so that specialist populations appear at the top and bottom of the panel and generalist populations appear in the middle. The dilution rates at which panels (A-D) were recorded are shown with vertical lines. Washout occurred at $D = 8.0$. Parameters: $k_{i1} = k_{i2} = k_x = 1.0$, $K_1 = K_2 = 1.0$, $k_g = 1.0$, $RT = 0.1$, $k_m = 0.1$, $k_{m1} = k_{m2} = 0.1$, $k_{m12} = 0.5$, $c_{s1}^+ = c_{s2}^+ = 1.0$, $c_p^+ = 0$, $\mu_{s1}^0 = 10.0$, $\mu_{s2}^0 = 8.0$, $\mu_p^0 = 0$, and mutational diffusion coefficients of 0.001 on each axis.

The pathway interaction term in the Network II maintenance energy expansion given with the constant k_{m12} is responsible for the niche partitioning found at low dilution rates. A positive value of k_{m12} promotes specialization because it imposes an energetic cost on bacteria that express both metabolic enzymes, in addition to the costs for each enzyme separately. With low dilution rates, substrate concentrations are low, so the available metabolic energy is low, and k_{m12} is large enough to promote specialization. In contrast, the interaction cost is smaller relative to the metabolic energy at higher dilution rates, thus lessening its influence and promoting generalization.

The relationship between the two specialist populations at low dilution rates is expressed with the community matrix, $\mathbf{A}$, which quantifies the influence of a change of one population size on the growth rate of another population [19]. In this model system, populations only interact via extracellular chemical concentrations, so perturbing one population size does not have an immediate effect on other populations. Instead, the effect is directly proportional to the duration of the perturbation:

$$\begin{aligned}
 A_{pp'} &\equiv \frac{\partial \dot{X}_p}{\partial X_{p'}} = X_p \frac{\partial r_p(\mathbf{c})}{\partial X_{p'}} = X_p \nabla_{\mathbf{c}} r_p(\mathbf{c}) \cdot \frac{\partial \mathbf{c}}{\partial X_{p'}} = X_p \nabla_{\mathbf{c}} r_p(\mathbf{c}) \cdot \frac{\partial \mathbf{c}}{\partial X_{p'}} dt \\
 &= -X_p \nabla_{\mathbf{c}} r_p(\mathbf{c}) \cdot \mathbf{u}_{p'}(\mathbf{c}) \Delta t
 \end{aligned} \tag{8}$$

$A_{pp'}$ is the element of the community matrix for the effect of phenotype p' on phenotype p . The matrix for the specialist populations shown in Figure 4A was calculated using eq. 8, where the values of X_p and c were taken from the simulation results and numerical derivatives were taken of the growth function. Considering just the two most populated phenotypes, the matrix is:

$$\mathbf{A} = \begin{bmatrix} -0.588 & -0.0006 \\ -0.0004 & -0.437 \end{bmatrix} \Delta t \quad (9)$$

The first row and column are for the population that expresses pathway 1 and the second row and column are for the population that expresses pathway 2. The negative values on the main diagonal of $\mathbf{A}$ imply that population growth rates decrease when the population size is made larger than the steady-state value and vice versa, leading to negative feedback. The small negative values on the off-diagonal imply that the two populations are in weak competition with each other [19]. In this case, they are not competing for nutrients, but for the ability to get rid of waste products where the product inhibition on the growth rate arises from eq. 6. The eigenvalues of eq. 9 are very nearly the same as the diagonal terms; their negative values confirm that the community of specialist populations is stable to population size fluctuations [19].

3.3 Network III

In the third network, the metabolic modules are arranged sequentially rather than in parallel (Figure 1), such that a bacterium could metabolize S_1 to S_2 , S_1 to P , or S_2 to P , where S_1 is a high energy nutrient and S_2 is a low energy nutrient. For simplicity, we return to adding only a single substrate to the chemostat (negligible amounts of S_2 and P are also added to avoid numerical errors arising from the logarithmic term in eq. 6). The rate constant for the import or export of the intermediate metabolite is made a third evolvable parameter to allow a wider range of phenotypes although it does not contribute to the maintenance energy. This network represents *Escherichia coli* bacteria grown on glucose, which can export or import the intermediate metabolites glycerol and acetate [10]. It also represents the yeast *Saccharomyces cerevisiae*, which can ferment glucose to ethanol to release a small amount of energy or respire glucose to carbon dioxide and water to release much more energy [20].

Niche partitioning with Network III is similar to that found for Network II, with the bacterial community composed of two specialist populations at low dilution rates and a single population at high dilution rates (Figure 5). While not shown in the figure, the original data show that the value of k_{i2} evolves to its maximal value for both specialist populations, implying that one population metabolizes substrate S_1 to S_2 and exports S_2 , while the other population imports S_2 and metabolizes it to product. At high dilution rates, k_{i2} evolves to its minimal value. Here, the single population metabolizes S_1 fully to product without letting the S_2 intermediate escape to the surroundings. When the dilution rate dependence is simulated using decreasing flow rates, the transition from a single population to two populations occurs within 0.1 units as it does for increasing rates, indicating minimal or no bistability.

The transition from specialist populations to a single population occurs for a similar reason as for Network II. At low nutrient levels, the pathway interaction cost is sufficiently large compared to available energy that bacteria grow faster if they just metabolize S_1 to S_2 , rather than metabolizing it all the way to product. This opens up a niche for a second specialist phenotype which metabolizes S_2 to product. At high dilution rates, the pathway interaction cost is minimal compared to the cost of losing S_2 to the environment, so cells grow faster if they include both metabolic modules and shut off S_2 transport.

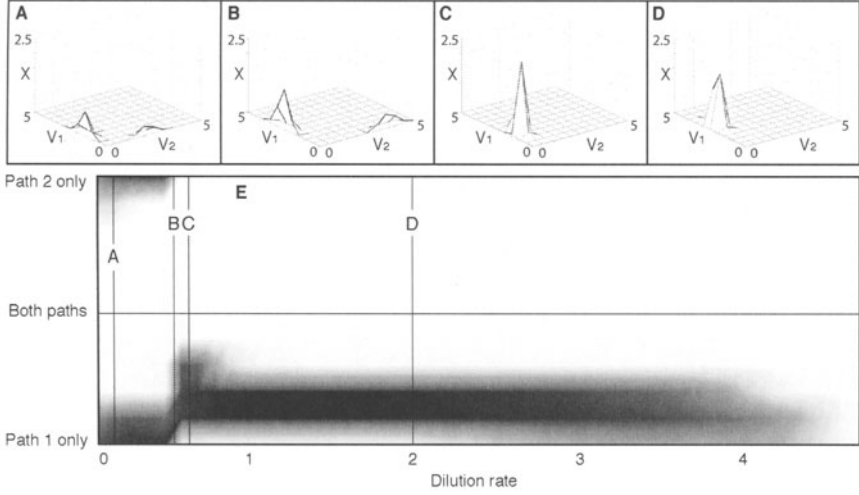


Figure 5. Steady-state population distributions across phenotypes for Network III as a function of the dilution rate. See the caption for Figure 4. The specialist populations shown in panels (A) and (B) evolved to have a value of k_{12} equal to 2, which is the maximum permitted, while the generalist populations shown in panels (C) and (D) have a k_{12} value equal to 0.01, which is the minimum value allowed. Washout occurred at $D = 4.9$. Parameters are the same as for Figure 4, except for k_{12} which is an evolvable parameter here and the following: $c_{S1}^\dagger = 0.98$, $c_{S2}^\dagger = c_P^\dagger = 0.01$, and $\mu_{S2}^\circ = 4.0$.

The community matrix for the specialist populations shown in Figure 5A is

$$\mathbf{A} = \begin{bmatrix} -0.0644 & 0.0015 \\ 0.0677 & -0.1282 \end{bmatrix} \Delta t \quad (10)$$

As before, the first row and column are for the “path 1 population” and the second row and column are for the “path 2 population”. The negative values on the main diagonal again indicate that each population is independently stable. However, the positive values on the off-diagonal show that these populations are mutualistic rather than competitive [19]. The benefit of the path 1 population on the path 2 population, quantified with the value in the lower left corner of $\mathbf{A}$, arises from the reliance of the latter phenotype on the metabolic product of the former phenotype. The metabolic energy available to the path 1 population is larger when the path 2 population reduces the concentration of S_2 in the medium, providing the much smaller benefit quantified in the upper right corner of $\mathbf{A}$. The eigenvalues of the matrix are -0.063 and -0.130 , indicating that this bacterial community is stable to population size fluctuations.

4. Discussion and conclusions

The model networks examined here are quite simple but are rich enough to yield interesting behaviors, including evolutionary optimization and niche partitioning that is dependent on the chemostat dilution rate. While minimal use was made of it in this work, the fact that the networks are based on the laws of thermodynamics rather than empirical observations is appealing. Because of it, one has a greater freedom in exploring parameter space and there is no fundamental reason

why behaviors found with these networks, or with any of a wide variety of similar models, could not be found with biological experiments.

Using Network I, the maximum metabolic reaction velocity was found to evolve to a final value in which the growth function is equal to the dilution rate for this phenotype, and has a lower value for all other phenotypes. This allows it to be identified as an evolutionarily stable strategy. This final phenotype is also the one that minimizes the substrate concentration in the chemostat and maximizes the product concentration. Assuming that the growth function is suitably well-behaved, the latter result can be derived from the former. Labeling the stable phenotype as p^* , the derivative of the steady-state chemical concentrations with respect to the phenotype at p^* is:

$$\left. \frac{dc}{dp} \right|_{p^*} = \frac{\partial c}{\partial r_p(c)} \left. \frac{\partial r_p(c)}{\partial p} \right|_{p^*} = 0 \quad (11)$$

The second equality follows from the fact that the latter partial derivative is zero, because the growth rate is maximal at p^* (see Figure 3). Similarly, the negative curvature of $r_p(c)$ at p^* can be used to show that evolution proceeds to minimize the substrate concentration while maximizing the product concentration, as was found in the simulations and is observed experimentally [8]. The result in eq. 11 can be readily generalized to all systems that obey the basic population balance model that was defined by eqs. 3 and 4, including those with multiple stable coexisting phenotypes (assuming there is a single steady-state and that functions are reasonably well-behaved). Since the chemical concentrations in the medium are stationary with respect to the phenotype at the evolutionary end-point, any thermodynamic function that depends on just these concentrations must also be stationary. It is likely that an optimizing function could be found for Networks II and III that is analogous to the substrate minimization that was found for Network I.

Both Networks II and III show coexistence at low dilution rates and single populations at high rates. Coexistence is not a necessary consequence of low dilution rates, which was confirmed by running simulations with decreased values of the interaction term in the maintenance energy, k_{m12} . This moves the transition between one and two populations to a lower dilution rate, eventually reaching zero, so that it becomes impossible to achieve coexistence. In contrast, there are never coexisting populations at chemostat washout, except in cases of perfect symmetry in the growth equation or growth rates that are identical by coincidence. As washout is approached, the medium chemical concentrations approach the feed concentrations, c^f . Because coexisting populations in this model only interact with each other via chemical concentrations, these interactions are reduced to zero at washout. Meanwhile, the growth function becomes $r_p(c^f)$, which is likely to be maximal for only a single phenotype. This maximum value is the washout dilution rate and the phenotype where it is maximum is the sole population that exists just before washout.

These results suggest various experiments. In particular, bacterial evolution has been observed using continuous culture, resulting in either a single population or coexisting populations. If the dilution rates were varied, would it be possible to experimentally vary the degree of niche partitioning? Our results indicate that the answer is yes.

Acknowledgements

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Chapter 3

Predictive Modelling for Fisheries Management in the Colombian Amazon

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A group of Colombian indigenous communities and Amacayacu National Park are cooperating to make regulations for sustainable use of their shared natural resources, especially the fish populations. To aid this effort, we are modeling the interactions among these communities and their ecosystem with the objective of predicting the stability of regulations, identifying potential failure modes, and guiding investment of scarce resources. The goal is to improve the probability of actually achieving fair, sustainable and community-managed subsistence fishing in the region.

Our model fuses common-pool resource non-cooperative games with principles of self-organizing commons management by allowing agents to affect the existence of game rules as well as choosing whether to act within the bounds of those rules. Sustainable management is threatened by both economically rational individuals, who cheat the system when it profits them, and by malicious individuals, who wish to destroy the system for their own obscure reasons. With our model, we hope to evaluate the stability of a system of regulations in simulation by measuring the impact of malicious agents on the behavior a population of rational agents employing a strategy of measured response.

1.1 Overview

Along the Colombian section of the Amazon river, a group of small indigenous communities and Amacayacu National Park are experimenting with the design and implementation of regulations intended to recover and maintain the integrity and productivity of their shared natural resources, especially the fish populations on which they depend. We are modeling the behavior and stability of management scheme options for this system with the objective of developing guidelines for strategic future investment of time, energy, and money. The goal is to improve the probability of actually achieving fair, sustainable and community-managed subsistence fishing in the region.

Sustainable long-term use of common pool resources is an inherently difficult political challenge. The Amacayacu communities face the additional complications of complex and poorly-understood ecosystems, uncontrolled demographic growth and cultural change in the population of legitimate resource appropriators, weak and often corrupt national and regional institutions, and primitive transportation and communication infrastructure. Balanced against these are the positive factors of a relatively small and well-defined population of users, appropriation practices that can be monitored relatively effectively at relatively low cost, recognition of the legitimacy of local regulations by regional and national institutions, and an explicit commitment on the part of the appropriator population to developing fair, sustainable, and democratic ground rules for natural resource use.

We approach this problem from the perspective of self-organizing commons management principles[4] and present a first-draft model for human/fish interactions in the Amacayacu region based on common-pool resource non-cooperative games,[6] with the addition of institutional level choice to our model. Predictions from this model can be derived through simulations which introduce a small number of malicious agents, and compared against the evolving situation of the Amacayacu communities. If successful, this model can then be used as an aid for decision-making in solving the resource management problems facing the Amacayacu communities

1.2 The Amacayacu Fisheries Dilemma

There are two types of fisheries in the Amacayacu region. The majority of activity is in the subsistence fisheries. A broad range of species are involved, likely more than 100, ranging in size up to a few kilograms. Subsistence fishing takes place mostly in the two tributaries bordering the park (Q. Mata Mata and Q. Amacayacu) and in the lakes contained within the islands of Mocagua and Zaragozilla. The open river, on the other hand, is harvested primarily for commercial purposes, yielding large catfish which are sold in the city of Leticia, 50 kilometers distant. Although these command a lucrative price compared to the smaller, bonier fish from the subsistence fisheries, the subsistence fisheries are significantly more important to the viability of the communities.

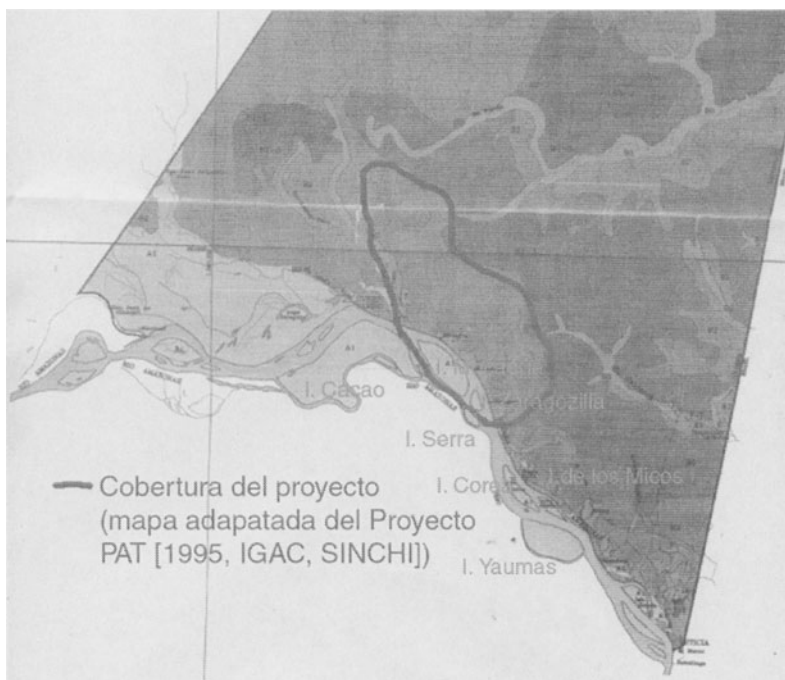


Figure 1.1: Amacayacu fisheries management project area (blue outline)

In recent years, the user communities have perceived a major decrease in the productivity of the subsistence fisheries, coincident with major demographic growth and the widespread introduction of fishing nets. The causation is unclear, and the subject of current research, although the use of nets appears to have a disproportionately large impact on the productivity of the fisheries.

Unfortunately, quantitative information about the fisheries is virtually non-existent. This presents a major challenge to any conservation effort, as there is little known about the biology or ecological interactions of the species being harvested, or indeed even exactly how species are being harvested regularly. Harvest records are only beginning to be compiled — establishing a system of records is a main objective for the management project in the coming year.

1.2.1 User Communities

The six communities which have participated in the project (Macedonia, Mocagua, Zaragoza, El Vergel, Palmeras, and San Martin de Amacayacu) are spread along 25 kilometers of the Colombian bank of the Amazon. Together they comprise approximately 2500 inhabitants, ranging from 183 in Palmeras to 826 in Macedonia.¹ Child mortality has plummeted due to improved health

¹2002 survey data, unpublished

care, but there is not yet a corresponding cultural change in birth-rate, so the population is growing rapidly.

Although there are no formal restrictions on where members of a given community can fish, in practice each community fishes a rough territory nearby, overlapping with its upstream and downstream neighbors. In addition, there are occasional problems with poachers from the Peruvian side of the river.

Interaction between communities is relatively scarce. This is partly due to the lack of enabling infrastructure — there are no roads, only a few occasionally functional satellite telephones, and boat motors and gasoline are expensive — and partly due to insularity on the part of the communities — it is more likely for people from non-neighboring communities to meet on excursions to the Leticia.

There is a high level of poverty in the communities, where much of the economic activity is non-monetary. Other local industries besides fishing include subsistence farming, ecotourism, and production of traditional crafts for sale.

1.2.2 Management Project History

Management of the fisheries is an outgrowth of other conservation efforts in the region. Isla Mocagua is also inhabited by the wattled curassow (*crax globulosa*), an endangered species of bird approximately the size of a turkey. Beginning in 2000, Project Piuri (after the Spanish name for the species) enlisted local aid in data-gathering and monitoring to prevent hunting of the birds. Spurred by the apparent success of Project Piuri, members of the involved communities began wondering whether they could improve the fisheries of the island as well.

Under the fisheries management project, begun in 2002, nets are banned from use in all subsistence fisheries. To enforce the ban, round-the-clock teams of monitors are deployed in the fisheries, with the authority to confiscate and burn nets from violators. Each community is responsible for monitoring a portion of the fisheries,

After only a few months of monitoring, there was widespread agreement that the fishing had greatly improved. The project has already weathered several crises, but consensus among the communities is still fragile.

1.3 Self-Organizing CPR Management

Despite stereotypes to the contrary, many communities avoid the tragedy of the commons and develop long-term sustainable common pool resource management schemes. For example, the *huerta* of Valencia, Spain, have been operating as a self-governing irrigation system since the year 1435.[5]

Analysis of a self-organizing CPR management system proceeds on three levels: **Constitutional Choice** is the highest level, in which participants determine how to go about devising their institutions. Below that is the level of **Institutional Choice**, in which participants make collective choices about regulations for interacting with the CPR — who can draw units, how conflicts

will be resolved, and what sanctions will be imposed for violations. Finally **Operational Choice** is the level at which participants actually interact with the CPR, deciding whether or not to obey or enforce the regulations.[4]

By contrast, analyses like the classical tragedy of the commons assume that the Constitutional and Institutional levels are fixed by an outside party, so that participants can only make choices at the Operational level, greatly limiting their options.

In fact tragedy of the commons situations do occur, a fact which self-organizing CPR management accounts for by identifying ways in which successful and failed CPR management systems tend to differ. Ostrom[4] identifies a set of eight design principles for successful self-organized CPR management systems:

1. Clearly defined boundaries
2. Proportional equivalence between benefits and costs
3. Collective-choice arrangements
4. Monitoring
5. Graduated sanctions
6. Conflict resolution mechanisms
7. Minimal recognition of rights to organize
8. Nested enterprises

Systems which follow all of these principles tend to be very successful, systems which only partially follow the principles tend to be fragile and unstable, and systems which follow few or none tend to fail badly.

In the case of the Amacayacu communities, all eight of these principles are on their way to being satisfied. Governmental authorities have given legal recognition and broad authority to the project, which is organized at both the community and regional level, and an ongoing process of collective choice within the communities is supporting the efforts at present. The fisheries under management are in well-defined locations, with a clearly identified population of legitimate users, and a system of monitoring established. The remaining principles (proportionality, sanctions, and conflict-resolution) are still in the process of being established.

1.4 Modeling Challenges

Modeling the Amacayacu fisheries presents major difficulties stemming from complexity and lack of knowledge about the ecosystem as well as from the shifting body of rules allowed by self-organization of the user community.

The major issues in modeling the fisheries stem from lack of information. Many different species of fish are harvested, and little to no information is known about the reproductive biology and ecological interactions of any given species. What is known is largely phenomenological information gathered by the user community: for example, cleaning surface vegetation off of the ponds significantly increases the harvestable fish population, but the mechanism is entirely unclear. Additional complexity is added by large seasonal variations in the fisheries as the river floods and retreats, and possible multi-year cycles for which historical data is sparse at best. Finally, the Amacayacu fisheries are not isolated from the larger Amazon, and the degree of interaction between them and the local, regional, and continental ecosystem is unknown.

The major issues in modeling the user community stem from the fluxing political situation. Because the national and regional institutions tend to be weak and sometimes corrupt, there is no powerful authority issuing or enforcing regulations. As a result, the main regulatory authority lies with the user community, resulting in a tight coupling of constitutional, institutional, and operational choice levels. Furthermore, the communities' general cynicism, that rules are unenforceable and that local actions cannot affect the environment, has been shaken by the success of Project Piuri and the perception of improving fisheries. Finally, with a total population of only a few thousand across all six communities, the group is small enough for actions of single users to have a large impact, particularly at the level of institutional choice, but large enough that any given user is likely to have no direct relationship with many of the other users.

A further complication comes from invading poachers from the Peruvian communities on the other side of the river. Not only do the poachers take fish, but their free-riding challenges the Amacayacu communities commitment to conservation.

1.5 System Model

Our system model is predicated on two major hypotheses:

Aggregate Biology Hypothesis: *Given the large number of species involved, the biology of individual species may be generalized and the fish resource modeled as harvestable biomass.*

System Dynamics Hypothesis: *Gross system dynamics are determined by the interaction of five factors: individual belief in regulations, economic rationality, social networking, physical geography, and observable ecological variables.*

The model consists of three components: the population of resource users, the environmental system from which units of resource can be harvested, and the rules regulating interaction between users and the environment. The specifics below represent a first draft of the model. It has been kept intentionally simple, minimizing the number of hidden variables, with the intention of simplifying synchronization with the evolving field data.

The environment is modeled as a collection of villages and fishing grounds. Traveling between any two places costs time proportional to the distance. At fishing grounds, users can choose to fish either with a net, yielding high returns at the cost of high impact, or with a spear, yielding low returns but low impact.

Our model of the fish population is fairly radical, due to the many species involved, the strong coupling with the surrounding Amazon region, and the observed rapid impact of environmental changes in the fishing grounds. Rather than model the underlying population, we model the biomass of “catchable fish”. Instantaneous conditions at a fishing ground regulate the sustainable density of catchable fish (e.g. net-fishing decreases density, clear vegetation increases maximum) Catchable fish then diffuse between the larger Amazon system and each fishing ground based on the ratio of density to sustainable density.

Each game is a day. Users must begin and end their days in their home villages. In between, they expend time to try to maximize fish, by choosing a combination of travel, net-fishing, and spear-fishing that expends all of the available time.

Rules are represented by a collection of expert system IF/THEN rules. Every user interprets the set of rules with belief values, representing whether the user believes the rule is enforceable — the expected probability of enforcement is the sigmoid of the belief ($s(b) = \frac{1}{1+e^{-x}}$). Rule belief is affected by two mechanisms: observation and gossip. If a user observes the antecedents of a rule being fulfilled, then if the consequence is also fulfilled, belief increases by one. If, on the other hand, the consequence is not fulfilled, belief decreases by one. Gossip, on the other hand, acts by diffusion of belief values between users at the same location.

There are two types of users. The vast majority act economically rationally, employing a strategy of measured response[6]. Under measured response, a user determines the Nash equilibrium of a situation and the optimal strategy within bounds of the rules, then combines them proportional to the enforceability of the rules. A small minority, however, exhibit malicious behavior, collaboratively choosing actions to minimize compliance with the rules (this will usually also minimize the total value extracted from the resource).

Evaluation is on the basis of robustness against malicious users. In general, it is the case that with enough malicious users, belief in the rules will be destroyed and the system will settle to the Nash equilibrium. The higher a percentage of malicious users in the population that a system can sustain without belief in the rules collapsing, the more robust that system is.

1.6 Contributions

Preliminary results from the model suggest that it can display behavior characteristics similar to the real fisheries management system. Further testing of the hypotheses, however, is awaiting more data, particularly the harvest records from the coming year.

If the hypotheses prove justified, we can then apply the model to assist in making decisions and detecting problems in the fisheries management project.

One area of immediate applicability is cost-benefit estimates for investment of scarce resources (e.g. is it better to have more monitors, or radios to make communication between communities easier?). Simulations may also be helpful in predicting what types of problems are likely to arise, allowing better prevention. Finally, studying how systems collapse in simulation may provide diagnostics for early warning signs of serious problems and prescriptions for treatment.

The inclusion of institutional choice in the form of individual belief in regulations may be of broader interest. If it proves to be a useful model, it greatly simplifies the modeling of institutional choice, enabling better understanding and easier use of self-organizing CPR management systems.

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Chapter 4

Complexity and Diversity of Digraphs

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1. Introduction

There has been a great deal of ferment in ‘Complexity Science’ in recent years, as chronicled in the proceedings of the New England Complex Systems Institute’s International Conference on Complex Systems [Minai & Bar-Yam 2006, 2008] and those of the Santa Fe Institute [Nadel & Stein 1995, Cowan 1994]. We have been primarily focused on developing metrics of complexity relevant to chemistry, especially synthetic chemistry [Bertz 2003a–c]. Our approach involves abstracting a molecule or a plan for its synthesis as a graph and then using the tools of graph theory to characterize its complexity and diversity.

Mathematicians generally use the vertex-edge convention; however, following Harary [1969], authors in other fields often use the point-line convention, which we adopt here. A *graph* G consists of a finite set $V(G)$ of *points* (*vertices*) together with a set $E(G)$ of *lines* (*edges*), which are unordered pairs of distinct points of $V(G)$. A line $x = p_1p_2 = p_2p_1$ in G joins points p_1 and p_2 , which are *adjacent points*. In a *multigraph* any pair of points may be joined by more than one line, i.e., a *multiple line*. Two lines that share a point are *adjacent lines*, e.g., p_1p_2 and p_2p_3 . Point p_1 and line $x = p_1p_2$ are *incident* to each other, as are p_2 and x . The points in $L(G)$, the *line graph* of G , represent the lines of G , and two points in $L(G)$ are joined whenever the corresponding lines in G are adjacent.

When the lines of a graph are directed lines, i.e., ordered pairs of distinct points, they are called *arcs*, and the graph is called a *directed graph* or *digraph* D . Arc (i, j) or simply $p_i p_j$ is the arc from point p_i , the *tail*, to point p_j , the *head*. *Multidigraphs* allow multiple arcs, for example, two arcs from p_1 to p_2 . The *in-degree* of p_i , $in(p_i)$, is the number of arcs terminating at p_i , and the *out-degree* of p_i , $out(p_i)$, is the number of arcs originating from it. Since each arc has one head and one tail, for any digraph we have $\sum_i in(p_i) = \sum_i out(p_i)$. The *degree* d_i of point p_i in a graph (digraph) is the number of lines (arcs) incident to it; thus, in a digraph $d_i = in(p_i) + out(p_i)$.

A *walk* of length $n - 1$ is a sequence of points $p_1, p_2, p_3, \dots, p_n$ that are joined by arcs $p_1p_2, p_2p_3, \dots, p_{n-1}p_n$. A *path* P_n on n points is a walk where each point and hence each line is distinct. In a *pseudopath* one or more of the arcs are oriented in the opposite direction from the rest. *Semipaths* are comprised of paths and pseudopaths. In a *connected graph* (digraph) all pairs of points are the endpoints of some path (semipath). A *cycle* C_n , also called an n -cycle or n -ring, is a sequence of arcs $p_1p_2, p_2p_3, \dots, p_{n-1}p_n, p_np_1$ such that all n points are distinct. We include $p_1p_2p_1$ as a 2-cycle. A *loop* is a line that joins a point to itself in a 1-cycle. A *tree* is a connected graph without cycles. Walk counts have been used to measure complexity [Rücker & Rücker 2001], as have trees (vide infra).

Two graphs G and H are *isomorphic*, $G \cong H$, if and only if there exists a one-to-one correspondence between their point sets that preserves adjacency. An *invariant* $I(G)$ of graph G is a number associated with G that has the same value for any graph H isomorphic to G . For example, the number of points, the number of lines and the number of pairs of adjacent lines are graph invariants. A *subgraph* S of graph G is a graph that has all its points in $V(G)$ and lines in $E(G)$. We include G itself and also P_1 , the trivial path of length 0, in the set of all possible subgraphs of G . A *spanning subgraph* of G is a subgraph that contains all the points of G . A spanning subgraph that is a tree is a *spanning tree*.

A molecule can be abstracted as a *molecular graph* M by representing its atoms as points and the bonds between them as lines. Chemical graph theory ordinarily uses *hydrogen-suppressed graphs*, which do not include any hydrogen atoms or the bonds to them. Multiple bonds are represented by multiple lines and lone pairs of electrons by loops. Different atoms can be indicated by coloring the points, e.g., some typical colors are black (●) for carbon, red for oxygen, blue for nitrogen, etc. We use white (○) for a heteroatom (e.g., oxygen) when color is unavailable.

We have introduced two methods to measure the complexity of graphs, including molecular graphs. The first was the ‘all possible subgraphs method,’ where N_S is the number of kinds of connected subgraphs, i.e., the number of non-isomorphic ones, and N_T is the total number of connected subgraphs, isomorphic and non-isomorphic [Bertz & Sommer 1997, Bertz & Herndon 1986]. The second was the ‘edge cover method’ [Bertz 2001, Bertz & Zamfirescu 2000], which is not discussed here.

2. Results and Discussion

The problem with the methods introduced above is their vulnerability to the ‘combinatorial explosion,’ e.g., the number of subgraphs increases exponentially with the number of lines. In order to simplify the problem, we have investigated subsets of all possible subgraphs such as the number of non-isomorphic trees (‘kinds of trees’), T_S , and the total number of trees (isomorphic and non-isomorphic), T_T , [Bertz 2003c, Bertz & Wright 1998]. The number of spanning trees has been used as an index of complexity [Gutman 1983]; however, it is not sensitive to branching [Nikolić 2003], an essential aspect of molecular complexity. Various indices weight the complexity factors differently, and it is useful to have a range of them when confronting practical problems.

A particularly simple tree is P_3 , the path on three points or equivalently the path of length 2, the use of which greatly reduces computational complexity. Gordon and Kennedy [1973] introduced the number of subgraphs isomorphic to P_3 as an index of branching in a model of polymer properties. In chemical terms it is the number of ways to ‘cut’ the propane skeleton out of a molecule, i.e., the number of paths of length 2 in the molecular graph.

In order to extend this approach to digraphs, we must consider the possible kinds of ‘paths of length 2’ in them. As shown in Figure 1, there are two types of directed paths of length 2, namely $p_1p_2p_3$ in **A** and $p_1p_2p_1$ (or $p_2p_1p_2$) in **D**. In addition there are two pseudopaths of length 2, **B** and **C**. The center point in **A** has $in(p_2) = out(p_2) = 1$ and is a *carrier*, as are both points in **D**. A point is a *sink* when all arcs are directed towards it, e.g., the center point in **B**, where $in(p_2) = 2$ and $out(p_2) = 0$. A point is a *source* when all arcs are directed away from it, e.g., the center point in **C**, where $in(p_2) = 0$ and $out(p_2) = 2$. Endpoints p_1 and p_3 in **B** are sources, and in **C** they are sinks.

For a simple example one can easily count each of the subgraphs **A–D** and calculate the triple (a,b,c) , where a is the number of subgraphs isomorphic to **A** plus twice the number isomorphic to **D**, b is the number of subgraphs isomorphic to **B**, and c is the number of subgraphs isomorphic to **C**. This approach quickly becomes tedious as the size of the digraph increases.

The task of computing (a,b,c) is facilitated by methods based on the adjacency matrix [Harary 1969]. The *adjacency matrix* A of a digraph D on n points with point set $V(D)$ and arc set $E(D)$ is the $n \times n$ matrix $A(V, E)$, where element $A(i, j) = 1$ if arc

$(i, j) \in E(D)$ and $A(i, j) = 0$ otherwise. Each entry of $A^k(i, j)$ is the number of directed paths from p_i to p_j that contain k arcs. Thus, an entry of $A^2(i, j)$ is the number of directed paths of length 2 from p_i to p_j , and since $i = j$ is permitted, both **A** and **D** are counted.

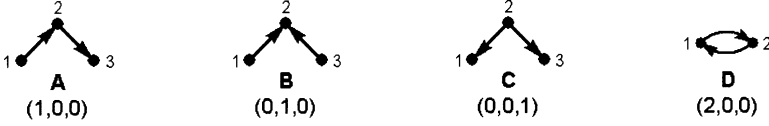


Figure 1. The four possible connected digraphs with 2 arcs and their triples (a, b, c) .

The transpose A^T of matrix A is obtained by interchanging its rows and columns. Then, $AA^T(i, j)$ represents the number of pseudopaths isomorphic to **B**, where endpoints p_i and p_j are sources, and $A^T A(i, j)$ represents the number of pseudopaths isomorphic to **C**, where they are sinks. Finally, for any digraph D we obtain the triple (a, b, c) by computing a as the sum of all entries in A^2 , b as the sum of all entries in AA^T and c as the sum of all entries in $A^T A$.

Alternatively, to reduce the computational time imposed by matrix multiplication, we note that ‘local’ information is sufficient to compute (a, b, c) . The in-degree and out-degree information for every point p of digraph D with point set $V(D)$ can be extracted efficiently from its adjacency matrix or equivalently from an adjacency list [Gibbons 1991]. Thus, $a = \sum_{p \in V} [in(p) \times out(p)]$, $b = \sum_{p \in V} C(in(p), 2)$ and $c = \sum_{p \in V} C(out(p), 2)$, where $C(k, 2)$ represents the combinations of k objects taken two at a time (k choose 2).

We have enumerated a total of 199 connected digraphs on four points with from zero to six 2-cycles. If we neglect the directions of the arcs, then there are 53 non-isomorphic multigraphs underlying them. The *underlying multigraph* results when the arcs in a digraph are converted into lines; a 2-cycle becomes a double line in this process. Then, we have 53 ‘families’ with from one to sixteen members, and Figure 2 shows one example from each. Figure 3 shows all ten digraphs from one of them.

For complexity considerations it is useful to compute the sum, $h = a + b + c$, the total number of semipaths of length 2, which is also given by equation 1, where h_i is the contribution of point p_i to h . The directionality of the arcs in a digraph is lost in computing h , which is the same for the underlying multigraph. Therefore, h characterizes the entire family of digraphs with a given underlying multigraph. For any graph G , $h = \eta$, the number of lines in the line graph, $L(G)$.

$$h = \sum_i h_i = \frac{1}{2} \sum_i d_i (d_i - 1) \quad (1)$$

It appears that the number of semipaths of length 2 is the simplest index of complexity that increases monotonically with all the factors that increase the complexity of a multidigraph: the number of points n , the number of arcs m , the

number of multiple arcs m_k comprised of k arcs, the number of rings r , and the degree of branching d_i at point p_i . For all trees on n points, $\sum d_i = 2m$ is constant, as $m = n - 1$. Therefore, branching is determined by the degree sequence in a graph or digraph.

Examining the first row of Figure 2, there is a general increase in complexity as one goes from left to right—with one exception. According to h , the ordering of **3** and **4** should be reversed. This makes sense when one considers the complexity factors: the number of points ($n = 4$), the number of arcs ($m = 5$) and the number of rings ($r = 1$) are the same for both, so that we must consider the degree sequences. For digraph **3** the degree sequence is 3, 2, 2, 1, whereas for digraph **4** it is 2, 2, 2, 2. On the basis of the highest degree, we conclude that **3** is more branched than **4** and consequently more complex. A caveat is the observation that the highest degree alone does not determine complexity, e.g., **9** has four arcs and degree sequence 4, 2, 1, 1, whereas **10** has 5 arcs and degree sequence 3, 3, 3, 1. Here, the ordering based on h also appears to be correct.

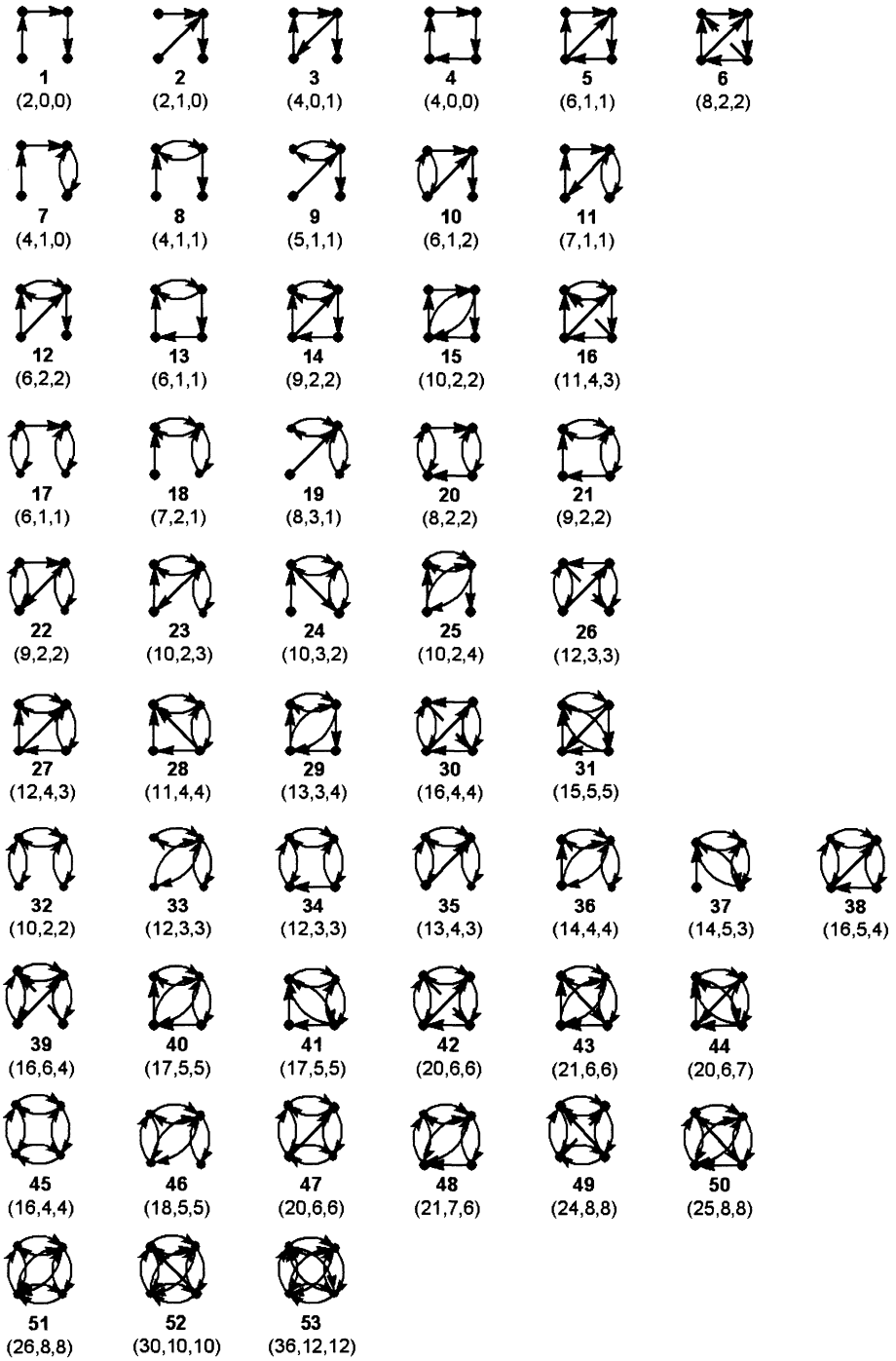


Figure 2. Representative digraphs with from zero to six 2-cycles.

Figure 2 contains many examples of digraphs with the same value of h . There are 13 degenerate pairs: (3, 7), (10, 11), (12, 18), (15, 32), (23, 24), (27, 28), (29, 35), (30, 45), (31, 38), (36, 37), (40, 41), (42, 47) and (43, 44); there are three degenerate triplets: (5, 13, 17), (6, 19, 20) and (14, 21, 22); and there is one degenerate quadruplet: (16, 26, 33, 34). The four digraphs in the quadruplet are differentiated by the total number of trees, T_T , including $T_1 \equiv P_1$; thus, **16** ($T_T = 51$) > **26** (46) > **34** (43) > **33** (30). They are not completely differentiated by the number of kinds of trees: $T_S = 12, 11, 9$ and 9 , respectively.

Except for **A** and **G**, all the digraphs in Figure 3 are uniquely characterized by their triples. Here, the order of numbers matters, e.g., (5,1,2) is distinct from (5,2,1).

The triple (a, b, c) also reflects the diversity of connectivity within the corresponding digraph. There are four levels of diversity among the digraphs of Figure 3: **B** (2,3,3), **I** (3,2,3) and **J** (3,3,2) are more diverse than **C** (2,2,4), **F** (4,2,2) and **H** (2,4,2), which are more diverse than **D** (5,1,2) and **E** (5,2,1), and they in turn are more diverse than **A** (6,1,1) and **G** (6,1,1). This order is based on equation 2 [Shannon & Weaver 1949, Bonchev & Trinajstić 1977], where H is the ‘information entropy’ and p_i is the probability of semipath i ; i.e., $p_1 = p_a = a/h$, $p_2 = p_b = b/h$ and $p_3 = p_c = c/h$. The values of H for the four levels are 1.56, 1.50, 1.30 and 1.06, respectively.

$$H = -\sum_i p_i \log_2 p_i \quad (2)$$

Quantities a , b and c are not equally relevant to all problems. We are especially interested in molecular complexity and synthetic complexity, i.e., the complexities of molecular graphs and synthesis digraphs, respectively. Hendrickson [1977] represented a synthesis plan by a *synthesis graph*, where the points stand for molecules and the lines for reactions that convert one molecule into another. Bertz [1986] refined this approach by introducing the *synthesis digraph*, which explicitly shows the directionality of the reactions involved and leads to additional qualitative and quantitative tools. In a synthesis digraph only directed paths from the available starting materials to the desired product can be fruitful [Bertz & Sommer 1993], and a is the relevant parameter, as each intermediate point must be a carrier. As far as h is concerned, a related quantity, η (vide supra), has been used as a predictor of relative synthetic efficiency [Bertz & Wright 1998, Bertz 1982, 1983].

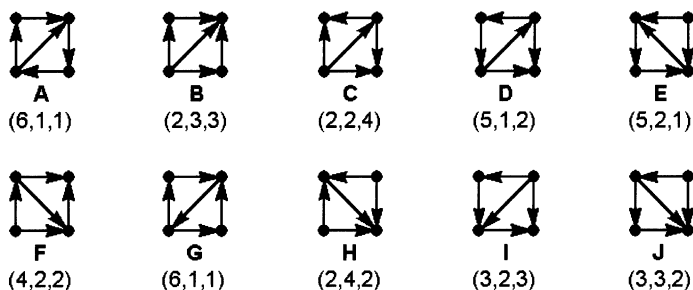


Figure 3. Digraphs with four points, five arcs and no 2-cycles ($A \equiv 5$, see Figure 2).

Electronegativity is one of the most important factors governing chemical reactivity [Pauling, 1960]. The bonds in molecules are polarized according to the electronegativities of the atoms involved, e.g., a carbon–oxygen bond is polarized towards the oxygen, as it has the higher electronegativity. Consequently, the oxygen atom has a partial negative charge and the carbon atom a partial positive one.

The *polarity digraph* P is obtained by replacing the lines in the molecular graph by arcs, where each arc goes from the less to the more electronegative atom. Polarity digraphs 1–3 in Figure 4a are hydrogen-suppressed graphs (vide supra), which may require some practice to visualize in chemical terms (see Figure 4b).

Polarity predicts the site of attack by a nucleophile (electron-rich species, e.g., hydroxide) on an ester, methyl acetate (1, Figure 4). Only electron pairs (loops) involved in the reaction are included here, and the positive counterions are not shown, as they are not directly involved. Attack occurs at the atom of the molecule (point of the polarity digraph) with the largest polarization, $\rho^+ = [(\text{out-degree}) - (\text{in-degree})] = 3 - 1 = 2$. (The superscripted plus sign indicates that the atom becomes more positive as the net outflow increases.) We give this definition because it is more ‘physical’ for chemical reactions, where the flow is negatively charged (i.e., electrons), than the alternative, $\rho^- = [(\text{in-degree}) - (\text{out-degree})]$.

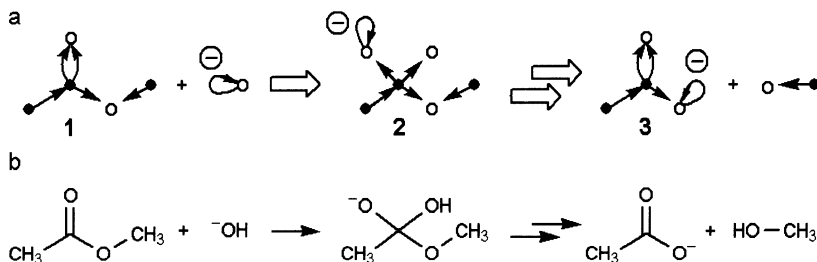


Figure 4. (a) Polarity digraphs for the hydrolysis of methyl acetate (1) by hydroxide (OH^-). (b) Conventional chemical equation corresponding to part (a).

3. Conclusion

Which measure of complexity or diversity is most useful depends upon the specific application. We have demonstrated that the simplest approach to the complexity of graphs, the number of paths of length 2, also gives useful results when extended to the complexity and diversity of digraphs. For some applications, the individual quantities a , b and c may be more useful than their sum, h . Another way to use these invariants is to calculate the information entropy, H , which is a useful measure of diversity. The polarity digraph is a new tool for chemical graph theory.

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Chapter 5

Complex Knowledge Networks and Invention Collaboration

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Knowledge and innovation flows as characterized by the network of invention collaboration is studied, its scale free power law properties are examined and its importance to understanding technological advancement. This research while traditionally investigated via statistical analysis may be further examined via complex networks. It is demonstrated that the invention collaboration network's degree distribution may be characterized by a power law, where the probability that an inventor (collaborator) is highly connected is statistically more likely than would be expected via random connections and associations, with the network's properties determined by a relatively small number of highly connected inventors (collaborators) known as hubs. Potential areas of application are suggested.

1. Introduction

Presently we are constructing ever increasingly integrated and interconnected networks for business, technology, communications, information, and the economy. The vital nature of these networks raises issues regarding not only their significance and consequence but also the influence and risk they represent. As a result it is vital

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to understand the fundamental nature of these complex networks. During the past several years advances in complex networks have uncovered amazing similarities among such diverse networks as the World Wide Web [Albert et al. (1999)], the Internet [Faloutsos et al.(1999)], movie actors [Amaral et al. (2000)], social [Ebel et al. (2002)], phone call [Aiello et al. (2002)], and neural networks [Watts and Strogatz (1998)]. Additionally, over the last few decades we have experienced what has come to be known as the information age and the knowledge economy. At the center of this phenomenon lies a complex and multifaceted process of continuous and far-reaching innovation advancement and technological change [Amidon (2002)], Cross et al. (2003) and Jaffe and Trajtenberg (2002)]. Understanding this process and what drives technological evolution has been of considerable interest to managers, researches, planners and policy makers worldwide. Complex networks offer a new approach to analyze the information flows and networks underlying this process.

1.1 Knowledge and Innovation Networks

Today, nations and organizations must look for ways of generating increased value from their assets. Human capital and information are the two critical resources. Knowledge networking is an effective way of combining individuals' knowledge and skills in the pursuit of personal and organizational objectives. Knowledge networking is a rich and dynamic phenomenon in which existing knowledge is shared, evolved and new knowledge is created. In addition, in today's complex and constantly changing business climate successful innovation is much more iterative, interactive and collaborative, involving many people and processes. In brief, success depends on effective knowledge and innovation networks. Knowledge collaboration and shared innovation, where ideas are developed collectively, result in a dynamic network of knowledge and innovation flows, where several entities and individuals work together and interconnect. These networks ebb and flow with knowledge and innovation the source and basis of technological advantage. Successful knowledge and innovation networks carry forth the faster development of new products and services, better optimization of research and development investments, closer alignment with market needs, and improved anticipation of customer needs resulting in more successful product introductions, along with superior competitor differentiation. [Skyrme (1999), Amidon (2002), and Cross et al. (2003)]

This paper discusses knowledge and innovation flows as represented by the network of patents and invention collaboration (inventors and collaborators) and attempts to bridge recent developments in complex networks to the investigation of technological and innovation evolution. The recent discovery of small-world [Watts and Strogatz (1998)] and scale-free [Barabasi and Albert (1999)] network properties of many natural and artificial real world networks has stimulated a great deal of interest in studying the underlying organizing principles of various complex networks, which has led in turn to dramatic advances in this field of research. Knowledge and innovation flows as represented by the historical records of patents and inventors, with future application to technology and innovation management is addressed.

1.2 Gaussian Statistics to Complex Networks

Patents have long been recognized as a very useful and productive source of data for the assessment of technological and innovation development. A number of pioneering efforts and recent empirical studies have attempted to conceptualize and measure the process of knowledge and innovation advancement as well as the impact of the patenting process on patent quality, litigation and new technologies on innovation advancement [(Griliches (1990), Jaffe and Trajtenberg (2002), Cohen and Merrill (2003)]. However, these studies have primarily relied upon traditional (Gaussian) statistical data analysis. Complex networks should reveal new associations and relationships, thus leading to an improved understanding of these processes.

Recent studies in complex networks have shown that the network's structure may be characterized by three attributes, the average path length, the clustering coefficient, and the node degree distribution. Watts and Strogatz (1998) proposed that many real world networks have large clustering coefficients with short average path lengths, and networks with these two properties are called "small world." Subsequently it was proposed by Albert et al. (1999) and Barabasi and Albert (1999) that many real world networks have power law degree distributions, with such networks denoted as "scale free." Specifically scale free networks are characterized by a power law degree distribution with the probability that a node has k links is proportional to $k^{-\gamma}$ (i.e., $P(k) \sim k^{-\gamma}$), where γ is the degree exponent. Thus, the probability that a node is highly connected is statistically more significant than in a random network, with the network's properties often being determined by a relatively small number of highly connected nodes known as hubs. Because the power law is free of any characteristic scale, networks with a power law node degree distribution are called scale free. [Albert and Barabasi (2002), Newman (2003), and Dorogovtsev and Mendes (2003)] In contrast, a random network [Erdos and Renyi (1959)] is one where the probability that two nodes are linked is no greater than the probability that two nodes are associated by chance, with connectivity following a Poisson (or Normal) distribution.

The Barabasi and Albert (BA) (1999) model suggests two main ingredients of self-organization within a scale-free network structure, i.e., growth and preferential attachment. They highlight the fact that most real world networks continuously grow by the addition of new nodes, are then preferentially attached to existing nodes with large numbers of connections, a.k.a., the rich get richer phenomenon. Barabasi et al. (2002) and Newman (2004) have also previously studied the evolution of the social networks of scientific collaboration with their results indicating that they may generally be characterized as having small world and scale free network properties.

1.3 Invention, Knowledge and Technology

Patents provide a wealth of information and a long time-series of data about inventions, inventors, collaborators, prior knowledge, and assigned owners. Patents and the inventions they represent have several advantages as a technology indicator. In particular, patents and patent citations have long been recognized as a very rich and fertile source of data for studying the progress of knowledge and innovation. Hence, providing a valuable tool for public and corporate technology analysis, as well as planning and policy decisions [Griliches (1990), Jaffe and Trajtenberg (2002),

Cohen and Merrill (2003)]. Nevertheless, patents and invention collaboration have undergone limited investigation, thus offering a very rich information resource for knowledge and innovation research that is even less well studied and is yet to be fully exploited [Jaffe and Trajtenberg (2002)]. A companion paper analyzes patents and patent citations from a complex networks perspective [Brantle and Fallah (2007)].

2 Invention Collaboration

Patents and invention collaboration data contains relevant information allowing the possibility of tracing multiple associations among patents, inventors and collaborators. Specifically, invention collaboration linkages allows one to study the respective knowledge and innovation flows, and thus construct indicators of the technological importance and significance of individual patents, inventors and collaborators. An item of particular interest is the connections between patents and invention collaborators. Thus, if inventor A collaborates with inventor B, it implies that inventor A shares or transfers a piece of previously existing knowledge with inventor B, and vice versa, along with the creation of new knowledge as represented by the newly patented invention. As a result, not only is a flow of knowledge shared between the respective invention collaborators, but an invention link or relationship between the individual collaborators is established per the patented invention.

The supposition is that invention collaboration is and will be informative of the relationships between inventors and collaborators as well as to knowledge and innovation. The construction of the invention collaboration network is discussed and it's bearing to knowledge and information. Next, summary statistics, probability distributions and finally the power law degree distribution is analyzed.

2.1 Bipartite Graphs and Affiliation Networks

An invention collaboration network similar to that produced by the movie actor network [Watts and Strogatz (1998)] may be constructed for invention collaboration where the nodes are the collaborators, and two nodes are connected if two collaborators have coauthored a patent and therefore co-invented the invention. This invention affiliation or collaboration relationship can be easily extended to three or more collaborators. The relationship can be completely described by a bipartite graph or affiliation network where there are two types of nodes, with the edges connecting only the nodes of different types. A simple undirected graph is called bipartite if there is a partition of the set of nodes so that both subsets are independent sets. Collaboration necessarily implies the presence of two constituents, the actors or collaborators and the acts of collaboration denoted as the events. So the set of collaborators can be represented by a bipartite graph, where collaborators are connected through the acts of collaboration. In bipartite graphs, direct connections between nodes of the same type are impossible, and the edges or links are undirected.

Figure 1 provides a bipartite graph or affiliation network representation with two sets of nodes, the first set labeled "patents" which connect or relate the second set labeled "invention collaborators" who are linked by the shared patent or invention. The two mode network with three patents, labeled P_A , P_B and P_C , and seven patent or invention collaborators, C_1 to C_7 , with the edges joining each patent to the respective

collaborators is on the left. On the right we show the one mode network or projection of the graph for the seven collaborators. It is noted that singularly authored patents would not be included in the bipartite graph and resulting invention collaboration network.

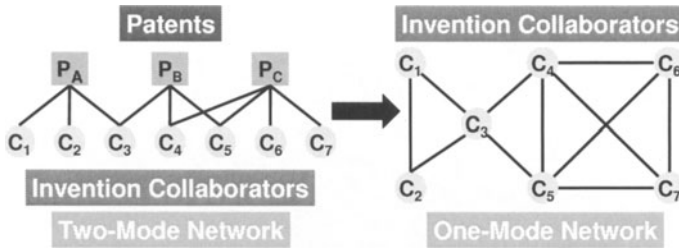


Figure 1 – Invention Collaboration Bipartite Graph or Affiliation Network

2.2 Knowledge and Innovation Flows

Patents and invention collaboration constitute a documented record of knowledge transfer and innovation flow, signifying the fact that two collaborators who coauthor a given patent, or equivalently co-invent said invention, may well indicate knowledge and innovation flowing between the respective collaborators along with the creation of new knowledge and innovation as represented by the new invention. The patent invention link and collaboration knowledge and innovation flow is illustrated in Figure 2 and can be easily extended to three or more collaborators. Thus, knowledge and innovation information made publicly available by the patent has not only flowed to the invention, but has significantly influenced the invention's collaborators. Several network measures may be applied to the collaboration network in order to both describe the network plus examine the relationship between and the importance and significance of individual inventors and collaborators [Newman (2004)].

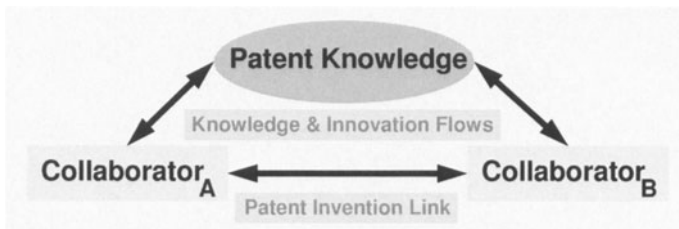


Figure 2 – Knowledge & Innovation Flows and Patent Invention Links

2.3 Patents, Inventors and Data

The invention collaboration network is constructed using the inventor data provided by the NBER (National Bureau of Economic Research) patent inventor file [Jaffe and Trajtenberg (2002)]. This file contains the full names and addresses of the inventors for patents issued from the beginning of 1975 through the end of 1999, comprising a twenty-five year period of patent production and invention collaboration. This includes approximately 4.3M patent-inventor pairs, 2.1M patents and 1.4M inventors.

2.4 Invention Collaboration Distribution

2.4.1 Power Law Degree Distribution

Figure 3 provides the probability degree distribution for the invention collaboration network on logarithmic scales. It may be seen that the best fit line for this distribution follows a power law distribution with an exponent of 2.8. Hence it is concluded that a power law provides a reasonable fit to the data. It is noted that a truncated power law distribution with an exponential cutoff may provide a suitable representation, with an associated improvement in the explanation of total variance ($R^2 \approx 1.0$). This systematic deviation from a power law distribution is that the highest collaborating inventors are collaborating less often than predicted and correspondingly the lowest collaborating inventors are collaborating more often than predicted. A reasonable rationale for this deviation is that in many networks where aging occurs, show a connectivity distribution that possess a power law organization followed by an exponential or Gaussian decay distribution [Amaral et al. (2000)].

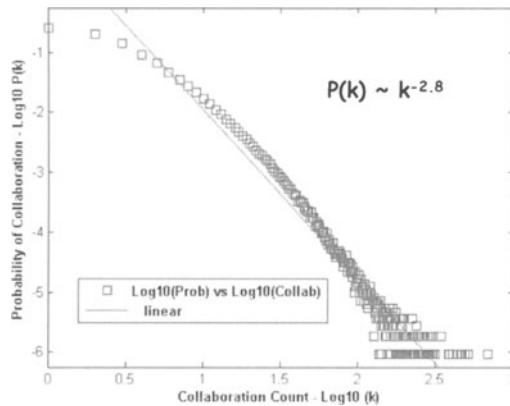


Figure 3 – Invention Collaboration: Collaborators Per Inventor

The improved fit of the truncated power law with exponential cutoff model, may be attributed to a distinction in the objectives of invention patenting versus scientific publishing. As a result, patent invention collaboration with the sharing of patent rights, further dividing any potential economic rewards and financial gains might have a minimizing or at least optimizing effect on any incentive to increase the number of collaborators. It would be expected that inventors would evaluate and weigh the potential technical contribution against the economic and financial impact of the prospective collaboration on the invention and its shared ownership. Again, with respect to scientific publication this objective is much less of a consideration.

For the patent invention collaboration network the degree exponent of the number of patent invention collaborators is approximately 2.8. Thus, it is demonstrated that the number of invention collaborators roughly follows a power law distribution. That is, the numbers of collaborators per inventor falls off as $k^{-\gamma}$ for some constant $\gamma \approx 2.8$, implying that some inventors account for a very large number of collaborations,

while most inventors collaborate with just a few and smaller number of additional collaborators. These results are consistent with the theoretical and empirical work concerning scale free networks where a degree exponent of $2 < \gamma < 3$ is predicted for very large networks, under the assumptions of growth and preferential attachment.

3 Summary, Discussion and Conclusions

Knowledge and innovation as typified by the network of patents and invention collaboration and the significance of this network to the advancement of technology is discussed. This area of research while traditionally investigated via statistical analysis may be further advanced via complex network analysis. The scale free power law property for the invention collaboration network is presented, where the probability that an inventor or collaborator being highly connected is statistically more significant than would be expected via random connections or associations. Thus the network's properties now being determined by a relatively small number of highly connected inventors and collaborators known as hubs.

Immediate areas of potential application and continued investigation include: technology clusters and knowledge spillover [Saxenian (1994), Porter (1998), Jaffe et al. (2000), Jaffe and Trajtenberg (2002)] and patent quality, litigation and new technology patenting [Cohen and Merrill (2003), Lanjouw and Schankerman (2004)]. Analyses of invention collaboration and application to these areas from a complex network analysis perspective should provide a deeper understanding as to their underlying structure and evolution which may influence both private and public policy decision making and planning initiatives.

Significant effort and research has been placed into investigating the organization, development and progression of knowledge and innovation, and its impact on technology advancement. Complex network analysis offers tremendous potential for providing a theoretical framework and practical application to the role of knowledge and innovation in today's technological and information driven global economy.

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Chapter 6

Random Evolution of Idiotypic Networks: Dynamics and Architecture

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The paper deals with modelling a subsystem of the immune system, the so-called idiotypic network (INW). INWs, conceived by N.K. Jerne in 1974, are functional networks of interacting antibodies and B cells. In principle, Jernes' framework provides solutions to many issues in immunology, such as immunological memory, mechanisms for antigen recognition and self/non-self discrimination. Explaining the interconnection between the elementary components, local dynamics, network formation and architecture, and possible modes of global system function appears to be an ideal playground of statistical mechanics. We present a simple cellular automaton model, based on a graph representation of the system. From a simplified description of idiotypic interactions, rules for the random evolution of networks of occupied and empty sites on these graphs are derived. In certain biologically relevant parameter ranges the resultant dynamics leads to stationary states. A stationary state is found to correspond to a specific pattern of network organization. It turns out that even these very simple rules give rise to a multitude of different kinds of patterns. We characterize these networks by classifying 'static' and 'dynamic' network-patterns. A type of 'dynamic' network is found to display many features of real INWs.

1.1 Introduction

The immune system is a complex adaptive system. By its macroscopic number of constituents at different levels of organization (groups of cells, cells, and even individual molecules), it appears as a natural playground for statistical physics. Much progress has recently been made understanding complex systems by classifying their underlying network topologies [2]. It has been argued that, though detailed interactions between a system's components may be rather complicated, much can already be understood by analysing the system's network structure. Naturally, network structures are frequently closely related to processes that govern network growth [1].

In this paper, we explain a model for so-called INWs in the immune system. For this, our 'programme' follows the above idea: we devise a very simple cellular automaton based minimal model hoping to capture the essential parts of the real system. We analyze the network structures arising from this simple set of rules. Finally we relate the emergent structures in our model to structures observed in the immune system.

The organization of the paper is as follows. We start by introducing some basic concepts from immunology. Building on this, we next explain our abstract model. Then, in §1.2 an analysis of the model is presented. We conclude the paper with a discussion of the biological relevance.

1.1.1 Idiotypic networks

Immune response against a broad class of antigens (bacteria, viruses, fungi, etc.) is triggered by antibodies and B cells. A B cell carries exactly one type of antibody on its surface. Antibodies and B cells of one 'type' (determined by the structure of the binding region of the antibody) define an idio type.

The process of antigen detection and elimination can be described as follows. Accidentally, the invading antigen meets with a complementary antibody. Then, the antibody and antigen form a complex, marking the antigen as 'hostile' for later removal by other groups of cells (e.g. macrophages). If a B cell with the complementary type of antibody on its surface encounters antigen, the B cell becomes stimulated, grows into a clone and finally becomes a production unit for its specific type of antibody.

It is Jerne's fundamental idea leading to INWs [7], that antibodies can not only recognize antigen, but also other anti-antibodies which are complementary. This causes the stimulation of the respective B cells and leads to ongoing self-balanced immune activity even in the absence of antigens. These mutually recognizing idiotypes build the INW. The dynamics of idiotypes within the network is frequently described by Lotka-Volterra-like equations:

$$\frac{dx_i}{dt} = x_i \left[-\gamma_i + f \left(\sum_j m_{ij} x_j \right) \right] + \chi_i, \quad (1.1)$$

where i is an index labeling idiotypes, x_i idiomtype i 's concentration, γ_i its inverse lifetime, f a function describing stimulation and death of B cells and antibody production by stimulated B cells, χ_i an influx rate of new idiotypes from the bone marrow. The coefficients m_{ij} are the elements of the adjacency matrix of the INW.

It is a common approach to model an idiomtype or vertex of the INW by a bit string $(i_1, \dots, i_d)$ of length d [5]. Estimates for the number of all conceivable idiotypes lead to a realistic bit chain length of $d \approx 35$ [9]. In a very abstract way the bit-string is thought to represent a discretization of the antibodies binding regions. Since binding is based on complementarity, only bit-strings which are complementary are allowed to interact. More precisely, if binding requires complementarity in all but k positions we set $m_{ij}^{(k)} = 1$ if $d_H(i, j) \leq k$ and $m_{ij}^{(k)} = 0$ otherwise, where $d_H(\cdot, \cdot)$ stands for the Hamming distance.

By introducing the set of vertices as the set of bit-strings and links as defined by the above 'matching rules' one obtains a base graph $G_d^{(k)}$ of all possible idiotypes, the so-called *potential repertoire*. The set of vertices which are present at a given time, the *actual repertoire* Γ , is only a relatively small subset of the possible repertoire, determined by the dynamics in the system. The remainder of the work will deal with describing how rules for interaction dynamics lead to the shaping of the actual repertoire within the potential repertoire.

As introduced in Eq. (1.1) there are two mechanisms driving the population dynamics of idiotypes. First, in the bone marrow, new types of idiotypes are continuously formed. A good approximation is to assume that the formation of new idiotypes is uniform and random. In other words, the probability over time that a given type i is formed is independent of i and constant.

A second mechanism shaping the actual repertoire comes from the interaction of the idiomtype populations. This is usually modeled by a 'bell-shaped' function f in (1.1), meaning that only idiotypes which experience at least some, but not too much stimulation from their neighbours are allowed to survive¹. Equipped with these two building blocks we now formulate the abstract model.

1.1.2 The model

Instead of considering idiomtype population densities as in (1.1) an idiomtype i can be present ($s_i = 1$) or absent ($s_i = 0$). In the first case, the corresponding vertex on the base graph is occupied, in the latter case it is empty. We account for the dynamics in the network by introducing the following two rules:

- (i) Introduce I new vertices into the network by randomly selecting I empty vertices and occupying them. This step is thought to model the influx of new idiotypes from the bone marrow.

¹Stimulation of a B cell requires the cross linking of two of its surface receptor antigens. Thus, on the one hand, for low concentrations of a complementary structure, e.g., antigen, every antigen binds to one receptor only. On the other hand, for high concentrations there is much competition about the B cells receptors leading to most antigens being bound to only one receptor. Hence, in both cases cross linking is effectively prevented.

- (ii) Check the neighbourhood of every occupied vertex v . If it has less than t_l or more than t_u neighbours, the corresponding idiootype is under- or overstimulated, respectively. Consequently, it will die out and we set $s_v = 0$ in the next timestep. The update in step (ii) will be performed in parallel.

The threshold values t_l and t_u , the influx I , and the values of the bit chain length d and the number of mismatches are the model's parameters. Since it is possible to mount an immune response against already a very small concentration of antigen, we use $t_l = 1$ in the remainder of this paper.

The threshold t_u prevents unlimited growth of the network. Conversely, the threshold t_l only leads to adjustments in the network, if a vertex is taken out due to violating the maximum number of neighbours rule first. Then, however, it may initiate a cascade of idiotypes dying out. This is so, if a vertex with t_u neighbours is adjacent to a vertex with t_l neighbours, which in turn has a neighbour with t_u occupied neighbours and so on (corresponding to a chain for $t_u = 1$). In this sense, the lower threshold introduces an intermediate term memory of a perturbation.

We note that the algorithm bears some similarity to Conways "game of life" [3]. Major differences lie in the following points: (1) we study the algorithm on a regular graph not associated with a notion of space and (2) the influx as above introduces a 'global birth' rate, that allows disconnected structures to emerge. Further, I serves as a selection pressure. For low I it forces the system into organized patterns. However, for too high I it causes disorder. This can be understood as follows. The higher the influx, the more likely it becomes that an occupied vertex gets many new neighbours. Thus, the higher the influx, the higher the probability that the occupied vertex becomes removed and the higher the chances that an extinction cascade is initiated. That is, only organized arrangements of occupied and empty sites, in which chances for long extinction cascades are minimized, can survive for a long time.

1.2 Static and Dynamic patterns

We start by investigating the dynamics on the first non-trivial type of base graphs, i.e. on the graphs $G_d^{(1)}$. It turns out, that for a given bit chain length and given values of (t_l, t_u) the dynamics of occupied and empty sites can be classified by a set of thresholds for the influx I . For very low I , typically organized 'metastable' structures emerge. Increasing I , a pattern of occupied and empty sites is formed which is characterized by utmost stability against perturbation. In this type of pattern, a vertex once occupied remains occupied. Thus, apart from fluctuations, the pattern is comprised of a permanent arrangement of empty and occupied vertices. Hence we classify it as a static pattern. Increasing I beyond a threshold I_c , networks tend to become random. For a more detailed analysis the reader is referred to [4].

Apart from the influx I , the structure and particularly the connectivity of the base graph also play an important role in determining which pattern is allowed

to emerge. The coordination number of the base graphs $G_d^{(k)}$ can be tuned by changing the number of allowed mismatches k . One finds that for $k \geq 2$ the ‘phase diagram’ becomes much more complicated than in the case of $k = 1$.

Associated with every pattern there is a typical average time $\langle \tau_{\text{life}} \rangle$ (‘lifetime’) during which a once occupied vertex remains occupied. We find that changes in pattern may lead to dramatic changes in average lifetimes, letting average lifetimes appear as a good indicator of changes in pattern structure. Fig. 1.1

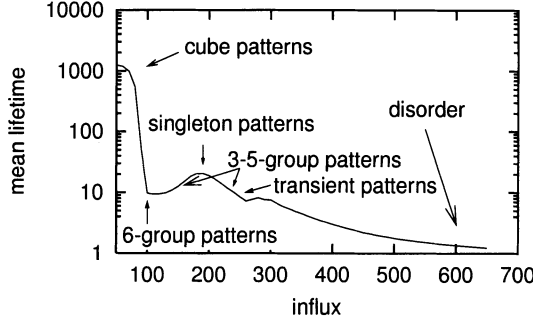


Figure 1.1: Data for the mean lifetime (log-scale) vs. influx obtained from simulations on $G_{12}^{(2)}$ with $(t_l, t_u) = (1, 10)$. Successively, the system forms cube-patterns, multiple group patterns, singleton patterns, and again multiple group patterns. Then patterns become transient and finally a randomness driven regime is entered. Every change of pattern structure leads to a change of typical average mean lifetimes of occupied vertices. Thus this diagram gives a good representation of the ‘phase diagram’ of the system in the influx direction. From [4].

shows simulation data for the dependence of $\langle \tau_{\text{life}} \rangle$ on the influx I . A more detailed investigation reveals transitions from ‘cube pattern’ to 6-group and multiple group and singleton patterns, followed by disorder for high I . It turns out that while cube pattern represent a type of pattern very similar to static pattern found on base graphs with $k = 1$, multiple group pattern are a completely different type of network organization. Unlike the previous case, vertices are now no longer permanently occupied or empty, but change from one state to the other with a typical average frequency.

The key for understanding the multiple group pattern lies in an analysis of the 6-group pattern. For a more detailed investigation, we introduce average occupancy $r_o(v) = 1/(T_1 - T_0) \sum_{t=T_0}^{T_1} s(v)$ and change rates $r_s = 1/(T_1 - T_0) \sum_{t=T_0}^{T_1} \delta_{s_t(v)s_{t+1}(v)}$. Fig. 1.2 displays data for the mean occupancy rate obtained from a simulation on $G_{12}^{(2)}$ for an influx $I = 100$. Clearly, mean occupancy rates cluster around 6 distinct values of $r_o^{(i)}$, $i = 1, \dots, 6$. By introducing cut-offs we accordingly define 6 groups of vertices $S_i = \{v \in G | r_o^{(i-1)} \leq \langle r_o(v) \rangle \leq r_o^{(i)}\}$, $i = 1, \dots, 7$, where $r_o^{(0)} = 0$ and $r_o^{(7)} = 1$. Further experiments show it’s not only that vertices of a group have approximately the same mean occupancy rate. Indeed, a similar picture as that in Fig. 1.2 could be presented for many other

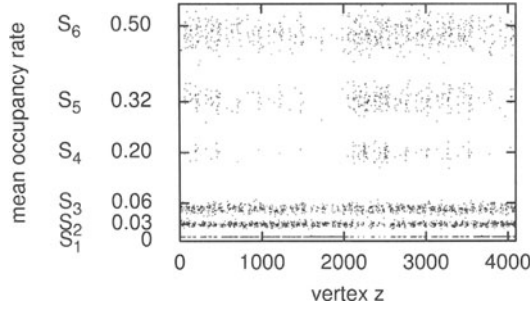


Figure 1.2: Mean occupancy rates of vertices z derived from a simulation on $G_{12}^{(2)}$ with $(t_l, t_u) = (1, 10)$ and $I = 100$. Six groups of vertices $S_1, \dots, S_6$ can be distinguished by their mean occupancy rates. From [4].

characteristics, such as mean frequencies of vertices of being singletons, belonging to clusters of small size or to the giant component, mean connectivities or mean lifetimes.

This analysis reveals the following structure of the the groups $S_1, \dots, S_6$:

- (a) Vertices of S_4, S_5 and S_6 typically have long lifetimes, belong frequently to small clusters, very seldom to the giant cluster and, in total, have only small numbers of occupied neighbours. Between 20% and 50% of the sites are occupied at a given time.
- (b) Vertices of S_2 and S_3 have intermediate lifetimes and are almost always located in the giant cluster. Moreover, they always have a high number of occupied neighbours. Nevertheless, only approx. 5% of the sites in these groups is occupied at a time.
- (c) Vertices of S_1 are almost never occupied. If they perchance are occupied, they tend to have a very high connectivity.

To further understand the interplay between different groups, we introduce inter- and intra-group degrees $\partial_{|S_i} v$ counting the number of occupied neighbours a vertex v has in group S_i . From this, one derives the arrangement of the groups on the base graph as visualized in Fig. 1.3. Both the actual arrangement of the groups on the base graph as also the properties (a)–(c) suggest a division of the actual repertoire as follows.

There is a densely connected core which consists of S_2 and S_3 . This core lies in the centre of the network, almost all other vertices have, if occupied, a connection to it. In other words: the core provides the minimum amount of stimulation needed that a vertex of another group can survive. Yet, while sustaining the remainder of the network, the size of the core is also restricted by it. Because a vertex of the relatively small core typically has many connections in the group and to the outside, increasing its size leads to overstimulation.

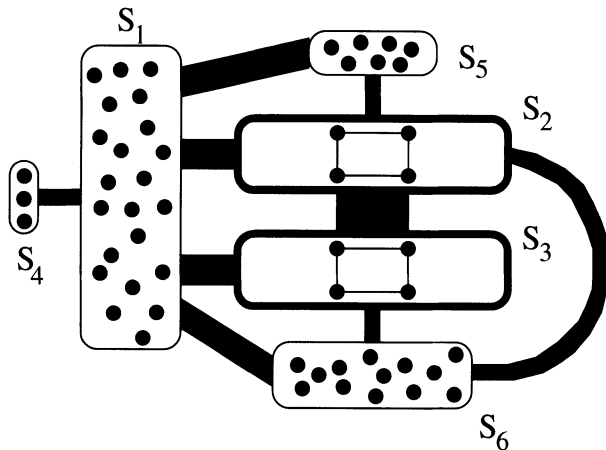


Figure 1.3: Visualization of the network structure of the groups $S_1, \dots, S_6$ on the base graph $G_{12}^{(2)}$. Groups are represented by boxes. The squares inside boxes indicate many connections of vertices of a group into the same group, isolated circles visualize that vertices have no other neighbours in the same group. The thickness of the connecting lines between the groups gives a measure for how many links connect vertices of the respective groups. Because of their importance for the existence of a giant component in the actual repertoire, the core groups S_2 and S_3 are bounded by fat lines. From [4].

Lying at the ‘outside’ and scarcely connected to themselves, the groups S_4 – S_6 form the periphery of the network. In turn, the size of these groups is determined by the amount of stimulation that they receive from the influx and from the core. Having typically only one connection to another occupied vertex, vertices in these groups are only loosely connected to the core.

A third functional unit is formed by group S_1 , vertices of which are almost never present.

1.3 Connection to Biology

Though recent studies, e.g., [8] hint to the importance of INWs for the immune system’s function, detailed structural investigations are very scarce and address systems which are too small to allow for general conclusions. However, by analyzing requirements for system function, general ideas about what the topology of a healthy INW should look like have been developed [10]. It is supposed, that INWs should comprise a densely connected core, the so-called ‘central immune system’ (CIS) and a collection of weakly connected small clusters of clones, the ‘peripheral immune system’ (PIS). While the CIS is assigned a vague role as a ‘regulatory part’ (being, e.g., responsible for the prevention of autoimmunity), the PIS is thought essential for establishing memory of previous antigen encounters.

Already the simple rules in our model allow the self-organization of a network which reproduces the above scenario. We interpret the highly connected core

of these networks as the CIS and the loosely interlinked periphery as the PIS of the INW. Idiotypes in the periphery groups were found to be long-lived, i.e. in principle capable of representing memory. Most of the time they are isolated. Their population survives by occasional stimulation from the core and stimulation through the influx of new random idiotypes. This mechanism could work together with other mechanisms for the stimulation of isolated clones [6].

The model further illustrates the role which the interplay between CIS and PIS could play in the regulation of the structure of an INW. In a healthy system a balance is maintained between both. Extensive growth of the CIS is prevented by the restricted stimulation available from the CIS. Likewise, the growth of the CIS is prevented by overstimulation, which is a consequence of the high connectivity of new nodes in it and the connections formed with the PIS.

More speculatively than the above interpretation, we conjecture that the group S_1 could be identified with a “mirror image of the individual’s molecular self”. The group is thought to represent all idiotypes complementary to (and hence attacking the) self. Our model also shows, that, in principle, such a group could be suppressed by the remainder of the network.

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Chapter 7

Constructing scale-free networks by a matrix stability approach

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In this paper, we present a method to evolve Scale-free (SF) networks as interaction networks of systems which are distinguished by their stability if perturbed out of equilibrium. Based on linear stability analysis of fixed points we use the largest real part of any eigenvalue as a measure for system stability. Our construction method involves two key mechanisms: (i) growth, one node at a time, and (ii) a directed search selecting the more stable systems, only allowing for at most small deteriorations of stability at each growth step. We explore the model's parameter space, explaining under which conditions a SF network topology emerges. The model for the first time relates stability of a dynamical system to a SF topology of its underlying interaction network.

1.1 Introduction

Scale-free (SF) networks have been found to occur in very diverse contexts. Examples are found in artificially created systems such as the WWW, transport flow systems or social networks, and also in many biological regulatory networks such as, metabolic, protein folding and genetic networks (for an overview see [1, 4]). It is this striking universality which makes one look for widely applicable general principles leading to the formation of these networks. In principle, two processes for their formation are known: (1) preferential attachment [3](and

modifications thereof, including, e.g., *a priori* assigned node fitnesses, additional rewiring or link deletion steps, and node aging – for a summary see [4]) and (2) optimization with respect to diameter and link number, distinguishing SF networks as networks which enable best communication for limited cost [5]. In this paper we develop a third mechanism, relating a SF interaction network of a dynamical system to its stability to perturbation away from equilibrium.

In previous studies, SF networks have been shown to be very robust to random attacks, but prone to heavy damage from attacks targeted at nodes with many neighbours (so-called ‘hubs’) [2]. Stability measures employed in these studies, however, have focussed only on topological properties. By showing that SF networks can also be understood as architectures of ‘robust’ dynamical systems, we hope to add another viewpoint to understanding why SF networks appear to be so universal in nature.

Consider an arbitrary set of N non-linear first order differential equations

$$\dot{x}_i = -\gamma_i x_i + F_i(\{x_j\}), i = 1, \dots, N, \quad (1.1)$$

where autonomous growth rate terms $\gamma_i x_i$ have been separated. We assume that after allowing for sufficient relaxation time the dynamics lead to a fixed point x^* . If the system approaches a limit cycle with period T_{limit} , we assume a ‘coarse-grained’ view of the system, only considering averages $\bar{x}(n) = 1/T \int_{(n-1)T}^{nT} x(t) dt$ over a time $T \gg T_{\text{limit}}$. For our purposes this allows us to treat the latter situation in the same way as that of the fixed point. For a small perturbation Δx from the fixed point linear stability analysis yields:

$$\frac{d}{dt} \Delta x_i = \sum_j \left(-\gamma_i \delta_{ij} + \frac{\partial F_i}{\partial x_j}(x^*) \right) \Delta x_j. \quad (1.2)$$

Thus, if the largest real part of the eigenvalues of the matrix M^1 with elements $m_{ij} = -\gamma_i \delta_{ij} + \frac{\partial F_i}{\partial x_j}(x^*)$ is below zero, small perturbations die out exponentially and the fixed point is stable. In the following we choose $\gamma_i = -1, i = 1, \dots, N$, considering a system of variables (or ‘species’) which are self-regulated and assume that Eqs (1.1) have been normalized with respect to internal growth rates.

As an alternative view on the above procedure, one could also assume that Eqs (1.1) are asymptotically linear for large x , non-linearities only occurring in a relatively small range of x ’s. In this region we think of the system as operating in a ‘normal’ regime. Following this view, the meaning of the above notion of stability is more than local, but describes the systems ability to return to normal modes of behaviour after a large perturbation. The smaller the real part of the dominant eigenvalue, the faster the system returns. Conversely, larger than zero eigenvalues indicate that the system explodes.

We note furthermore that, by omitting all diagonal entries the matrix M defines a graph. Nodes of the graph are the ‘species’ (or variables in the dynamical system). If $m_{ij} \neq 0$ node i is connected to node j . A positive link means that

¹In the context of analysing ecosystems this matrix is referred to as ‘community matrix’.

i furthers the growth of the population of j , likewise a negative link indicates suppression of j by i .

The remainder of the paper is as follows: in §1.2 we introduce and discuss the framework of our model. In §1.3 we analyze typical networks generated by the model. In a wide range of parameter values SF networks are formed. We explore the dependence of the network structure on parameters and try to find the steps in our model which prove essential to the formation of SF topologies. The paper concludes with §1.4 by summarizing the results and outlining implications.

1.2 Model framework

We undertake to construct graphs with positive and negative links, trying to minimize the real part of the dominant eigenvalue of the matrix M associated with the network. Our approach is to ignore all details of the underlying equations (1.1) and to concentrate only on the system's linearization near a fixed point. This is very similar to [7, 8]. We start with a system of $N_0 = 4$ disconnected nodes ($m_{ij} = -\delta_{ij}, i, j = 1, \dots, 4$) and continue adding nodes, one at a time. After each addition stability is checked and acceptance or rejection depends on how the dominant eigenvalue of M is changed.

To be more precise, our construction procedure consists of the following steps:

- (i) Add a node to the network and let it form a positive and a negative in- and a positive and a negative out-link to randomly selected nodes of the 'old' network (cf. Fig. Fig. 1.1). In this paper, we restrict the model to link strength $m_{ij} = \pm 1$. For continuous link strength we refer to a later study (Brede and Finnigan in preparation).

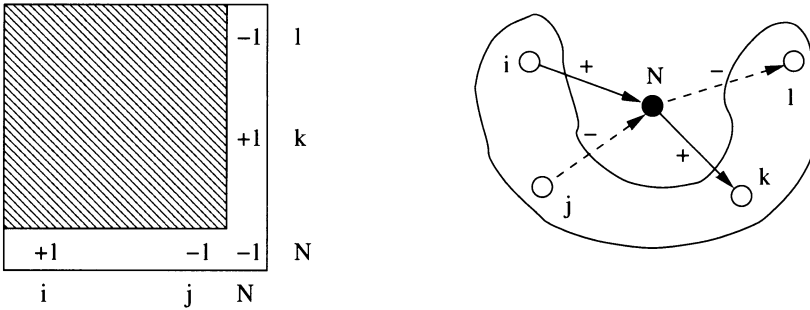


Figure 1.1: Visualization of the attachment process as described in the text. A new node leading to a graph of size N forms a positive in- and out-link with randomly selected target nodes i and k . Likewise it forms negative in- and out-links with j and l , which are also selected at random. The left hand figure shows changes in the matrix M caused by the attachment of node N .

- (ii) Calculate the dominant eigenvalue $\lambda_{\max}(N+1)$ of M . If $\lambda_{\max}(N+1) > \epsilon = 0$ the configuration is rejected. If $\lambda_{\max}(N+1) < \lambda_{\max}(N)$, the new

configuration leads to more stability and will be accepted. Otherwise, if $\lambda_{\max}(N+1) > \lambda_{\max}(N)$, the acceptance probability is given by

$$p_{\text{accept}} = \exp(-\beta(\lambda_{\max}(N+1) - \lambda_{\max}(N))), \quad (1.3)$$

where β is an inverse temperature-like parameter. A high value of β in (1.3) allows only ‘small’ deteriorations in stability. Sometimes accepting an ‘unfavourable’ configuration is found necessary to avoid getting trapped in the search. In case of rejection a new configuration of size $N+1$ is generated in step (i).

- (iii) Unless the desired system size has been reached, continue with (i). If some configurations is encountered, such that no new node can be added according to (i) and (ii) we restart with $N_0 = 4$.

By construction, every graph has the same number of negative and positive links, hence $\langle m_{ij} \rangle_{i \neq j} = 0$. Furthermore, since $m_{ii} = -1$ it holds $\text{Tr}(M) = \sum_i \lambda_i = -N$ giving $\bar{\lambda} = 1/N \text{Tr}(M) = -1$. It follows, that all eigenvalues of a constructed matrix are found in $[-N, 0)$ and $\lambda_{\max} \in [-1, 0)$. A consequence of this is that a stable matrix always has a narrow eigenvalue distribution, centred around -1 . Since $\text{Tr}(M) = -N$, any matrix having eigenvalues far smaller than -1 will also have a number of eigenvalues $\lambda_i > -1$, reducing stability.

The algorithm can be interpreted in two ways. First, it can be understood as a directed search, trying to construct as stable a system as possible. Neglecting the system’s growth, it is then very similar to a Metropolis algorithm as commonly used in the study of spin systems. Second, it could also be conceived as a network evolution, mimicking the stepwise assembly of a real system’s components over a long period of time. After each node addition, the system again settles into a stationary state. Then, under the challenges of external (thermal) fluctuations the stability of this state is measured. If the system becomes unstable the new component can’t be successfully added. In this interpretation, β summarizes elements of randomness in the above process. We think of two major sources of noise. First, depending the details of the external fluctuations, the evaluation of the stability of a real system is prone to errors. Second, a new node might be added, before the last configuration could be tested ‘properly’. We also consider such events as noise. Clearly, the above interpretation assumes a separation of time scales between typical times between node additions and the systems relaxation time, i. e. is valid for $T_{\text{node}} \gg T_{\text{relax}}$.

1.3 Results

To understand the influence of the selection process of step (ii) we start by calculation the degree distribution of a network which is formed by only applying step (i). Without loss of generality, we don’t distinguish between positive and negative links and calculate the in-degree distribution. Since every new node has two in-links, nodes of degree smaller than two are due to the initial conditions

and don't affect the asymptotic limit. Consider the mean number $\langle n_i(t) \rangle$ of nodes with degree i at timestep t . Following the rate equation approach of Krapivsky et al. [6] one obtains

$$\langle n_i(t+1) \rangle = \langle n_i(t) \rangle - \langle 2/N(t)n_i(t) \rangle + \langle 2/N(t)n_{i-1}(t) \rangle, \quad (1.4)$$

where $N(t)$ stands for the total number of nodes in the network after iterating step (i) for t times. Assuming that the $\langle n_i(t) \rangle$'s grow linearly with network size, i. e. $\langle n_i(t) \rangle \sim p_i N(t)$, Eq. (1.4) asymptotically results in

$$p_i = \frac{1}{2} \left(\frac{2}{3} \right)^{i-1}. \quad (1.5)$$

Thus, without selection of stable networks the growth process of step (i) always leads to an exponential degree distribution.

Fig. 1.2 contrasts the behaviour of the degree distribution as expected from Eq. (1.5) with simulation results obtained for a high and a low value of β . With

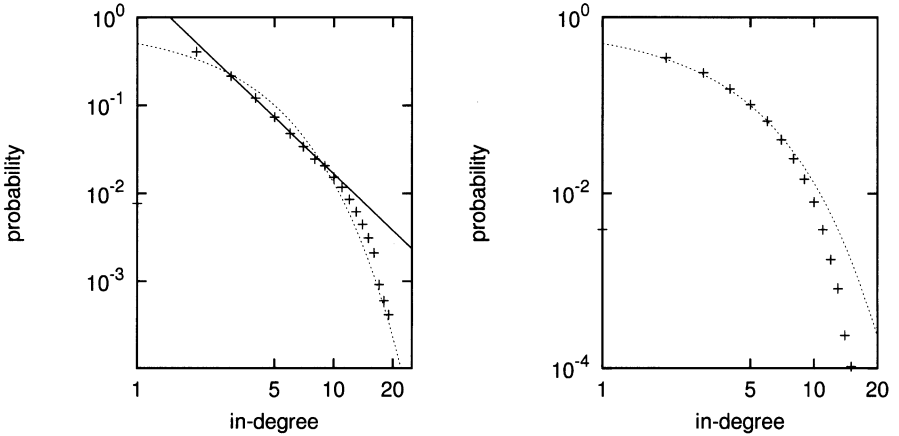


Figure 1.2: Simulation data for the degree distribution of graphs of size $N = 100$ constructed by the model as explained in the text. The left panel displays data for high $\beta = 50.0$, in the right panel data for $\beta = 1.0$ are shown. The dotted line indicates an exponential distribution as given by Eq. (1.5). For high β up to a finite size cut-off, both the in- and the out-degree distributions obey a power law $p_i \sim i^{-\gamma_{\text{in}}}$ with exponents $\gamma_{\text{in}} = \gamma_{\text{out}} = 2.14 \pm .03$. Contrariwise, simulation data obtained for small β are in very good agreement with Eq. (1.5). The data represent averages over 1000 independent configurations.

low selective pressure for stability, the degree distribution is —apart from a finite size cut-off— in very good agreement with Eq. (1.5). However, for high β , the network turns out to be SF with exponent $\gamma_{\text{in}} = \gamma_{\text{out}} = 2.14 \pm .03$. Exponents in the range between -2 and -3 are frequently observed in empirical network studies, see [1].

Simulations show, that over a wide range, the value of β does not influence the exponent γ . However, dropping below a critical value of β networks are no longer SF, but exponential. To quantify this transition in network structure, we introduce a degree entropy

$$S_{\text{deg}} = - \sum_i p_i \ln p_i \quad (1.6)$$

and investigate the dependence of $\langle S_{\text{deg}} \rangle$ on β . Fig. 1.3 displays simulation

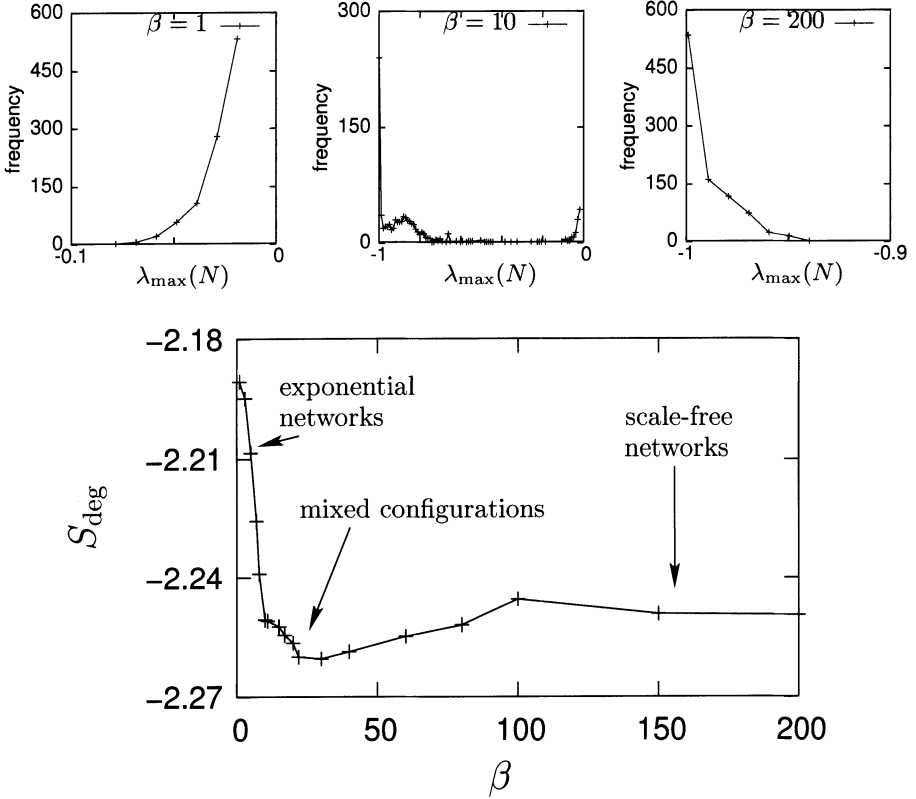


Figure 1.3: The lower panel displays simulation data for a system of size $N = 50$ showing the change of the degree entropy with β . The upper panels give the $\lambda_{\max}(N)$ -histogram for three representative situations: for $\beta = 1$ almost any walk ends close to $\lambda = 0$ (corresponding to networks with exponential degree distribution), for $\beta = 10$ a fraction of the walks stays at the initial condition $\lambda = -1$, while some have already reached $\lambda = 0$ or are in between, and finally, for $\beta = 200$ no walk escapes from $\lambda = -1$ (i. e. every network constructed is SF). Every datapoint corresponds to averages obtained from 1000 independent runs.

data for a network of size $N = 100$. The data show a sharp drop from the initial exponential degree distributions to an intermediate minimum at $\beta \approx 20$ to the typically SF behaviour of networks generated for high β . As also shown

in Fig. 1.3 the transition between different types of networks is triggered by a transition in the behaviour of typical walks performed by the largest eigenvalue $\lambda_{\max}$ as the system grows². This can best be visualized by the probability distribution, that a realization of the process reaches a final point $\lambda_{\max}(N)$.

For small β , where the pressure to stay close to the initial point $\lambda = -1$ is low, almost all walks end very close to $\lambda = 0$. As β increases, more and more realizations of the process don't get away from $\lambda = -1$. Further, in some instances $\lambda = 0$ is not reached, leading to a second extremum in the $\lambda_{\max}(N)$ -distribution. Choosing larger and larger values of β more and more realizations don't escape from $\lambda = -1$ consequently diminishing the proportion of walks reaching $\lambda = 0$ or being trapped in between.

A closer investigation of the above situation reveals that only networks with maximum eigenvalues 'close' to the optimum $\lambda = -1$ are SF. Further, the farther away a network configurations maximum eigenvalue is from -1 , i. e. the closer to $\lambda_{\max} = 0$, the closer the network structure becomes to that of an exponential network. From this point of view, for low β almost all networks are exponential. Increasing β , 'mixed configurations' in which part of the networks are still exponential while another fraction already is SF, occur. For larger and larger β the fraction of SF networks increases and finally dominates.

The algorithm described above contains three key elements: (a) network growth, (b) rejection of unstable configurations, and (c) a tendency to keep the eigenvalue distribution narrow, as expressed by Eq. (1.3). We next try to identify which of these mechanisms prove essential for the construction of SF networks.

To investigate the influence of (a) we fix the network size and explore the influence of the selection for most stability alone. We start with a random directed network composed of an equal fraction of positive and negative links, which has the same connectivity $p = 4/N$ as all other networks constructed above. The directed search towards optimal stability is implemented by rewiring K links to randomly selected new target nodes, thereby keeping the links' sign. Acceptance or rejection of network configurations is decided on the basis of Eq. (1.3). It turns out that all networks constructed in this way, still have a peak in the degree distribution. From this one can conclude that growth is a key factor in the formation of SF networks.

To verify the importance of (b), we replace the constraint of accepting only networks with $\lambda_{\max} < \epsilon = 0$ in step (ii) with $\epsilon = 1$. Depending on the choice of β the peak of the larger values of $\lambda_{\max}(N)$ now can also be found in the interval $[0, 1]$. However, the fundamental results do not change. Independent of the choice of ϵ the range of β values where SF networks are found remains valid.

As already explained above in the analysis of the phase diagram for the network evolution depending on β , it is essential to keep the degree distribution narrow, as achieved by choosing high values of β . The detailed functional form of Eq. (1.3), or even that unfavourable configurations are accepted at all, however, do not seem to be important. Replacing, e.g., the probabilistic acceptance by

²The network evolution and thus also its projection on $\lambda_{\max}$ is a Markov process.

accepting every configuration with maximum eigenvalue close to -1 still allows the formation of SF networks.

1.4 Conclusions

We have presented a model for growing interaction topologies of dynamical systems that are distinguished by their high stability. We identified two essential mechanisms for constructing stable SF networks in this way: (a) a growing system and (b) a tendency to keep the eigenvalue distribution ‘narrow’. The latter requirement was implemented by only accepting newly attached nodes if the attachment leads to either more or slightly less stability in comparison to the old configuration. This algorithm can be interpreted in two ways. First, one can understand it as a directed search, constructing an ensemble of matrices with smallest possible largest eigenvalue. On the other hand, this way of assembling a system one element at a time could also be thought to mimick the evolution of a natural system. We speculate that —apart from preferential attachment and optimization for communication— selection for most stability against perturbation could be one of the key mechanisms explaining why SF network topologies are so common in nature.

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Chapter 8

Fractal Statistics of Modeled Zoning Patterns in Calcite

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1. Introduction

In recent years, the phenomenon of oscillatory zoning has been established in more than 70 rock-forming and accessory minerals having been formed in different geological media [Shore & Fowler, 1996]. Observations of oscillatory zoning in solution-grown calcite crystals are reported by Reeder *et al.* [1990]. In these calcites periodic zonal variations in Mn^{2+} content were not correlated with changes in any bulk solution parameters, and it was interpreted that the oscillatory behavior developed autonomously. Wang and Merino [1992] describe a dynamic model for calcite grown from an aqueous solution containing growth-inhibiting cations such as Mn^{2+} . This model, based on a feedback involving H^+ accumulation, surface adsorption, and calcite growth inhibition is able to autonomously produce oscillatory changes of Ca^{2+} and H_2CO_3 concentrations adjacent to a calcite growth surface without large-scale changes in bulk water chemistry. After a series of simplifying assumptions this model can be reduced to an autonomous system of two ordinary first-order differential equations with five parameters:

$$\begin{aligned}\frac{du}{dt} &= 1 - u - \lambda(1 + \beta_1 v + \beta_2 v^2)u \\ \theta \frac{dv}{dt} &= -v + \gamma \lambda(1 + \beta_1 v + \beta_2 v^2)u\end{aligned}\tag{1}$$

Here, u and v are scaled concentrations of Ca^{2+} and H_2CO_3 , respectively, next to the crystal surface; θ is the ratio of diffusivities of Ca^{2+} and H_2CO_3 ; λ is scaled value of rate constant; β_1 and β_2 are positive constants to adjust the ability of H^+ to inhibit calcite growth; and γ is a positive constant; all quantities are dimensionless. A qualitative analysis made by Wang & Merino [1992] and Bryksina & Sheplev [2001] predicts the existence of numerous oscillatory solutions to the equations describing the system.

In this work we use a computer package MATHEMATICA to integrate the system (1) numerically and to calculate the concentrations of Ca^{2+} (u) and H_2CO_3 (v) with respect to time. According to the assumptions made by Wang and Merino [1992] the amount of a trace element (such as Mn^{2+}) incorporated into calcite is proportional to the amount of a trace element adsorbed on the growth surface and depends on pH at the growth front. The

oscillatory pH leads to an oscillatory variation of trace elements (including Mn^{2+}) in calcite crystals. We calculate the H^+ content at the crystal surface using the equation [Eq. 18, p. 590; Wang and Merino, 1992] together with H_2CO_3 (v) concentrations obtained from (1). As the Mn^{2+} content is inversely proportional to the H^+ content, the next step is to construct a synthetic image to simulate cathodoluminescence. Here the Mn^{2+} concentrations are fitted to a 255 gray level scale and assigned colors from black to the yellow orange region of the spectrum where yellow is assigned the highest values, orange intermediate values and black the lowest values. The zoning is then reproduced as a 2 dimensional synthetic image. In general terms a wide range of zoning patterns can be created where zones are defined by color and widths of zone by the gradient of color change. In this way it is possible to visualize the oscillatory zoning produced by the Wang-Merino model for different parameter values and the zoning patterns can be used for both qualitative and quantitative comparisons. The aim of this work is to use fractal statistics to quantitatively characterize oscillatory zoning patterns produced by the Wang-Merino dynamic model for different physical parameters.

2. OZP1

The results of numerical integration of the system (1) when the parameter values correspond to OZP1 (Table 1) are presented in Figure 1. As it follows from a qualitative analysis [Wang & Merino 1992; Bryxina & Sheplev 2001], system (1) in this case has a unique steady state, which is an unstable focus. The scaled concentration of Ca^{2+} (column *a*) shows an asymmetric profile with a gradual sloping increase followed by a sharp decline. The plot in column *b* shows the behavior of the dynamic system (1) on the phase plane $\{\text{Ca}^{2+}, \text{H}_2\text{CO}_3\}$. We see here the phase trajectory, which began at the steady state $\{0.22; 1.56\}$, moves away from it with oscillations of increasing amplitude, and then go to a closed trajectory, which we call a universal limit cycle and which is characterized by oscillations with constant amplitude.

Table 1. Parameter values used to generate OZP.

Type of OZP	θ	λ	β_1	β_2	γ
OZP1	0.1	0.01	70	100	2
OZP2	0.2	0.01	60	80	2
OZP3	0.25	0.01	30	80	2
OZP4	0.35	0.011	40	100	1.5

Column *c* in Figure 1 shows a graphic representation of the zoning pattern. From a “petrographic” perspective, if this was view of a crystal, the growth history would be from left to right and the pattern would be described as an oscillatory zoning pattern. The zones would be described as showing an asymmetric gradational change in color from yellow to orange followed by a sharp boundary.

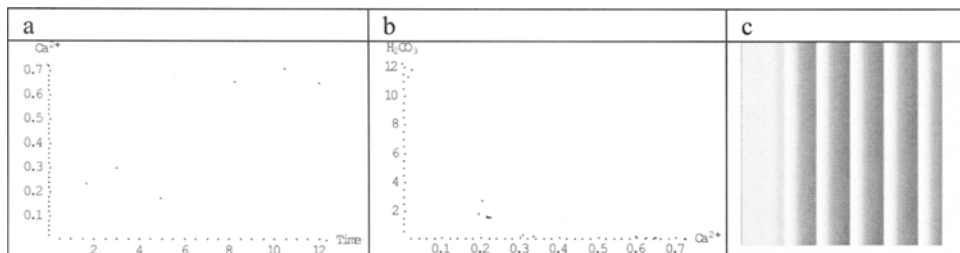


Figure. 1. Behavior of Wang-Merino dynamic model at the parameter values: $\theta=0.1$, $\lambda=0.01$, $\beta_1=70$, $\beta_2=100$, $\gamma=2$. Starting point: $u=0.22$, $v=1.56$. (a) Scaled concentrations of Ca^{2+} depending on time. (b) Phase portrait of the model. (c) OZP generated by the model.

3. OZP2

At the parameter values for OZP2 (Table1) there is also one steady state of the dynamic system (1). As it follows from [Wang & Merino 1992; Bryxina & Sheplev 2001] this steady state is a stable focus. Here the model produces oscillations with decreasing amplitude for Ca^{2+} concentrations (Fig. 2a). The phase trajectory corresponding to these oscillations is a convergent trajectory in the phase plane (Fig. 22b), which goes from an initial point $\{0.5; 1.5\}$ to steady state with coordinates $\{0.29; 1.43\}$. The 2 dimensional pattern (Fig. 2c2) shows symmetrical gradational zones of color that decrease in intensity.

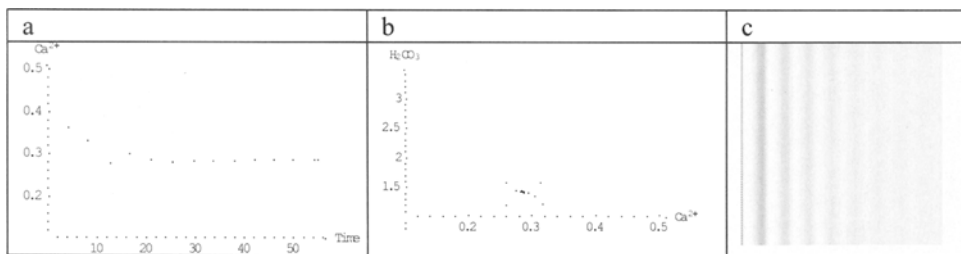


Figure. 2. Behavior of Wang-Merino dynamic model at the parameter values: $\theta=0.2$, $\lambda=0.01$, $\beta_1=60$, $\beta_2=80$, $\gamma=2$. Starting point: $u=0.5$, $v=1.5$. (a) Scaled concentrations of Ca^{2+} depending on time. (b) Phase portrait of the model, (c) OZP generated by the model.

4. OZP3

In contrast to OZP1 and OZP2, three steady states can be generated by the dynamic model (1) using the parameter values for OZP3 (Table1). In this case the phase trajectory of the system depends very much on the starting point chosen for solving of dynamic system. Some starting concentrations do not result in the creation of a periodic solution which

means there will be no zones. Depending on the starting point the system may evolve to one or another steady state separated on the phase plane by what is known as a saddle which is itself a steady state. There are two special trajectories called the separatrix of the saddle. When starting points lie on one trajectory, the steady state is an attractor, and when the starting points lie on another trajectory, this steady state is a repeller. From all another starting points the solution will not reach this steady state.

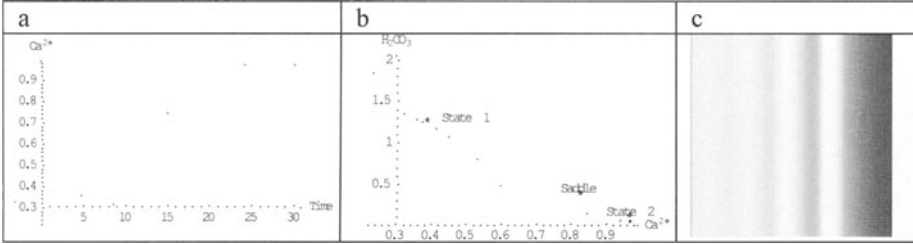


Figure 3. Behavior of Wang-Merino dynamic model at the parameter values: $\theta=0.25$, $\lambda=0.01$, $\beta_1=30$, $\beta_2=80$, $\gamma=2$. Starting point: $u=0.4$, $v=1.2$. (a) Scaled concentrations of Ca^{2+} depending on time. (b) Phase portrait of the model. (c) OZP generated by the model.

Location of a saddle and another two steady states on the phase plane $\{\text{Ca}^{2+}; \text{H}_2\text{CO}_3\}$ are shown in Figure 3b. For State1, and the region around State 1, concentrations of Ca^{2+} are low ($u=0.39$) and the system will evolve from what is an unstable focus. State2 has the highest Ca^{2+} concentration ($u=0.97$) and the system will evolve to a stable node, which attracts the system. The third steady state (a saddle) exists between State 1 and State 2 at intermediate Ca^{2+} concentrations but does not produce oscillatory zoning. When we take the starting point $\{0.4; 1.2\}$ close to State1, the system (1) evolves away from State 1 in an oscillatory fashion and is finally drawn gradually towards a constant value (State 2). But if a starting point is chosen somewhat farther from State1, for example at point $\{0.45; 1.3\}$ on phase plane $\{\text{Ca}^{2+}; \text{H}_2\text{CO}_3\}$, then the system moves from the starting point to the constant value without oscillations, which means there will be no zones.

Figures 3a shows oscillations with increasing amplitude (OIA) depending on time for scale concentrations of Ca^{2+} . The zoning produced by the model in this case is shown in the Figure 3c, where we see symmetric zones of increasing color intensity changing to finally to a zone of homogenous color.

5. Bifurcation Values of Parameters (OZP4)

Figure 4d shows oscillatory zoning produced by the Wang-Merino model at the bifurcation values of parameters for the model (OZP4, Table1). Bifurcation values of the parameters are some critical values, which when changed can cause qualitative differences in the behavior of the dynamic model.

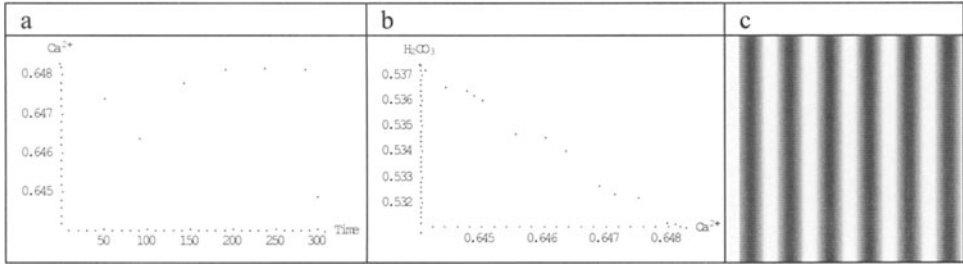


Figure. 4. Behavior of Wang-Merino dynamic model at the parameter values: $\theta=0.35$, $\lambda=0.011$, $\beta_1=40$, $\beta_2=100$, $\gamma=1.5$. Starting point: $u=0.646$, $v=0.534$. (a) Scaled concentrations of Ca^{2+} depending on time. (b) Phase portrait of the model. (c) OZP generated by the model.

To find these parameters we use the results of the qualitative analysis of dynamic model (1) obtained by [Bryxina & Sheplev 2001]. In this analysis they took into consideration not only the linear part of system (1) but also the non-linear part, and calculated Lyapounov coefficients L_1 , L_2 and L_3 . They showed that L_1 and L_2 may have zero values at some parameter values of the model, but if $\sigma = 0, L_1 = 0, L_2 = 0$, then L_3 was < 0 for any parameter values of the model. Also they showed that the number of parameters of the dynamic model (1) can be reduced to four by the following substitution:

$$x = 1 - u \quad y = \beta_1 v \quad B = \beta_1 \gamma / \theta \quad g = 1 / \beta_1 \gamma \quad \beta = \beta_2 / \beta_1^2 \quad (2)$$

Bifurcation values of the parameters are found from the conditions: $\sigma = 0$, $L_1 = 0$, $L_2 = 0$. The expressions for σ , L_1 , L_2 depending on the parameters of the model can be found in Bryxina & Sheplev [2001]. As we have four parameters (λ, B, g, β) and only three equations, one parameter must be fixed, for example $\beta = 0.0625$. This value of the parameter β is obtained from the fifth equation in (2), when we take $\beta_1 = 40$ and $\beta_2 = 100$, at which three steady states can be generated by dynamic model (1). From the equations $L_1 = 0$ and $L_2 = 0$ we find $\lambda = 0.011$ and $g = 0.017$, and from equation $\sigma = 0$ we find the value of the parameter $B = 172.75$. Using (2) we can return to the primary parameters remembering that there is an option to choose one parameter. So, taking $\beta_1 = 40$ and $\beta_2 = 100$ we calculate $\theta = 0.35$ and $\gamma = 1.5$.

There are three steady states of the dynamic model (1) at the bifurcation parameter values (OZP4, Table1): a multiple focus, a saddle and a stable node. Figure 4a shows the solutions of dynamic system (1) at the bifurcation parameter values, when starting point is closed to the steady state $\{0.646; 0.534\}$, which is a multiple focus. The phase trajectory (Fig. 4b) in this case is a closed line or a limit cycle. Depending on the starting point, the solution of the dynamic model approaches the limit cycle (by oscillations) or tends to the steady state with the highest Ca^{2+} concentration ($u = 0.964$) which is a stable node (no

oscillations). Figure 4c shows the OZP produced at the bifurcation values of the parameters, where zones in terms of color are symmetrical and repeat each other along sample. Such zoning can be produced if there is no change in parameter values during some time. After a negligible change of the value of parameter θ , a multiple focus can be changed to an unstable focus at $\theta = 0.348$ and to stable focus at $\theta = 0.351$.

Output of Mn^{2+} concentrations ($c_{Mn^{2+}}$) from MATHEMATICA were normalized to a 255 color scale using:

$$\frac{c_{Mn^{2+}} \cdot 255}{\max}$$

where max was the maximum value of Mn^{2+} concentrations, this scale provided for visual representation and comparison of OZP1, OZP2 and OZP3. On the other hand, the magnitude of oscillations of Mn^{2+} concentrations for OZP4 was very small and the scale had to be stretched using

$$\frac{(c_{Mn^{2+}} - \min) \cdot 255}{\max - \min},$$

where min was the minimum value of Mn^{2+} concentrations. Figure 4d shows symmetrical zoning from light to dark in OZP4. However, this in fact would be very faint in comparison to the other patterns.

3. Self-Affine Fractals

Halden and Hawthorne (1993) were the first to apply fractal geometry to the description of oscillatory zoning in minerals. Fractal geometry has been applied to a wide range of phenomenon in recent years [Mandelbrot 1982, Feder 1988]. And now fractal analysis seems to be the most promising tool in study of oscillatory zoning [Holten *et al.* 1997, Holten *et al.* 1998, Bryxina *et al.* 2002]. Fractal analysis characterizes this phenomenon statistically, providing a quantitative characterization of zoning in natural specimens. The single-space series or single valued function $y(x)$, for example gray level function, can be characterized by fractal dimension D and by Hurst exponent H , which are connected by the equation

$$D = 2 - H, \quad 0 < H < 1$$

One of the methods of determination of fractal dimension is the method of standard deviation [Feder 1998; Meakin 1997]. The standard deviation of a function $y(x)$ is defined as

$$w(l) = \sqrt{\langle y^2(x) \rangle_l - \langle y(x) \rangle_l^2},$$

where $\langle \dots \rangle_l$ denotes an average over all sections (x_0 to $x_0 + l$) with a length l . The function $y(x)$ is self-affine fractal with fractal dimension D , if its standard deviation $w(l)$ can be scaled as

$$w(l) = l^H.$$

The Hurst exponent equal to 0.5 suggests a statistically random process. At $H > 0.5$, the time record or single-space series is persistent, i.e., the system has a tendency to oscillate between “extreme” values that would be constrained by a limit cycle. The data in this case have a positive correlation between preceding and subsequent events. Alternatively this may be expressed as an increasing or decreasing trend in the past favoring an increasing or decreasing trend in the future, i.e., a clearly expressed tendency at relatively low “noise”. If, on the other hand, $H < 0.5$, the record is anti-persistent, the increments are negatively correlated, and the data themselves seem to be highly “noisy”.

Table 2 shows the values of Hurst exponents (H), fractal dimension (D) obtained from the “images” of OZP models 1 through 4 and time-scales, on which these OZP have persistent fractal behavior.

Table 2. Values of Hurst exponents (H) and fractal dimension (D) for synthetic images and time-scale corresponding to calculated values of H .

Type of OZP	H	D	Time-scale
OZP1	0.83	1.17	0.99
OZP2	0.8	1.2	1.43
OZP3	0.88	1.12	8.79
OZP4	0.94	1.06	22.6

As it might have been expected the values of Hurst exponent are greater than 0.5, because we considered oscillatory solutions of the model. The tendency, however, is that the largest value of Hurst exponent corresponds to a limit cycle (OZP4). The next value of Hurst exponent corresponds to an unstable focus changing to stable node (OZP3) followed by a value for the unstable focus changing to the universal limit cycle (OZP1) then to the smallest value of Hurst exponent corresponding to the stable focus (OZP2). These values of Hurst exponent are calculated on a specific time-scale, which are presented in the fourth column of Table2. When the process of forming of oscillatory zoning in calcite corresponds to the regime described by OZP4, the time during which the system has persistent behavior, or in another words, the time during which the system “remembers” what was in past and what will be in future, is equal to 22.6. This quantity is approximately equal to a half of the period of the limit cycle (43.8). This means that OZP4 would form very slowly in comparison to other OZPs. The fastest process for forming of oscillatory zoning corresponds to the regime for OZP1.

5. Conclusion

If the dynamics of the Wang and Merino model can be used as a reasonable analogue for Mn distribution in natural and synthetic calcite, we might anticipate a mineral could show a range of qualitatively and quantitatively different patterns but they would essentially be

“variations on a theme”. Furthermore, they should have some quite specific characteristics that we should be looking for and describing and quantifying.

In a natural system there is no reason why we could not find all four types of zoning in one crystal. This could come about if the system were opened to changes in solution chemistry where the “starting point” for growth was reset; or, if θ , the diffusivity ratio of Ca^{2+} and H_2CO_3 were to change, either in response to temperature variation or the concentration gradients of other elements in the system, then one pattern might evolve in to another. This would suggest that sequences of zoning patterns could be used to compare and contrast crystals in a “stratigraphic” sense. Also we need now to make careful observations of the zones with respect to whether concentration, or intensity of color in the case of cathodoluminescence, is increasing or decreasing and whether the zones show gradational or sharp boundaries.

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Chapter 9

Complexity and Army Transformation

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1.1. Introduction

On 12 October 1999, the U.S. Army began a journey down a new path to innovation, when General Eric Shinseki presented his vision of Army Transformation at the 45th annual meeting of the Association of the United States Army. In this speech, General Shinseki described the Army as an organization consisting of heavy forces with excellent staying power but poor strategic responsiveness, light forces with excellent responsiveness but poor staying power, and a logistics system with an excessively large footprint. His proposed solution, a comprehensive change of the Army resulting in full-spectrum dominance and strategic responsiveness, would occur so quickly as to “be unnerving to some.” [Shinseki, 1999] While this prediction has turned out in some ways to be true, it is not necessarily the speed of change that is unnerving to many of the people studying Army Transformation.

1.2. Army Transformation

1.2.1. What is Army Transformation?

General Shinseki's concept of Army Transformation centered on a strategy of moving from today's Army, the “Legacy Force,” through an “Interim Force” that would provide some of the desired innovations relatively quickly, culminating in the “Objective Force” as the ultimate realization of the transformation ideal. The desired innovations would be achieved by harnessing the ongoing “Revolution in Military Affairs” (RMA). In keeping with Donald Rumsfeld's vision of Department of Defense Transformation, the Objective Force would possess new capabilities making it ideally suited to function in the “emerging operational environment.” Lighter combat vehicles would conduct “operational maneuver from strategic distances,” capable of

"early arrival in a crisis...decisively attacking and defeating the center of gravity of any adversary." Objective Force units would "*see first, understand first, act first and finish decisively as the means to tactical success* (emphasis in the original)." These tactical capabilities would be provided by "unprecedented intelligence, surveillance and reconnaissance capabilities," and "instantaneous dissemination of commander's intent coupled with broad access to the Common Operating Picture (COP) on a non-contiguous battlefield." As a result of these new capabilities, the Objective Force would be responsive, deployable, agile, versatile, lethal, survivable and sustainable [U.S. Army White Paper, 2003].

1.2.2. The problem with Army Transformation

A detailed study of Army Transformation reveals that the process currently lacks a theoretical basis for change [Calhoun, 2004]. This is apparent in its top-down, leader-directed nature, the lack of objective experimentation, and the reliance on hoped-for future technological solutions to offset built-in limitations of the Future Force. In stark contrast to the Complex Responsive Process (CRP) view of innovation in organizations [Stacey, 2001], leadership is control-oriented and hierarchical; emergent patterns of innovation are overlooked or actively discouraged. The U.S. Army's awareness of complexity theory and emergence is similar to that of general society's, although complexity is a key component of the curriculum at the Army's School of Advanced Military Studies. Incorporating the principles of complexity theory into the transformation process will be a difficult, but critical task.

The notion of an RMA appears to be substituting for scientific theory as the intellectual foundation of Army Transformation. While historians still argue whether an RMA occurred during various periods in military history [Rogers, 1995], the Army has embraced the notion of an ongoing RMA. Nevertheless, analysis of Army Transformation reveals that the existence of the RMA is both unlikely (analysis of several hundred years' history reveals that every significant Western military revolution was "uncontrollable, unpredictable and unforeseeable." [Knox and Murray, 2001]) and risky (it is questionable whether one should declare that an RMA is currently in existence, because this can distort cultural perceptions and set unrealistic expectations regarding the efficacy of the hoped-for "revolutionary" innovations).

In the decade following the 1991 Gulf War, the increasingly widespread belief in American technological superiority led many to predict that the "information revolution" would soon lift the fog of war. By the late 1990s, business information management practices were seen as potential military solutions, as described in books such as *Network Centric Warfare*. In keeping with this trend, Army Transformation currently relies on the promise of technology, in the form of information superiority and Precision-Guided Munitions (PGMs), to overcome the reduced survivability of the lighter-skinned combat vehicles of the future. Paradoxically, the very emphasis on technology that leads some to believe PGMs will reduce the need for sizeable ground forces has created the opposite situation in recent combat experience: "Ever-more lethal precision engagement technology is driving our opponents increasingly into cover and increasingly into complex terrain--and these are the postures that demand

the largest proportion of dismounted strength in the American combined arms mix. Hence the demand for dismounted infantry in Army combat units is likely to rise over time." [Biddle, 2004] This is but one example of many that point to flaws in an innovative process that relies on technological solutions.

What is particularly troubling about this concept is that it not only dominates future vision, but it has migrated to the present, where it is shaping current Army doctrine [McMaster, 2003]. Similarly, the emphasis on future technology has become so ubiquitous that services must adopt the same language if they hope to appear "relevant and ready" in the competition for defense funds.

History abounds with examples of the failure to effectively innovate. The dangers are evident--procurement programs are expensive and lengthy, and once a major force redesign is adopted, it will take many years and a great deal of money to change course if the chosen path takes the Army in the wrong direction. The hierarchal approach of Army Transformation ensures the stakes are even higher. The top-down method is not without precedent, and is not necessarily destined to fail, but it is questionable whether the risk is warranted: "The lesson may well be that if you are right, top-down leadership will allow you to get it very, very right. If you get it wrong, however, you will get it very, very wrong." [Murray and Millett, 1996]

1.3. Historical case studies

1.3.1. Innovation in the Napoleonic Era

The French Revolution caused a dramatic paradigm shift in the nature of warfare. Armies made up of a motivated citizenry mobilized quickly and fought with great zeal. [Lynn, 2000] The resulting transformation, well under way by 1793, gave France's armies unprecedented size, discipline and flexibility. Dramatic changes in culture, perception and organization occurred through the self-organizing process of pattern formation caused by the changing nature of complex interactions during the period of Revolution. It only remained for Napoleon to capitalize on and complete the process of transformation:

... Thirdly, the Revolution provided Napoleon with a promotion system open to talent. The importance of this legacy cannot be overestimated; it was the caliber of the truly "natural" leaders who emerged from the ranks of the Revolutionary Armies to command battalions, *demi-brigades*, divisions, corps and armies, that made Napoleon's achievements possible. [Chandler, 1966]

The changing nature of culture and interactions in the new popular conscript armies enabled self-organization and innovation through emergent patterns of action. The other European armies of the period resisted the changes engendered by France's revolutionary fervor, clinging to traditional views of army organization and social distinction between the officer and soldier class. In contrast, soldiers in the French army were no longer viewed as socially inferior:

...the new French armies now consisted of citizen soldiers who were equal in social rank to the officers and refused to be brutalized; they had to be led by example. Moreover, the disruption of the officer corps because of the Revolution as well as the exigencies of war itself created a demand for good officers, many of whom rose through the ranks. [Epstein, 1994]

The dramatic changes caused by the Revolution resulted in the enabling of change agents throughout all levels of the army. Recognition that personal achievement could gain an individual promotion on merit encouraged excellence and initiative. Emergent patterns of action resulting from the changing nature of the complex interactions in the organization were not suppressed--on the contrary, they were encouraged.

Perhaps the best illustration of the adherence of the Napoleonic system to the principles of complexity is the Marshalate. The meteoric rise of soldiers like Lannes, Murat, and Massena--much like Napoleon's own--resulted from the empowerment of change agents at all levels; similar promotions on merit would have been unthinkable in any other contemporary European army. Napoleon's Marshals embodied the CRP view: through the *corps d'armee* system, each commanded a redundant formation that was fully capable of independent action. This lent an unprecedented degree of operational flexibility and mobility to Napoleon's armies, because it simplified logistic requirements and allowed operation on an initially broad front. Separate corps could fight independently for extended periods, while the army adjusted its activities to deal with emergent contingencies. Marshals were frequently detached on "corps of observation" missions, encouraging the action of change agents at subordinate levels of command to exercise initiative to attain independent goals.

Napoleon's army embodied the cultural transformation of the French Revolution, maximizing the potential enabled by the changing nature of the complex interactions within the organization. Control was de-emphasized both within the ranks, by adopting the revolutionary suppression of class distinction and adopting concepts of promotion on merit; and at the leadership level, through establishment of the Marshalate and the *corps d'armee* system. Unprecedented flexibility to cope with emergent exigencies while on campaign, as well as a general sense of the empowerment of change agents at all levels of the army, were the result. Command and control was relatively hierarchal in comparison to modern armies, but in comparison to the undistributed armies of the time [Schneider, 2000], no other European army possessed the level of decentralized control that existed in the *Grand Armee*. Redundancy provided through overlapping and complementary *corps d'armee* ensured durability of combat formations; while difference resulting from the capability for independent action under decentralized control enabled emergent patterns of self-organizing action as the organization operated at the edge of chaos.

1.3.2. Innovation in the German Army

Much like innovation in the Napoleonic period, change in the interwar German army was heavily influenced by the social and political environment of the period, and a

large body of military theory that expanded upon the foundation built by Clausewitz after the Napoleonic wars. Like the rest of the world, Germany viewed interwar transformation through the lens of its World War I experience. Unanswered questions surrounded the new lethality of the "empty battlefield," [Schneider, 1987] the debated role and usefulness of the tank in future wars, the nature of political-military relations, and the difficulty of transforming and mobilizing a new army under the rigid constraints of the Treaty of Versailles. As the evolving nature of the contemporary battlefield forced armies to become progressively more distributed, Germany correspondingly inculcated change agents at the lowest levels of its organizations. This enabled emergent patterns of change during the interwar transformation processes, resulting in adoption of a highly decentralized tactical method that emphasized independent action of change agents at the junior leader level.

The manner in which Germany evaluated doctrinal concepts following World War I demonstrates its emphasis on the activity of change agents throughout the army. Perhaps the most universal and enduring concept influencing the German Army's interwar transformation was a thorough and honest process of critical self-evaluation. During the interwar years, the German army formed fifty-seven committees of officers with tactical and operational experience to conduct critical surveys of nearly every major area of combat operations, emphasizing "solid, realistic estimates of what had actually occurred, not on what generals might have believed to have happened." [Murray and Millett, 1996] The resulting reports formed the basis of Germany's innovative process--a foundation of honest, critical self-analysis, rather than one of cultural bias and parochialism. To further ensure its discourse on war did not diverge from reality, the German army thoroughly tested its new doctrinal concepts in experimental units and during many comprehensive maneuvers: "...a typical German Army captain or major in 1940 would have participated in more multidivisional maneuvers than the average British or French general." [Corum, 1992] When attempting to incorporate new technologies, the Germans relied on foreign analysis where it was available, but they emphasized exploiting their own lessons learned through testing of these technologies in experimental units [Habek, 2003]. Remarkably, they avoided parochialism in even the most contentious areas of debate; for example, the most vocal armor advocates emphasized the tank's role as an integral member of the combined arms team, avoiding the pitfalls of the armor-centric view emphasized by contemporary British theorists [Murray and Millett, 1996].

After decades of debate and experimentation, *Auftragstaktik* emerged as the conceptual foundation of German tactics. This is reflected in the emphasis on "considerable independent tactical authority for junior leaders," both officers and non-commissioned officers, in the 1921 Army Regulation 487, *Leadership and Battle with Combined Arms* [Corum, 1992]. As described by Williamson Murray:

Post-World-War-I German doctrine consequently emphasized conceptions that were starkly different from those of the British and French. The first was a belief in maneuver. The second emphasized an offensive mind set; the third demanded that commanders decentralized operations to the lowest level possible. The fourth required officers and NCOs to use their judgment on the battlefield;

the fifth stressed that leadership at all levels must always display initiative [Murray and Millett, 1996].

The basic philosophy embodied in *Auftragstaktik* traces its roots to Clausewitz' emphasis on fog and friction in combat, emphasizing decisive action with limited information in an environment characterized by meeting engagements. War was not viewed as a predictable event subject to centralized control and specialized units. Rather, tactical and operational methods were developed in peacetime to conform to war's inherently chaotic nature, emphasizing the ability to operate in a state of self-organized criticality, where flexibility and initiative were maximized to enable emergent patterns of action. As a result, the German Army was comfortable operating in a state of self-organized criticality at the edge of chaos. Its emphasis on decentralized Control, embodied in *Auftragstaktik*, made the German army particularly suited to take advantage of the fleeting emergent opportunities that typified the complex environment of modern warfare.

1.4. Complexity and Army Transformation

Army Transformation is a relatively new name for what is traditionally an ongoing process of innovation in military organizations. The new name is symbolic of an effort to harness revolutionary change. Caught up in the fervor over the notion of an I-RMA, the overall focus of the process has become the search for technological panaceas, built on an intellectual foundation of eliminating uncertainty in war. History shows a more balanced approach would combine the search for improved technological capabilities with equal vigor in improved operational and organizational design, honest experimentation and critical self-assessment. Instead, Army Transformation has resulted in the migration of future concepts to current doctrine; force structure changes are currently driven by the need to create more units to satisfy overseas commitments; the few experiments that occur are manipulated to make future vision a current "reality;" and critical thinking is rejected in favor of the inculcation of transformation dogma.

The Army understands how to encourage emergence during combat operations. Leaders at all levels are taught to display initiative and find innovative solutions to problems, retaining freedom of action within the guidance of the commander's intent. It is the commander's intent that maintains cognitive tension, allowing the various elements of the complex system of a military organization to pursue their distinct aims in combat, while maintaining a unity of effort through pursuit of the commander's aims. This same spirit must be inculcated within the peacetime Army. Instead of perpetuating the tendency to establish constricting layers of bureaucracy and control, the Army must engender an environment that keeps the spirit of initiative and innovation alive in peace as well as in war. This can best be accomplished by embracing complexity theory as the intellectual foundation of Army Transformation.

Significantly the U.S. Army had success with a less control-oriented approach during the transformation of the late 1970s and early 1980s. During this period, due to

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the post-Vietnam Army's decline, a major effort to overhaul Army doctrine resulted in the publication of FM 100-5, *Operations*. While many senior leaders were intellectually engaged in the innovative process, it was not top-driven as it is today. On the contrary, it was characterized by intense debate, critical thinking, honest analysis of contemporary warfare and experimentation, and the contributions of change agents at all levels within the Army and the civilian community [Naveh, 2000]. During this period, transformation's "chief characteristic was pluralism in its ideas and organizations, reflecting the dynamics of economic markets and democratic politics, rather than control from atop by any single plan. While this process was turbulent and confusing, it worked." [Binnendijk, 2002]

CRP theory provides an intellectual foundation upon which Army Transformation could be based. This theoretical shift would provide a positive influence on culture through a guiding Common Body of Metaphor (CBM) that recognizes the manner in which human organizations best achieve positive change. If the U.S. Army adopts CRP theory as the theoretical basis for organizational innovation, it will engender an operational and tactical mindset in which change agents at all levels are comfortable operating in a state of self-organized criticality at the edge of chaos--in peace and in war--where they are optimized to achieve beneficial adaptation in the form of self-organized patterns of emergent behavior. In contrast to transformation efforts that focus on technological innovations, inculcation of a complexity CBM will enable the U.S. Army to see the innovations already resident within the organization, waiting to emerge, rather than pinning hopes on the unproven technologies of the future.

As difficult as it may be for an Army culture based on bureaucracy and control, the key lesson of CRP theory may be that an innovative organization will achieve more by doing less. Society's prevailing worldview is still dominated by the linear approach of Newtonian physics and the reductionist, time-reversible assumptions of the scientific method--but the major discoveries of the past twenty years in complexity demonstrate that a new conception of the way the world works is in order. Complexity demonstrates that an innovative process based on prediction and certainty is fundamentally flawed--Clausewitzian friction is a permanent feature of war. It is only by facilitating emergence through the inculcation of a CBM based on CRP theory that the U.S. Army can achieve the evolutionarily advantages provided by operating, in peace and in war, at the edge of chaos.

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Chapter 10

A Model of Biological Attacks on a Realistic Population

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The capability to assess the impacts of large-scale biological attacks and the efficacy of containment policies is critical and requires knowledge-intensive reasoning about social response and disease transmission within a complex social system. There is a close linkage among social networks, transportation networks, disease spread, and early detection. Spatial dimensions related to public gathering places such as hospitals, nursing homes, and restaurants, can play a major role in epidemics [Klov Dahl et. al. 2001]. Like natural epidemics, bioterrorist attacks unfold within spatially defined, complex social systems, and the societal and networked response can have profound effects on their outcome. This paper focuses on bioterrorist attacks, but the model has been applied to emergent and familiar diseases as well.

1 Introduction

While physical “simulation” exercises can provide valuable insights on bioattacks, they are limited in number, size, scope, and scenarios due to cost, time, and cognitive constraints. It is faster, more cost-effective, and comprehensive to do computer

simulations, which allow larger numbers of complicated, out-of-the-box scenarios to be examined systematically.

Computational models have been built to explore outbreak impacts for over 30 years. SIR models [Anderson and May 1991] typically assume homogeneously mixing populations. Recent models address the spatial dimension [Lawson 2001]. Cellular-automata models, such as the individual-based model of smallpox epidemics [Epstein 2004] allow spatial operation and discontinuities. The geometry of cellular automata, however, could cause incorrect modeling of disease spread. System dynamics models can capture the general epidemic dynamics. This is similar to the discrete event simulation models such as the model of antibiotic distribution used to examine post-exposure prophylaxis [Hupert et. al. 2002]. The sensor-action models such as the Measured Response bioterrorism simulator based on Synthetic Environment for Analysis and Simulation (SEAS) [Chaturvedi and Mehta 1999] can model individual-based sensing and action pairs. Due to its “genome”-based sensing-action pairs, however, SEAS has a fundamental weakness of capturing only the reactive, psychological, and behavioral content, ignoring knowledge-intensive, deliberative, and network-intensive reasoning inherent in humans and socio-technical and economic systems. As it is based on SEAS, SEAS-derived Synthetic Environment for Computational Experimentation (SECE) also has this weakness. SEAS can be used for model aggregate events with large enough sample, but not for critical social and knowledge networks or superspreading events—both of these need to be addressed properly to tackle bioterrorism and other socio-technical problems. Episims model of the Los Alamos National Lab uses transportation networks simulation to estimate contact graphs that are assumed to be social networks [Eubank et. al. 2004] and assumes viral load as the basis for disease spread. Most bioattack models simulate a single disease or only bioattack diseases, make homogenous-mixing and perfect-information assumptions, discount factors such as the urban geography, how people are embedded in social and knowledge networks, and ignore knowledge-intensive, networked reasoning.

BioWar is a model that combines computational models of social networks, communication media, and disease transmission with demographically resolved agent models, urban spatial models, weather models, and a diagnostic error model to produce a single integrated model of the impact of a bioterrorist attack on a city. Unlike traditional models that look at hypothetical cities, BioWar is configured to represent real cities by loading census data, school district boundaries, and other publicly available information. Moreover, rather than just providing information on the number of infections, BioWar models the agents as they go about their lives with their social-networked and knowledge-rich reasoning. This enables on the observation of factors such as absenteeism, insurance claims, over-the-counter drug purchases, and hospital visit rates, among others. In this paper, we will only describe the core submodels of BioWar.

2 BioWar Model

BioWar is a city-scale spatial multi-agent network model capable of simulating the effects of weaponized biological and chemical attacks. Recent work has demonstrated that the failure to take social networks and locations into account leads to incorrect estimates of disease spread and response policies [Morris 2004][Klov Dahl et al. 2001]. BioWar is socially (embedded in social, knowledge, and task networks) and spatiotemporally more realistic than previous bioterrorism attack models, as it enables:

- Heterogeneous population mixing, defined by social networks.
- Simultaneous modeling at multiple levels (pathogen dispersion, knowledge evolution, multiple layers of local, state, and federal authorities, etc.).
- Detailed modeling and simulation of individuals, social networks, and reasoning.
- Data driven dynamics: real-world data can be used as input to simulation with minimal processing and simulation outputs match the data formats.
- Human-in-the-loop and social & knowledge network in the loop operations.

Figure 1 shows the components of BioWar.

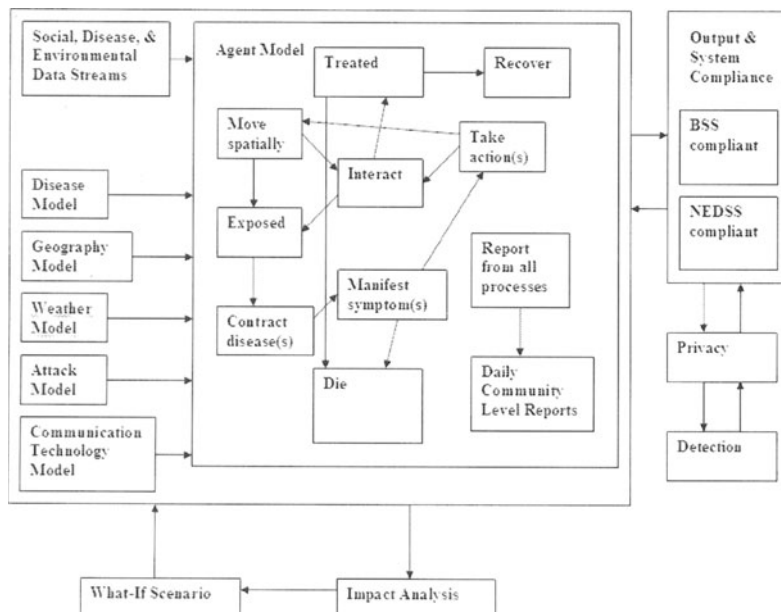


Figure 1: The design of BioWar.

The agent-model takes as input the social, disease, and environmental data streams. It integrates various models of disease, geography, attack, weather, and communication technology. The agent-model itself is a knowledge-intensive reasoning engine governing how agents interact, move, and seek and receive treatments. All data are screened for privacy and anonymity.

3 Agent-level Disease Model

The current version of BioWar simulates 62 diseases—four weaponized diseases and 58 naturally-occurring diseases—simultaneously in a population. We use a symptom-based general disease model. Each disease has its own set of symptoms, timing of disease phases, variability in presentation based on age, gender, and race, and contagiousness. Each symptom has its own severity and progression timing. Each instance of a disease infecting an agent is individually represented and progressed through time. Diseases propagation is probabilistically determined by agent risk factors influenced by demographic and occupation variables, the transmissibility of the disease, and the spatial and temporal proximity of uninfected agents to infected agents. Our disease model generates epidemic (or EPI) curves as output.

Each infectious disease progresses through up to five phases:

- Incubation: the period before the agent begins presenting symptoms due to a bacterial or viral infection.
- Early symptomatic (prodromal): the period of time during which an infected agent may experience mild or non-descriptive symptoms.
- Late symptomatic (manifestation): the period of time during which an infected agent may experience severe and/or disease-specific symptoms.
- Communicable: the period of time during which an infected agent may infect other agents. This phase may overlap with the above phases. Noncontagious diseases such as anthrax do not have this phase.
- Recovery/death: a period of time during which an infection resolves or causes death.

In constructing our disease model, we used data and accounts on anthrax releases [Inglesby et al. 2002] and disease knowledge bases [Isada et. al. 2003]. We have also drawn on the experience of medical expert systems for diagnosis [Miller et. al. 1982].

3.1 Symptoms

In BioWar, symptoms are a factor governing behavior and determine the initial diagnosis of agents entering the medical system. This symptom-based disease model permits the representation of outliers and stochastic flux. The symptoms are assigned measures that influence which symptoms agents get and how that influences their behavior [Miller et. al. 1982]. The diagnosis is influenced by symptom severity and other factors such as other disease & symptom confounding, patient health history and demographics, and occupation. The true nature of the agent's health status is obscured to the agent so it only responds to sensed symptoms. Modulated by demographics, mild symptoms prompt a visit to a pharmacy, high ones to a doctor, and severe ones to the emergency department.

3.2 Dose-Response Relationship for Weaponized Pathogens

Relationships of the infection probability, illness duration, and onset-of-illness versus inhaled dose were recently published for anthrax, botulism, pneumonic plague and Venezuelan equine encephalitis [Rickmeier 2001]. At this stage, BioWar takes into account dose and age-of-agent for infection probability for inhalational anthrax

following formulas developed by Webb, Blazer, and Buckeridge [Webb and Blaser 2002][Buckeridge 2003] while for the other weaponized diseases the exponential model for infection probability is used.

4 Agent and Social Networks

The significance of social networks to contagious disease transmission is obvious. While non-contagious bioagents such as anthrax do not spread through social networks, social networks define the exposed subpopulation through co-location of agents at the time and place of an attack.

4.1 Representation of Agent

An agent is represented as a knowledge-rich reasoning engine that has roles such as mother, schoolmate, doctor, nurse, teacher, etc. Additionally, an agent has socio-demographic and economic status. An agent is located at specific spatio-temporal coordinates and exhibits behaviors. These behaviors include interaction (communicate, get infected, infect), recreation, going to school/work, seeking treatment, purchasing over-the-counter drugs, and moving to other places. Each agent has an ego net and natural biological rhythm (e.g., sleeping 8 hours a day). Moreover, an agent can exhibit symptoms, reason about options, and has mental model of diseases. The propensity of an agent to seek treatment is affected by socio-demographic position (age, race, gender, class, etc.), economic status, ego-networks, and severity of perceived symptoms. Note that even if an agent seeks treatment, treatment is not always available, such as when doctor office is closed. If an agent goes to pharmacy, the agent's symptoms determine drug purchase choices influenced by symptom severity, symptom-drug relationships, and agent demographics.

4.2 Social Networks

In BioWar, each agent is linked to other agents in the simulated population by a set of links (relationships) modeling a social network. Each link is a descriptor of a pair of agents and their relationship type. Agents may be linked unidirectionally or bidirectionally. Relationship types currently implemented are family (spouse, parent, child, sibling, other family), proximity based (co-worker, schoolmate, group member, neighbor), and voluntary (friend, advisor, other). The overall network size and distribution were drawn from Klov Dahl's study along with some target numbers for individual relationship counts [Klov Dahl 2002].

4.3 Agent Interaction

Agents interact with each other based on BioWar's CONSTRUCT model which describes the co-evolution and emergence of communication and knowledge networks, driven by homophily and expertise-seeking [Carley 1991]. The actions of agents are influenced by their knowledge-rich reasoning in addition to their social networks. Agents also interact with others nearby and also by random chance. As agents interact, they may exchange knowledge and diseases.

5 Results

BioWar is designed to be modular and portable, and currently runs under Linux, Windows, and Tru64 UNIX. The run time scales linearly with the number of agents. We have simulated runs for several cities, including San Diego, Pittsburgh, Norfolk, San Francisco, DC, and Hampton city of Virginia. The scenarios simulated include no attack, anthrax attack, and smallpox attack. The runs for the city of Hampton cover 100% of its 145,665 inhabitants without scaling. The length of the runs is 2 years, with each tick of the simulation being 4 hours. There are 1 weaponized disease and 58 naturally-occurring diseases, including seasonal flu strains. Figure 2 shows the run results for the city of Hampton, Virginia. When an anthrax attack occurs during a flu season (a 2.5 kg anthrax attack with an efficiency of 0.05 at 4pm of January 25, 2003, infecting 2122 people during a sports event at a stadium), it increases the doctor visit rate significantly for a short period of time after the attack. After an aerosolized smallpox attack occurs, infecting 2%-2.5% of the agents in a locality at 4pm of May 26, 2003, it results in a long aftermath and more deaths compared to the anthrax attack, due to the contagious nature of smallpox.

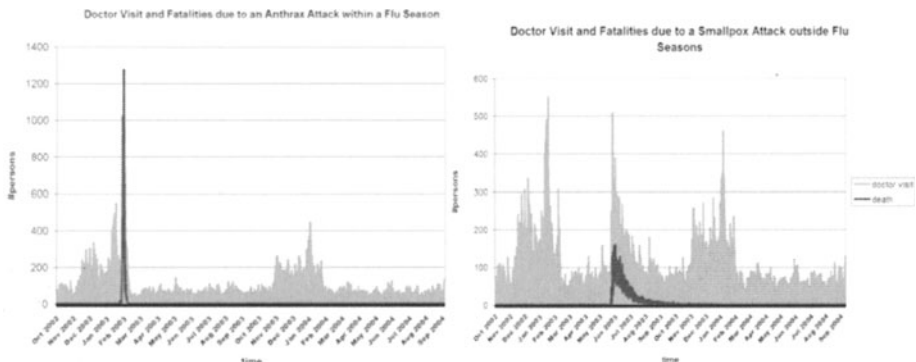


Figure 2: (Left) The number of deaths (dark) and doctor visits (grey) occurring with an anthrax attack. (Right) The number of deaths and doctor visits occurring with a smallpox release.

6 Model Validation

We have validated BioWar for anthrax and smallpox cases against existing epidemiological models (SIR—Susceptible-Infected-Recovered—model and its variant) and empirical data [Chen et. al. 2004][Chen et. al. 2006] for various response scenarios. Computer-assisted manual validation of a model such as BioWar is difficult to get right with respect to proper results and spent resources due to model complexity, emergence, human cognitive limitations, and large parameter space. This makes comprehensive automation necessary. A knowledge-intensive experimental approach has been created [Yahja and Carley 2006] for this purpose, implemented in a tool called WIZER for **What-If AnalyZER**. WIZER performs knowledge-intensive

virtual experiments—and real experiments if augmented with robotics interface—using its synergized simulation and inference engine. WIZER checks the outputs of simulation, reasons about the results, and adjusts simulation parameters, meta-models, and knowledge bases. In contrast to evolutionary computation [Fogel 2005] which relies on evolutionary operators, our knowledge-intensive experimental approach relies on scientific experimentation and knowledge accumulation to make progress. The experiment results can bring forth revolution.

7 Conclusion

Several improvements for BioWar were planned, including adding infrastructures such as road & air transport networks and organizational structures & responses. While more enhancements are in pipeline, current version of BioWar represents significant advancement over other models. This includes BioWar's ability to model socially defined mixing and spatiotemporal effects, critical networks, knowledge-rich & networked reasoning, and emergent properties & unexpected outcomes based on local interactions.

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Chapter 11

Cartography applications for autonomous sensory agents

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This paper proposes a coverage scheme for the rapid mapping of an area's characteristics by a group of mobile and autonomous sensory agents. It is assumed that the agents utilize the wireless medium for communication, and have limited computational, storage and processing capabilities. These wireless sensory agents collaborate among each other in order to optimize their coverage tasks and communications. In this paper, we present a scheme that helps maximize the system's efficiency through an adaptive coverage algorithm, where agents share information and collectively build a spatio-temporal view of the activity patterns of the area. Our scheme is particularly useful in applications where the events of interest exhibit an oscillatory behavior. Relevant applications include distant scouting and exploratory missions where the size and number of the scouting agents are crucial to the success of the mission.

1.1 Introduction

1.1.1 Preliminaries

In some scientific explorations the goal is to locate, quantify and analyze the magnitude of some local events or phenomena, and then keep looking for new events. This information allows the involved scientists to draw conclusions about the significance of an area with respect to a certain criteria. For example, the analysis of the locations and emission rates of geysers (such as the California

geysers) warns seismologists about upcoming earthquakes [9]. In another application, NASA [6] scientists are hoping to find life and other bio-sources on the frozen moon EUROPA [6]. The success of these missions hinges on first discovering areas of volcanic vents or hot water sources, underneath the frozen oceans of the planet, since these sources can provide the much needed warmth and nutrients for potential life forms, before sending in specialized underwater robots to collect life samples. These vents are the result of natural geological forces, and can exhibit either uniform or nonuniform oscillatory patterns of activity. Activity is identified by the emission of particles or liquids that becomes intense for some period of time, and then recedes back to a more tranquil state. In certain location or *spot*, the amount of particles emitted during a period of time is used as a criterion for determining how active or *hot* that spot is. Identifying the spatio-temporal pattern of activity of the different *hot spots* or *hs*, allows us to determine the *seasonal* behavior of the terrain. In other words, which parts of the terrain are going to be active and at what times. The physical constraints of the agents ranging from the limited battery supply to limited computational capability force us to adopt minimalistic and energy-efficient designs. Finally, the main advantage of using these exploratory scout agents is that they allow for following specialized agents to come and explore the best area, hence maximizing the quality of valuable scientific information yield vis-à-vis energy and time spent.

1.1.2 Challenges

The challenges for distant exploratory missions stem mainly from the fact that no human intervention is possible once the agents are deployed. This requires the agents to be autonomous, i.e. they must be able to self-organize into network(s), study the surroundings, discover the *hs*, relay the information in a timely manner and collaborate for keeping constant coverage of the area. Another important challenge is due to the tight physical space available in the transport ship that imposes restrictions on the physical size of the agents in addition to their possible deployable number. This minimalist physical design makes the agents resource-challenged devices, especially in terms of battery, memory, computational and communicational capabilities. Hence all proposed schemes for these types of applications have to take all these restrictions into consideration for energy efficient communicational, storage and computational algorithms.

1.2 Related work

There is a lot of work in the area of coverage and map-drawing for sensory agents, and the literature seems to be divided into two main approaches. The first approach views the coverage area from a mobility perspective where the deployment area is divided into a large grid-based framework. The network's performance is based on the actual physical location/coverage of all the grid's parts. The second approach considers the area in terms of control-based laws

and computational geometry of the spatial structures found in the area, using techniques such as Voronoi diagrams in order to direct the nodes in the proper direction. An interesting work is reported in [7] where the authors propose using Voronoi diagrams and the Delaunay triangulation method in order to configure the network based on agent locations in the network. Then they define an algorithm that calculates the maximal breach path, which represents the path that a target can take and be least covered by the sensor nodes, and another maximal support path as its contrary where it is most covered by sensor nodes. In [8] the authors define a mathematical model based on the agent's sensing abilities and then display results after using their model on tracking a target using multiple amount of sensors. They calculate the sensors' placement versus the breach and support paths presented in [7]. In [3] the authors present a grid-based analysis of the sensor's density relationship to the physical area coverage and how much sensor nodes have their areas covered by other sensor nodes. In [4] the authors present a dynamic clustering framework for the sensor networks with emphasis on putting a bound on finding an available path. A random-walk based mobility model is also presented. In [5] the authors study the effect of the range of radio transceivers on the general network connectivity and power consumption. They present an algorithm to determine the minimum required radio range and study the effects of random mobility on these values. In [10] a vision-based mobility approach is presented for robotic coverage tasks where the metrics are the percentage of area covered and distance traveled by the robot. The mobility is based on a zigzag pattern after the robots subdivide the area into smaller areas and landmarks. Finally, a good work on coverage and mobility is presented in [1] where the authors present a mathematical model for decentralized control laws that seek to coordinate between mobile sensor nodes covering an area. They define a node/agent sensing model and rely on randomly generated manifold formations and Voronoi diagrams in order to relocate the sensor nodes in positions that would give the sensor agent a good coverage and at the same time avoid agents crossing each other's paths.

1.3 Outline of the mobility algorithm

1.3.1 Architecture

In our system, ANTS [2] *autonomous network of tiny sensors*, we consider two types of agents: Workers and Leaders. Workers are smaller with less computational and battery powers than Leaders. Leaders act as data storage and process the information gathered by their Workers. Workers form clusters around a Leader, and the Leaders collectively act as a 2nd tier network for the whole system. The reason for such an architecture is to decrease the load of computation and communication at the Worker level in order to increase the longevity of the network. In simple comparisons with other systems, this specialization architecture has proven to increase the life of the network when compared to other architectures such as flat networks for similar scenarios [2].

1.3.2 Communication

Every Worker in the system defines its coverage area by its sensing radius' R_s , which, for simulation purposes, is limited to the its coordinate location or spot. The leader node on the other hand, defines its area of coverage by its radius (or range) of communication, R_c . As is the common practise for simplification, we consider both areas to have a square shape rather than a circle. The Leader has the capability of communicating with all Workers in its cluster. Inter-cluster and intra-cluster communication occur at the Leader-Leader and Worker-Worker levels respectively. Leaders use a combination TDMA and FDMA to communicate with cluster members, and CDMA to communicate with other Leaders. The frequency used by the cluster is determined by every cluster's Leader after negotiation with nearby Leaders to avoid interference.

1.3.3 Shingling

After the deployment of all the agents and the establishment of clusters in the network, every Leader agent collects information about every Worker node in its cluster including its location coordinates. Then it calculates and broadcasts back to all its Workers the value of the smallest distance separating any two Workers. This value is used by each agent to define the sides of a virtual square, centered at the agent's location. Every worker plans for its own route, but can broadcast to its Leader the coordinates for the plan, to receive back the step-by-step route details.

The agents view the deployment area in terms of a grid where each point coordinate corresponds to a triplet (N, E, T) . N stands for the value of the sensed phenomenon, E represents the geological characteristic such as elevation and terrain type, and its value defines the needed mobility energy and time cost for this location. Finally, T represents the time stamp when N and E 's values were valid. The sensed phenomenon could represent a multitude of natural occurrences, so the type of data value could be temperature, pressure, humidity and or chemical composition. Choosing the smallest distance between any two agents as the starting virtual square, ensures the creation for the first contiguous coverage area formed by the fusion of the two closest agents's coverage/virtual squares. It also sets a common minimum starting cycle coverage area for all the agents. This fact helps in the coordination and time synchronization of all the agents so that the Leader can have a sense of when all the nodes should cover their respective squares. Time delays resulting from the E factor found in the terrain is incorporated in future route planning.

Every Worker agent picks a starting location on its virtual square and proceeds to *cover* every coordinate location in the square following the order found in its route-coordinates list. At every coordinate location, the agent records the triplet values. An *hs* is discovered when the sensed phenomenon's value at a location exceeds a certain threshold of normalcy. The time to cover the initial virtual square will be then used as the standard cycle to discover the phases and periods of all the other *hs*' cycles. The first fused covered area that emerges

would contain at least two Worker agents and these Workers would belong to a sub-cluster. In subsequent cycles more fused areas will emerge and more sub-clusters will start to appear and grow and fuse together until the sub-cluster's membership becomes the same as the original cluster's. Simulations have shown us that when this happens, almost the entire target area would have been covered in its entirety at least once.

Before a Worker starts moving, it first checks first with its memory to see if the new proposed route has been recently covered by itself or any member of its sub-cluster. A Worker just needs to store in its memory the contents of two virtual square's triplet values, which can be easily stored as a doubly-linked list data structure. This way a Worker is guaranteed not to cross into its own recently covered area. Workers communicate with each other and Workers of the same sub-cluster add another identification variable to their transmissions. Workers negotiate among each other in order to avoid redundancy by simply checking if part of the route proposed by the neighbor Worker is found in their memories. This guarantees a minimum span of one cycle difference before the same agent returns to the same area. The Workers do transmit their findings after every cycle to their Leader for storage and spatio-temporal analysis. The challenge of discovering a varied oscillatory phenomena is to cover the area *like shingles* which usually overlap slightly. Once any *hs* is discovered during a cycle and its location made known, the *T* factor is noted, and if subsequently other Workers pass onto the same location, then the current *N* state of the location is noted to see when it was active and when it was not. The Leader node can then determine at which cycles or *seasons* it is most likely to be active. Refer to the following Figure 1.1 for a more illustrative explanation of our algorithm.

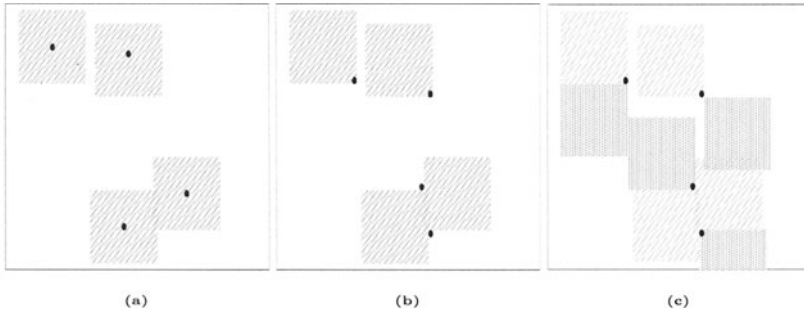


Figure 1.1: Mobility pattern of agents of a cluster of 4 agents.

(a) Shows the first mobility coverage with respect to the original agents' locations, (b) Shows the location of the agents after the first cycle, (c) Shows the second cycle coverage area .

The planned routes, communication and standard *shingling* between the Workers allow for the same sub-cluster members to have an estimate about the separating distance between them. Hence they can tailor their transmis-

sion variables to accomodate the needed amount of power to transmit efficiently across to other Workers. Also, since the Leader acts as a time-data repository, Workers can always query their Leader for information without the need of attaching vast amounts of data to their packets when communicating with each other. Finally the internal decision mechanism for Workers to decide on the location of their new starting point and the direction of their new coverage is based upon the need to go in the direction of newly discovered *hs*, other shingle areas and to the borders of the Leader's R_c area.

1.4 Simulation Results

In our paper, we are considering the EUROPA scenario, where we assume that the agents have been deployed on an ocean floor and the sensed phenomenon is temperature. In this section we will focus on two different cluster sizes for the same sub-area. In Figure 1.2 we show a (20x20) portion of the (100x100) locations map, where a 5-member and 15-member cluster are deployed with 30 hidden hotspots. The figures show the coverage progress of each cluster size. In Figures 1.3 and 1.4 we show average results, for a size 5 and 15 cluster members regarding the time it takes to discover what percentage of *hs* and total coverage as well. Note that only a fraction of these *hs* is active at any period of time. Note how the network quickly makes a complete sweeping coverage of the terrain first.

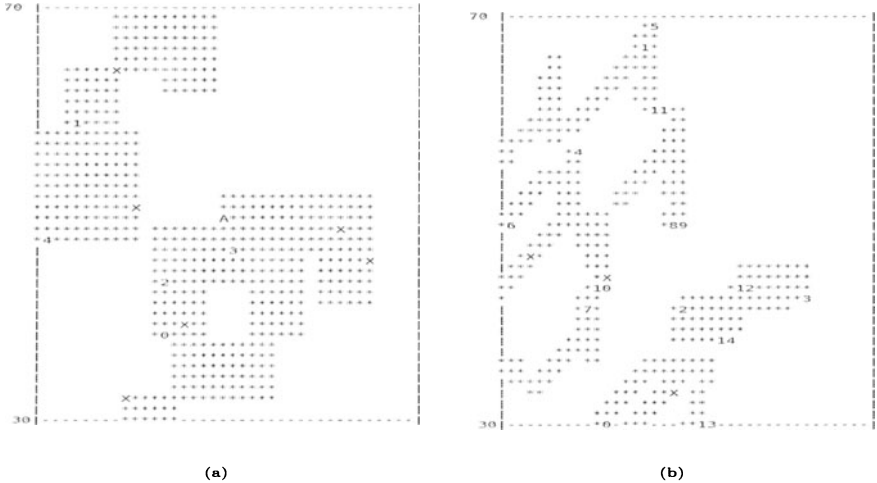


Figure 1.2: Showing clusters of sizes 5 & 15 around leader A, x represent hotspots. The y-axis & x-axis both range from 30 $\mapsto$ 70

- (a) Shows the coverage progress of a 5-member cluster after a few cycles, (b) Shows the coverage after few cycles of a 15-member cluster after same few cycles.

1.5 Conclusion

In this paper, we have described an approach to exploring and mapping an unknown environment's events especially when they exhibit oscillatory activity, and where the agents are resource-challenged. We have provided a real-world application scenario where these challenges are likely to arise. Our approach is based upon exploiting a fast overlapping mobility pattern, similar to shingling, that allows the agents to quickly cover the bulk of the target region area and also to create a contiguous coverage area. The use of a standardized area for mobility allows for communication cost reduction, and cyclic pattern discovery of hotspots. The information gathered by these agents, in addition to the E factor provides future missions with important information regarding the data cost and value of different locations at different times for path planning purposes.

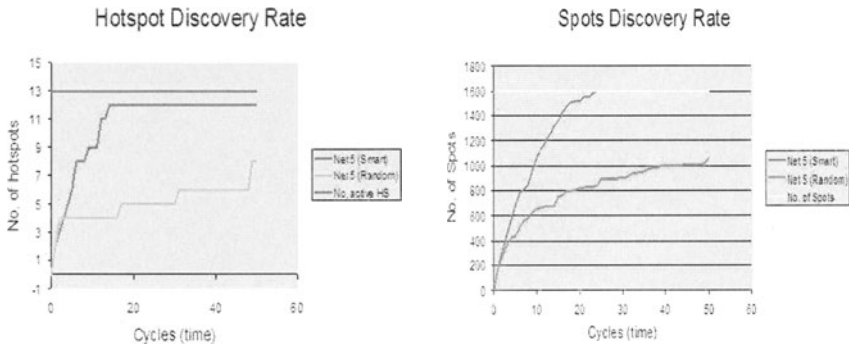


Figure 1.3: Showing the time taken v.s. rate of spots and hotspots discovered for a size 5 cluster.

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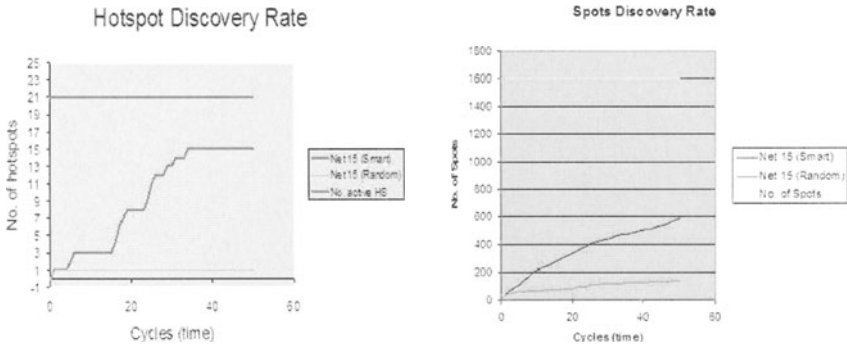


Figure 1.4: Showing the time taken v.s. rate of spots and hotspots discovered for a size 15 cluster.

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Chapter 12

Dissipation and Statistical Mechanics of granular gas : General framework and 1-ball case

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310.1. Introduction

Recently, a tremendous amount of works has been performed to investigate properties of granular gas (see [Goldhirsch 2003] for a review). This problem is fundamental because it is a frontier of statistical mechanics when dissipation becomes dominant; hence it asks the problem of what dissipation changes in the behavior of a statistical ensemble of particles in interaction: within which limits can one use the analogue of thermodynamics concepts to describe the behavior of these systems?

Indeed, dissipation is already taken into account in many different problems of physics, such as electronic transport, or as hydrodynamics of Newtonian fluids. This is why analogy with these problems has been the idea of theoretical understanding of granular gas [Savage & Jeffrey 1981, Haff 1983, Goldhirsch 2003]; and the description starts with a series of continuous equations imposing preservation rules of mass, momentum and energy transfer, with a distribution of particle speed assumed almost Maxwellian, because of the supposed local thermodynamics equilibrium.

However, the dissipation at work in granular systems is different from the other ones (Newtonian fluid, electronic transport,...) because it is directly generated by collisions. This cancels likely the validity of a series of approximations, despite what is often supposed. This will be recalled in the first part of the paper.

Indeed, one can illustrate the strong effect of dissipation just by looking to clustering of a granular gas: it occurs already at very small density of grains as shown by a recent micro-gravity experiments [Falcon et al. 1999] or using a pseudo-Maxwell demon experiment on earth [Jean et al. 2002]; so, links this clustering is linked to the change from a Knudsen regime (for which particles interact mainly with the boundaries) to the case of interacting particles [Evesque 2001]. The photos of the granular gas in 0g show also that the wall speed is faster than the typical ball speed

even when the density is so small that no cluster occurs, so that the excitation is of “supersonic” nature [Evesque 2001] . This asks about (i) the validity of a continuous description and (ii) the role played by the boundaries: does the box act as a thermostat or as a “velostat” [Evesque 2002], i.e. does it impose a speed or a kinetic energy? Also, do the system behaves in a similar way on earth as in micro-gravity?

This paper proposes a frame work to discuss some basic assumptions on the theory of dissipative granular gas, and shows with a simple experiment that a deep understanding about the limitations can be gained from very simple experiments (or simulations); this necessitates to avoid the use of unproved analogies. The 1-ball experiment reported here demonstrates that rotation cannot be forgotten. It has then true implication of theory of chaotic billiard.

The results, and their interpretation reported here, have been obtained from micro-gravity experiments. This makes them rare and quite expensive. But despite their cost, they have brought some new important findings which have not been described previously. And they enlighten the questioning. So they might not be so costly.

310.2. Basis for the dynamics of granular matter in a vibrating container

310.2.1. The Boltzmann equation

The mechanics of granular materials obey the general laws of mechanics, which can be described as free flights of particles in between collisions. When the time spent by a particle in free flight is much larger than the duration of the collisions, the number of complex collisions engaging 3 or more bodies at the same time is rare so that the collisions can be considered as binary collisions. In this case one speaks of the granular gas mechanics. Within this approximation of "dilute" condition, the solution of the N-particle problem can be integrated over the N-1 or N-2 particles which do not interact with the considered particle; hence the problem can be reduced to the one of finding the distribution function at time t of a single particle $f(q,p,t)$ and its evolution; here q and p are the position and momentums of the particle, in which rotations are included; one notes also v and m the particle speed and mass. This simplification requires also that topological constraint between successive collisions are small to allow neglecting correlations in between successive collisions.

So, starting from the N-particle Liouville equation, the evolution is described by the distribution function f of a single particle, with f obeying the Boltzmann equation:

$$[\partial/\partial t + \mathbf{v} \cdot \nabla_{\mathbf{r}} + \mathbf{F} \cdot \nabla_{\mathbf{p}}] f(p,q,t) = (\partial f/\partial t)_{\text{coll}} \quad (1)$$

The term $(\partial f/\partial t)_{\text{coll}}$ contains collisions between two balls and between the ball and the container wall, since both collisions can happen. The dynamics of the container can be described as an oscillating spring-mass system at constant energy with Hamilton equation $H = p_w^2/(2M_w) + kq_w^2/2$; the ratio k/M_w and the energy E_0 shall be adjusted to get the right frequency and amplitude; it is supposed here that $M_w \gg Nm$ to neglect the variation of amplitude due to repeated collisions, where m is the grain mass.

When the particle density gets larger, three-body, or 4-body,... collisions become more numerous, and the BBGKY expansion of the Liouville equation has to be used to compute the evolution, incorporating cross correlations of few different particles.

Nevertheless, the problem is completely solved in the dilute regime when one finds the correct distribution function f . It takes the form:

$$(\partial f / \partial t)_{\text{coll}} = \int dp_1 \int d\Omega \sigma(\Omega) [|v' - v_1| f(p')g(p_1) - |v - v_1| f(p)g(p_1)] \quad (2)$$

The right term of Eq. (2) is made of a sink term and of a source term; the sink describes collisions between both particles p and p_1 (leading to a rate of disappearance of p) and the source term describes collisions between particles p' and p_1 generating a particle with momentum p . $\sigma(\Omega)$ is the cross section of the collisions. The use of $g(p)$ in Eq. (2) allows to treat at the same time collisions with the wall, $g \neq f$, and collisions between two balls, $g = f$ if a statistical averaging is possible.

310.2.2. Classic gas of atoms

At this stage it is worth recalling some classic results about the statistical mechanics of a gas of atoms. Indeed, in the case of a gas, one looks for a stationary homogeneous solution of the Boltzmann equation, i.e. $\partial f / \partial t = 0$, $\nabla f = 0$. This imposes to search f satisfying $(\partial f / \partial t)_{\text{coll}} = 0$. But collisions between atoms obeys some simple rules of conservation, which are mass preservation, momentum preservation and energy preservation; furthermore, one gets also $\sigma(p_1, p_2 | p'_1, p'_2) = \sigma(-p'_1, -p'_2 | -p_1, -p_2) = \sigma(-p_1, -p_2 | -p'_1, -p'_2) = \sigma(p'_1, p'_2 | p_1, p_2)$. So Eq. (2) leads to :

$$(\partial f / \partial t)_{\text{coll}} = \int dp_1 \int d\Omega \sigma(\Omega) |v - v_1| [f(p')f(p'_1) - f(p)f(p_1)] = 0 \quad (3)$$

and Eq. (3) is satisfied if $f(p')f(p'_1) = f(p)f(p_1)$. In turn this condition is satisfied if f is such as its logarithm $\ln(f)$ is a linear combination of the invariant of the collisions, that writes $\ln(f) = A_m + B_p + C p^2 / 2m$, or as the Maxwellian distribution:

$$\ln(f) = D - (p - p_o)^2 / (2mk_B T) \quad (4.a)$$

$$\text{or } f = A_o \exp \{ -(p - p_o)^2 / (2mk_B T) \} \quad (4.b)$$

Eq. (4) is then a possible stationary solution. It remains to demonstrate that Eq. (4) is the solution. This is straight forward applying the H theorem of Boltzmann. This H theorem tells that any solution of Eq. (1) with $(\partial f / \partial t)_{\text{coll}}$ given by Eq. (3) evolves in such a way as its local entropy $-f \log(f)$ shall increase continuously. Hence, as Eq. (3) describes a stationary state (with a constant entropy), Eq. (4.b) is the exact solution.

310.2.3. Extension to the case of little dissipative systems:

When the system dissipates little and the number of collisions is large, the H theorem applies at least approximately at the local scale leading to a local convergence time which is short compared to the complete evolution time. In this case, the procedure to find f consists to apply a perturbation approach, starting from the Maxwellian unperturbed distribution. This is often used, for instance in the cases of electrons in metals, of the hydrodynamics of Newtonian fluids...

The reason why this approximation is valid in these cases comes from the great number of collisions that preserve energy; hence the system converges locally fast towards its local equilibrium. Then transport and dissipation occur together with the slow diffusion of heat.

310.2.4. The case of very dissipative systems is likely different

However, when each collision dissipates energy, the system dissipates efficiently, and the problem changes likely of nature because the collision rules do not obey anymore the law of conservation of energy. The first consequence is probably that the equilibrium distribution f is no more Maxwellian, because this distribution requires that energy is preserved during collisions, *cf.* demonstration of Eq. (4). We give elsewhere an example when looking at the problem of few grains [Evesque 2004].

An other well-known effect caused by dissipation is the non-preservation of the elementary volume $dq dp$ in the phase space. This comes directly from the Liouville equation and the Hamilton equation of motion. That leads to concentrate the dynamics on attractors, which are periodic orbits, strange attractors...

Indeed many typical examples are given in textbooks with oscillators, leading to circular orbits and chaotic dynamics... Here we propose a simple example of the reduction of the phase space; it has been obtained when studying the dynamics of a single ball in a vibrating box to calibrate a force sensor. But the reduction is so efficient, i.e. from 11-d to 1d, that it makes an elegant toy example. The reduction of freedom degrees is driven by the coupling between translation and rotation that occurs during collisions. So it demonstrates the importance of rotations in granular gas mechanics.

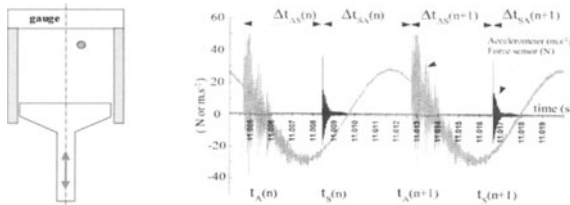


Figure. 1. A steady cell (length $L=10\text{mm}$, diameter $2R=13\text{ mm}$) contains a ball (diameter $d=2\pm 0.002\text{mm}$); the vibration of the piston can induce a periodic motion of the ball, in phase with the vibration. The knowledge of the collision times with the piston and with the gauge on top allows to measure the ball speeds and the restitution coefficient $v_{\text{out}}/v_{\text{in}}=-\epsilon$.

310.3. The case of a single ball in a container with a vibrating piston

The limit of a gas of non interacting particles can be studied when diminishing the density of the system, till the particles never meet. An other way is to reduce the dimension of the cell and to work with a very little number of particles. This is what is reported here. In this case one expects the system is connected to the problem of chaotic billiard. In 1d with no dissipation and in 0g, it becomes also the Fermi problem [Fermi 1949, Brahic 1971, Lichtenberg 1980]; or it is the bouncing ball case, in 1d under gravity and no top wall [Luck & Mehta 1993]. This 1-ball example in a vibrating box can also be used to test the effect of boundary conditions. Is the box playing the role of a velostat and imposes a definite mean speed [Evesque 2002]?

The cylindrical cell of Fig. 1 is fix in the lab frame; its bottom is vibrating ($z=b \cos(\omega t)$, $30\text{Hz} < f = \omega/(2\pi) < 120\text{Hz}$) and it is closed on top by an impact sensor to be

calibrated; it contains a sphere. An accelerometer is fixed to the piston, and measures $b\omega^2/g$ and $\omega/(2\pi)$. Its signal is perturbed by the impact of the ball with the piston, so that it allows measuring these times of impact t_{2n} and the position z_{2n} of the piston.

310.3.1. Determination of the restitution coefficient $\epsilon = -v_{out}/v_{in}$:

From the signals of Fig. 1 one can (i) determine the times t_{2n} & t_{2n+1} of impacts with the gauge and with the piston, (ii) measure the amplitude I_{2n} of impacts, (iii) compute the speeds v_{n+} and v_{n-} , before and after each impact n , (iv) calibrate I_{2n} vs. v_{2n} and determine $\epsilon_n = -v_{n+}/v_{n-}$ as a function of v_{n-} , for the gauge and for the piston. A typical example is given in Fig. 2 in the case of the sensor. Similar results are obtained with the piston. The experimental values of ϵ do not follow the law predicted by simulations aimed at mimicking granular gas in micro-g, i.e. the curve in Fig. 2.

More complete discussion about fluctuations amplitude and lack of perfect synchronisation are reported elsewhere [Evesque 2004].

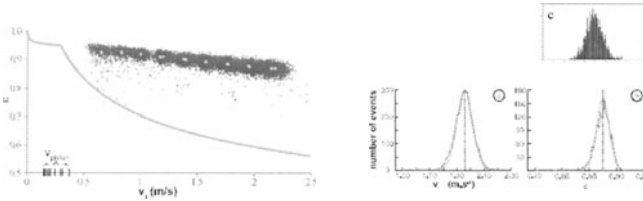


Figure. 2. Left: Variation of the restitution coefficient ϵ with the ball speed, for a 2mm diameter stainless steel sphere ($d=2.0 \pm 0.002\text{mm}$) hitting the sensor; the curve corresponds to predicted ϵ from simulations that try to mimic micro-g results without introducing ball rotation of [Falcon et al. 1999]. Right: Statistical distributions of the input velocity (a) of the ball with the sensor and of the restitution coefficient ϵ (b). The dotted curve corresponds to the Gaussian profile of same half-width at half-height. On top of (a) and (b), fig (c): normal dispersion on ϵ obtained from 1d simulation when adding some Gaussian noise on the measured time (the accuracy is 10^{-4} s on the piston and 10^{-5} s for the sensor). (from [Garrabos et al. 2004] except for fig. c which is from Cl. Ratier, G. Thoorens)

310.3.1. Effect of collisions on rotation and transverse motion:

One observes also the freezing of the transverse motion of the ball as soon as the ball hits the lid. This can not be seen from the sensor signals of Fig.1, but has to be observed optically either with the eyes or with a camera: performing the same experiment on earth at small enough amplitude (or without the lid), one sees the ball jumping from left to right erratically; but as soon as the ball starts hitting the top wall the vertical trajectory is stabilised and it evolves no more transversally. This demonstrates the freezing of the transverse degrees of freedom. We will show now that it demonstrates also the freezing of the rotation degrees of freedom.

The stabilisation of the vertical trajectory is due to the coupling between rotation and transverse motion during collisions. This coupling is a solid friction effect that acts on the ball to tend to impose a non sliding condition at the contact point during collision. Consider the case without a lid, sketched on Fig. 3: A transverse motion imposes some rotation after the first bounce; but the next bounce preserves the same ratio of lateral speed and rotation, so that the ball can keep on moving in the same

direction. With the lid, any transverse component of speed forces the ball to rotate in one direction, say spin +, at one wall but in the other direction, say spin -, at the opposite wall. This improves the dissipation and freezes rotation and transverse motion.

This effect can be generalised to ball-ball collisions in 2d or 3d: due to solid friction, and due to the fact that collision are non frontal, collision rules fix the ball spins at the end of each collision from the impact parameter at the beginning of the collision. Next collisions occur from other directions with different impact parameters so that an important part of spinning energy is lost during each collision. This effect is stronger in 3d than in 2d because the probability of frontal collision decreases with increasing the space dimension; and it does not exist in 1d. Hence one understands why dissipation looks quite large in 3d experiment on granular gas, much larger than in a 1d case. One expects approximately 40% energy-dissipation rate/collision.

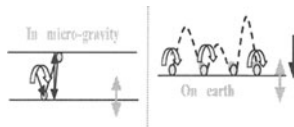


Figure. 3. Sketch of collisions with rotation with bottom and top walls (left), with only top wall (right)

It is rather strange that no simulation on granular gas or granular fluids has ever demonstrated and studied this effect, although this is essential to model correctly the physics of this system. In practice, until now (2004), most published simulations have just imposed some collision rules, nearly at random, in order to get a better fit with experimental data; very little introduce rotations, some introduce a tangent restitution coefficient instead [Goldhirsch, 2003]. Some others introduce a single speed-dependent normal restitution coefficient, just to fit the experimental results; this is the example given in Fig. 2, which is far to agree with the measured experimental points! So, simulations have not taken correctly care of this phenomenon.

The present effect is then a direct result of space research, even if it could have been obtained much more easily. This experiment points out also the effect of boundary conditions: indeed, the behaviour obtained in normal 1g condition without a lid (and in 3d) is different from the micro-g condition (which imposes to use a lid).

The effect of the lid is then to freeze a lot of degrees of freedom since the dimension of the phase space of this experiment passes from 11-d, (3 positions, 2 angles, 3 speeds, 2 rotation speeds and piston position), to 3-d (z , v_z and v_{piston}). Comparatively, resonance and periodic motion, which are observed in our experiments too, reduces the phase space much less: the synchronization links together the ball position z and the piston speed v_{piston} ; it relates also v_z and the impact times t_n to the length L of the box and to the period of the forcing; so the attractor becomes 1d instead of 3d. So, synchronization diminishes the space dimension from 3 to 1, *i.e.* 2 units, while the lid diminishes from 11d to 3d, *i.e.* 8 units!!

Reduction of dimensionality is classic in dissipative systems, as explained in books on chaotic strange attractors; however, it is peculiarly efficient in the present case. 3d simulations have been performed also with a Discrete Element code from Moreau and confirmed the experimental finding when friction is taken into account.

In classic billiard theory applied to statistical mechanics (which never takes account of rotation), the real shape of the cavity plays a significant role on the ergodicity/non-ergodicity of the problem. In particular, billiards having the shape of a sphere cap should not present stable orbits. It would be interesting to demonstrate that cavity with peculiar shape would result also in the destabilisation of the resonant trajectories, hence improving the ergodicity of the dynamics. In the same way, using non spherical particles, adding some important surface roughness or adding some hard convex fixed obstacles into the cavity should also improve the “quality of the ergodicity”. This is why perhaps the existence of a few balls, instead of a single one, may change the qualitative nature of the dynamics and force the problem of granular gas to be rather ergodic. However, this remains to be demonstrated.

At last, an other remarkable experimental result of the 1-ball experiment is that the speed v_z of the ball is always larger than the piston speed $b\omega$. In our terminology, it means a “subsonic” kind of excitation. The ratio $v_z/(b\omega)$ is much larger in the case of resonance than within erratic motion. This is in agreement with 1d simulations and theoretical description [Evesque 2001a]. This shows also that the “supersonic” excitation observed when a collection of beads fills the cell is linked to the dissipation due to ball-ball collision.

310.4. Conclusion

The physics of granular gas has been importantly investigated during these last 10-15 years, using many different approaches; the ones stand from a theoretical approach; some others from 2d and 3d experiments on earth and in weightlessness conditions; others use numerical simulations and confrontation between numerical calculation and experimental data.

But complete answers remain little in the literature at the moment. For instance if one is interested by the problem of simulations, one can get from the literature different procedures to simulate the gas of particles and its dissipation, starting with different collisions rules; one uses (i) simply a normal restitution coefficient, or (ii) two coefficients (a normal and a tangent restitution coefficient), while others (iii) include particle rotation, solid friction, But none of these works tend to define clearly the minimum ingredients to get the true limit behavior of a dissipative granular gas as it is encountered in experiments.

Here it is proved with the 1-ball experiment that accurate *ab initio* calculation shall contain ball rotation. Of course, one can still argue that 1d modeling is enough!

Gravity has to play an important role also, whose effect on granular gas behavior should gain to be clarified; indeed results in 1-g and in 0-g are often thought as equivalent, but the timescale and confinement are strongly affected by gravity. For instance the time scale of a bouncing varies as $t=v/g$ while it scales as L/v in 0-g; and the particles are confined on the bottom in 1g while confinement requires two

opposite walls in 0g. This asks the effect of boundary conditions: the presence of a second walls is crucial here; are lateral walls playing similar importance?,....

Here the 1d experiment demonstrates the major difference due to the second wall!

But the single ball system is not so well defined. For instance take the case of the 1d bouncing ball system in 1g without rotation: Theoretical study [Luck & Mehta 1993] leads to quasi-periodic orbits; but experiment finds complete chaos. Are rotation degrees of freedom involved in this change of behavior?

It is recalled in the present paper that Maxwellian distribution of gas speed is linked to the energy preservation rule which is far from being a characteristics of granular physics. In general it is considered that the moving box plays the role of a thermostat, but it is better described as a velostat, because it imposes the bead speed [Evesque 2002 & 2004].

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Chapter 13

The Nash Equilibrium Revisited: Chaos and Complexity Hidden in Simplicity

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The Nash Equilibrium is a much discussed, deceptively complex, method for the analysis of non-cooperative games (McLennan and Berg, 2005). If one reads many of the commonly available definitions the description of the Nash Equilibrium is deceptively simple in appearance. Modern research has discovered a number of new and important complex properties of the Nash Equilibrium, some of which remain as contemporary conundrums of extraordinary difficulty and complexity (Quint and Shubik, 1997). Among the recently discovered features which the Nash Equilibrium exhibits under various conditions are heteroclinic Hamiltonian dynamics, a very complex asymptotic structure in the context of two-player bi-matrix games and a number of computationally complex or computationally intractable features in other settings (Sato, Akiyama and Farmer, 2002). This paper reviews those findings and then suggests how they may inform various market prediction strategies.

1 Introduction

One of the particularly difficult aspects of the Nash Equilibrium is that the average economic practitioner, game theorist or other type of modeler is most likely to be familiar with a very truncated simplified version of John Nash's actual discovery. In business schools, for example, phrases like "a Nash equilibrium occurs whenever you have a strategy which cannot be dominated by any other strategy but which itself cannot dominate any other strategy".

In a scientific sense, all of these simplified conceptions, many of which are very useful heuristics or generalizations, really dance around the nature, structure and meaning of the Nash Equilibrium. While a detailed exploration of Nash's discovery is beyond the scope of the current paper, it is recommended that the interested reader download Nash's doctoral dissertation, "Non-Cooperative Games", which is the 28 page mathematical proof that constitutes the actual "Nash Equilibrium" (Nash, 1950). Additional simplified versions of greater or lesser complexity appear in various forms on the internet, such as the explanation given on Wikipedia.

Research on the Nash Equilibrium in its complete form is generally highly abstract and often involves a degree of complexity which makes that research rather daunting for anyone but the professional mathematician or mathematical economist. A good example of the complexity of research which has added valuable extensions to our knowledge of the Nash Equilibrium in a technical sense is the series of papers (in some sense competitive and in another sense incrementally building on the work of its predecessors) concerning asymptotic boundaries for Nash Equilibria in particular types of game-theoretic situations.

2 Asymptotic Boundaries for Nash Equilibria in Non-Cooperative Games

Quint and Shubik began their exploration of this element of the Nash Equilibrium in their 1997 paper, "A Bound on the Number of Nash Equilibria in a Coordination Game". Quint and Shubik's abstract states:

"We show that if y is an odd integer between 1 and $2n - 1$, there is an $n \times n$ bimatrix game with exactly y Nash equilibria (NE). We conjecture that this $2n - 1$ is a tight upper bound on the number of NE's in a "nondegenerate" $n \times n$ game. We prove the conjecture for $N \leq 3$, and provide bounds on the number of NE's in $m \times n$ nondegenerate games when $\min(m, n) \leq 4$." (Quint and Shubik, 1997).

For those not professionally familiar with this type of proof, the subject is made more accessible in the main body of the text, where Quint and Shubik further argue that:

In two-person game theory, perhaps the most important model is the so-called “strategic form” or “bi-matrix” game form of a game. The game is represented as a two-dimensional matrix, in which rows represent the (pure) strategies for one player and the columns those for the other. In each cell is placed a pair of numbers representing the payoffs to the two players if the corresponding pair of strategies is chosen. In the analysis of bi-matrix games, perhaps the most basic solution concept is that of Nash Equilibrium (NE). A pair of (mixed) strategies (p^*, q^*) is an NE provided the first player cannot do any better than to play p^* against the second player’s q^* , while likewise, the second player’s “best response” against p^* is q^* . In Nash’s seminal papers (1950, 1953), he proved that every bimatrix game has a NE mixed strategy.

Notice that this is a rather more precise definition of the concept of a strategy which cannot be dominated but which also cannot dominate other strategies in the game.

Quint and Shubik’s paper is important for a number of reasons. First, they provide a succinct explanation of the work done over the past fifty years on studying the Nash Equilibrium. In particular, they capture the essence of the problems inherent in defining the number of NE’s in a bi-matrix game. For those who have not followed this research, John Nash’s original work (1950) says that there has to be at least one “Nash Equilibrium” in such a game (Theorem 1, p. 5). In 1964, Lemke and Howson demonstrated that under a certain “nondegeneracy” assumption, the number of NE’s must be finite and odd (see also Sandholm et al.). Quint and Shubik note that this “oddness” property appears in various forms over the years, and then in 1993, Gul, Pearce and Stacchetti demonstrated that if a nondegenerate game has $2y-1$ NE’s, at most, y of them are pure strategy NE’s. Shapley argued as early as 1974 that in a 3×3 , non-degenerate game the maximum number of NE’s was seven, but provided no proof. Quint and Shubik also note that the situation is less clear for cases of $N > 3$. They argue that it is an open problem to fully characterize the numbers of NE that can occur and offer a partial solution in their 1997 paper.

3 Discovering New Nash Equilibria in Bimatrix Games

Perhaps the most interesting aspect of Quint and Shubik’s paper was that even while they were significantly extending knowledge about the Nash Equilibrium, they were too modest in their conjecture. Almost immediately following the Quint and Shubik paper, Bernhard von Stengel of the London School of Economics in a paper entitled “New lower bounds for the number of equilibria in bimatrix games” argued that: “A class of nondegenerate $n \times n$ bimatrix games is presented that have asymptotically more than $2^{1/4} n = p(n)$ Nash equilibria. These are more equilibria than the $2n - 1$ equilibria of the game where both players have the identity matrix as payoff matrix. This refutes the Quint-Shubik conjecture that the latter number is an upper bound on the number of equilibria of nondegenerate $n \times n$ games. The first counterexample is a 6×6 game with 75 equilibria...”

Subsequently, At the First World Congress of the Game Theory Society, von Stengel (2000) presented an improved computational method for finding the equilibria of two-player. His method was based on what he describes as the “sequence form of an extensive form game with perfect recall”. Von Stengel described this method as “improvements of computational methods for finding equilibria of two-player games in extensive form”, which was “based on the ‘sequence form’ of an extensive form game with perfect recall, a concept published by the author [von Stengel] in GEB in 1996, and in parts independently described by other authors (Romanovskii 1961, Selten 1988, Koller and Megiddo 1992).” The brunt of von Stengel’s presentation was to “show a number of results that demonstrate how to put this result into practice, in particular to achieve numerical stability.” This method, developed around algorithms for polytope computing, created algorithms which were capable of computing what von Stengel subsequently describes as “single equilibria that are (strategic-form) trembling-hand perfect and, for smaller games, allow for the complete enumeration of all equilibrium components.” From a purely computational point of view, this result is a very significant theoretical advance in the understanding and ability to calculate the complex structure of the Nash Equilibrium.

Credit for the final “blockbuster” on this subject shout go to Andrew McLennan and In-Uck Park, for their 1999 paper, “Generic 4×4 Two Person Games Have at Most 15 Nash Equilibria”. Here, the authors used an articulated cyclic polytope model to construct a series of lemmas that constrain the set of equilibria. Polytope computing, like quantum computing is one of the more powerful non-linear solutions which has been suggested for dealing with both this and other, recently discovered structural properties of the Nash Equilibrium which are, for contemporary, digital computing architectures, computationally intractable.

4 Non-Cooperative Meta-Games: The Rationality Trap

In a 2002 paper, Sato Yuzuru, Akiyama Eizo and J. Doyné Farmer present a novel view of the Nash equilibrium in the case of learning to play a simple, two player, rock-paper-scissors game. Their abstract argues rather modestly:

We investigate the problem of learning to play a generalized rock-paper-scissors game. Each player attempts to improve her average score by adjusting the frequency of the three possible responses. For the zero-sum case the learning process displays Hamiltonian chaos. The learning trajectory can be simple or complex, depending on initial conditions. For the non-zero-sum case it shows chaotic transients. This is the first demonstration of chaotic behavior for learning in a basic two person game. As we argue here, chaos provides an important self-consistency condition for determining when adaptive players will learn to behave as though they were fully rational.

While this sounds relatively straightforward, the actual constraints of rationality, whether the strong “instrumentally rational utility maximization” of neoclassical economics” or the more limited “bounded rationality” of neo-institutionalism and rational choice theory, have strong effects on the decision process and its end points. The pioneer in this field is, of course, W. Brian Arthur, developer of modern non-equilibrium economics. Without attempting to recapitulate this very large body of work, it is useful to look at a few key ways in which equilibrium assumptions about transactions, and strategies, when based on assumptions about the rationality of play on the part of the opposing players, encounter a great deal of difficulty. To the extent that these strategies (including strategies which attempt to find a Nash equilibrium) dictate one player’s choices by attempting to anticipate the choices or strategies of other players, they are not robust and their fragility can easily cause the entire game to become ill-defined (in economic terms this would be defined as “market failure”). As Arthur himself argues (1994):

The type of rationality we assume in economics--perfect, logical, deductive rationality--is extremely useful in generating solutions to theoretical problems. But it demands much of human behavior--much more in fact than it can usually deliver. If we were to imagine the vast collection of decision problems economic agents might conceivably deal with as a sea or an ocean, with the easier problems on top and more complicated ones at increasing depth, then deductive rationality would describe human behavior accurately only within a few feet of the surface. For example, the game Tic-Tac-Toe is simple, and we can readily find a perfectly rational, Minimax solution to it. But we do not find rational "solutions" at the depth of Checkers; and certainly not at the still modest depths of Chess and Go.

As a concrete example of how anticipatory strategies can rapidly degenerate, Arthur offers the following example:

There are two reasons for perfect or deductive rationality to break down under complication. The obvious one is that beyond a certain complicatedness, our logical apparatus ceases to cope--our rationality is bounded. The other is that in interactive situations of complication, agents can not rely upon the other agents they are dealing with to behave under perfect rationality, and so they are forced to guess their behavior. This lands them in a world of subjective beliefs, and subjective beliefs about subjective beliefs. Objective, well-defined, shared assumptions then cease to apply. In turn, rational, deductive reasoning--deriving a conclusion by perfect logical processes from well-defined premises--itself cannot apply. The problem becomes ill-defined.

Two classic examples of his kind of strategic mis-fire which are particularly interesting are Arthur’s “El Farol Bar Game”, and Epstein and Hammond’s (2002)

“line-up game” (for a more complete treatment of this problem see <http://necsi.org/events/iccs/openconf/author/papers/313.doc>). In these games, the El Farol Bar Game in particular (and its more computational cousin, the minority game) the structure is such that there is no equilibrium point which can mutually satisfy all players. This is not because the equilibrium is unattainable due to practical constraints but rather because in the manner described above, each player’s move changes the expectations and payoffs of the other players (a feedback loop not terribly dissimilar to some of Arthur’s path-dependent stochastic processes). In Epstein and Hammond’s “Non-explanatory Equilibria: An Extremely Simple Game With (Mostly) Unattainable Fixed Points” the equilibrium points of the game are so sparsely distributed (i.e., the phase space is so large) that even small increases in the number of players creates a solution basin of such high dimensionality that the problem becomes not just ill-defined but insoluble. Both of these cases involve complex structures where small, linear growth in one parameter drives exponential growth in another parameter, with that exponential growth often feeding back into the original iterative level of the process.

5 Chaos and Learning in a Simple Two-Player Game

To return to Sato, Farmer and Akiyama’s paper, their findings demonstrate that even a relatively simple game like rock-paper-scissors, may not, in fact, converge to the Nash equilibrium (which is the expectation for rational or instrumentally rational players). Given the problem of non-convergence, they argue that when players fail to learn the Nash equilibrium strategy in a multiple iteration or multiple generation game, it then becomes important to understand what the actual dynamics of the learning process in that situation are. For analytical purposes they treat the learning “trajectory” as the phase space representation of the degree to which player’s game choices (strategies and moves) either become asymptotic to the Nash equilibrium or fail to converge upon the Nash Equilibrium at all.

As we have discussed elsewhere and as the authors discuss in their paper at great length and full technical detail, the presence of the rationality meta-problem combined with the fact that, at least, in a typical zero-sum, mixed-strategy game like rock-paper-scissors, the fact that there is a conserved quantity (i.e., the payoff) leads to a Hamiltonian familiar from celestial mechanics. In this case the coupled replicator equations form a conservative system which cannot have an attractor. The implications of this relationship are profound. In the most critical case, the system becomes non-integrable and as chaotic trajectories extend deeper into the strategy space, regular and chaotic trajectories become so finely interwoven that there is a regular orbit arbitrarily close to any chaotic orbit. To exchange sides of the equation, computationally, as values of ϵ approach 0.5, any regular orbit is arbitrarily close to a chaotic orbit. Not only is this in certain very fundamental ways computationally intractable, but it makes a shambles of any predictive methodology for system trajectories.

6 Conclusion: The Complexity of Experience

If one follows Sato, Farmer and Akiyama's research in detail, one is confronted, in even this simple setting for the Nash equilibrium, with the full complexity of chaotic dynamics: heteroclinic orbits, Lyapunov spectra, conserved phase space across pairwise conjugate coordinates, and four dimensional simplexes. The question then becomes, what do we make of all this? Do we simply throw up our hands in frustration, or is there some insight from complex adaptive systems research which will allow use to make sense of the kinds of emergent behavior discovered by all of the foregoing researchers, and in some sense, within the context of this particular discussion, discovered originally by Nash himself (i.e., that the Nash equilibrium is an emergent property of an n -iteration, two-player, zero-sum game).

In recent years, a variety of quantitative techniques have been brought to bear on new Nash equilibrium problems (for a more complete treatment see <http://arxiv.org/ftp/arxiv/papers/0707/0707.0324.pdf>). Beginning with Eisert, Wilkins and Lewenstein's initial formulation of the quantum Nash equilibrium, followed by David Meyer's treatment, as well as those of Landsberg, Iqbal and Weigert, Flitney et al. and perhaps finishing with Cheon and Tsutsui's mapping of solvable quantum games on Hilbert space, it appears that quantum mechanics offers some remarkable tools, as well as some very complex answers, but answers nonetheless to these kinds of quandaries. In particular, quaternionic analysis, especially, the new form of quaternionic analysis developed by Peter Jaks, which distinguishes between left non-commutation and right non-commutation, offer especially hopeful and new solutions to these hitherto unexpected complexities in the Nash equilibrium. Similarly, quantum computing, which appears to be arriving far faster than originally predicted, offers the possibility of soon being able to compute problems which only recently were regarded as computationally intractable.

It may not be entirely comforting to realize that it is the nature of emergent phenomena to generate unanticipated outcomes and often unanticipatedly complex problems, even within the framework of complex adaptive systems research. However, one can also argue that it is a fundamental challenge of complexity science to develop novel approaches for solving such problems, particularly when it is an intrinsic characteristic of the problem that it cannot be anticipated in advance of new experimental or computational results.

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Chapter 14

Adaptation and Coevolution on an Emergent Global Competitive Landscape

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Notions of Darwinian selection have been implicit in economic theory for at least sixty years. Richard Nelson and Sidney Winter have argued that while evolutionary thinking was prevalent in prewar economics, the postwar Neoclassical school became almost entirely preoccupied with equilibrium conditions and their mathematical conditions. One of the problems with the economic interpretation of firm selection through competition has been a weak grasp on an incomplete scientific paradigm. As I.F. Price notes: "The biological metaphor has long lurked in the background of management theory largely because the message of 'survival of the fittest' (usually wrongly attributed to Charles Darwin rather than Herbert Spencer) provides a seemingly natural model for market competition (e.g. Alchian 1950, Merrell 1984, Henderson 1989, Moore 1993), without seriously challenging the underlying paradigms of what an organisation is." [1] In this paper we examine the application of dynamic fitness landscape models to economic theory, particularly the theory of technology substitution, drawing on recent work by Kauffman, Arthur, McKelvey, Nelson and Winter, and Windrum and Birchenhall. In particular we use Professor Post's early work with John Holland on the genetic algorithm to explain some of the key differences between static and dynamic approaches to economic modeling.

1 Introduction

The difficulty with the “Darwinian” biological metaphor is that in many cases, self-organization may exert a more powerful influence on evolution than selection. In other cases, change occurs not because of selection, but despite selection. In particular, through the use of a quantitative model of “fitness landscapes”, Kauffman is able to specify a number of evolutionary characteristics which are quite different than those of the Darwinist or Neo-Darwinist paradigm. The concept of coevolution on a dynamic fitness landscape is perhaps the most important from an economic point of view. As Kauffman explains: “Adaptive evolution occurs largely by the successive accumulation of minor variations in phenotype. The simple example of computer programs makes it clear that not all complex systems are graced with the property that a minor change in systemic structure typically leads to minor changes in system behavior. In short, as their internal structure is modified, some systems change behavior relatively smoothly and some relatively radically. Thus we confront the question of whether selective evolution is able to “tune” the structure of complex systems so that they evolve readily.” [2]

1.1 Adaptive Mechanics

The mechanism by which biological systems tune is the result of standard statistical mechanics, whereby ensembles move randomly through all phase spaces of the system over time. With respect to the random array of ensemble positions, we might think of economic or business systems which occupy nearby positions in a large market with many securities (a “densely packed” state space). Borrowing from random walk theory we could view the ability of a security to earn economic returns as the measure of its fitness. While this is a very simple metaphor it helps to tie the conceptual foundations of economics and finance to evolutionary biology in the sense that the elements of both systems can rest in peaks or valleys (in finance this would be equivalent to Jensen’s α , which represents the degree to which management (and by logical inference, corporate structure) either creates or destroys value in a firm. The peaks can be either local maxima or global maxima. In highly efficient markets stocks would reach their equilibrium prices rather rapidly and the fitness landscape would be highly correlated. In less efficient markets, for example markets like the long distance commodities trades we frequently see in international business, where there are significant information asymmetries and market inefficiencies, the landscape would tend to be “rugged” and multi-peaked. In such a situation, there are opportunities for large arbitrage (similar to the biologist’s “punctuated equilibrium”). In the context of a dynamic landscape where multiple entities interact and both their presence and their interactions affect the structure of the landscape.

2 Problems of the Standard Model

Two important points follow from Kauffman’s model. The first is the idea of *adaptation* that economic theories (particularly equilibrium-oriented theories which

model performance as the outcome of selection) often implicitly rest their theoretical structure upon. The standard economic model of adaptation creates an internally contradictory foundation for the economic phenomena it seeks to explain (for a more detailed treatment of this subject as well as extended references see [3]).

The second problem with the standard model is more technical and has to do with some of the formal mathematical properties of NK Boolean networks as well as with the mathematical limitations that coevolving populations impose on fitness landscapes. In this context, Kauffman's model treats adaptive evolution not merely as 'survival of the fittest', but rather as a complex, dynamical search process : [2]

Adaptive evolution is a search process—driven by mutation, recombination and selection—on fixed or deforming fitness landscapes. An adapting population flows over the landscape under these forces. The structure of such landscapes, smooth or rugged, governs both the evolvability of populations and the sustained fitness of their members. The structure of fitness landscapes inevitably imposes limitations on adaptive search. On smooth landscapes and a fixed population size and mutation rate, as the complexity of the entities under selection increases an error threshold is reached...the population "melts" from the adaptive peaks and flows across vast reaches of genotype space among near neutral mutants. Conversely on sufficiently rugged landscapes, the evolutionary process becomes trapped in very small regions of genotype space...the results of this chapter suffice to say that selection can be unable to avoid spontaneous order. The limitations on selection arise because of two inexorable complexity catastrophes...each arises where the other does not. One on rugged landscapes, trapping adaptive walks, the other on smooth landscapes where selection becomes too weak to hold adapting populations in small untypical regions of the space of possibilities. Between them, selection is sorely pressed to escape the typical features of the system on which it operates.

Kauffman's model leads to the prediction of two kinds of "complexity catastrophe". Type I catastrophes are the result of the fundamental structure of NK Boolean fitness landscapes. In a dynamic fitness landscape, as complexity increases, the heights of accessible peaks fall towards mean fitness. In terms of financial markets we might compare this to the fact that over long periods of time the β (a standard interpretation of *systematic* or market risk) of all stocks in the market has a tendency to drift towards a value of 1- the tendency of peaks to average out to small levels is equivalent to the tendency of securities to perform more or less identically to the market as a whole when viewed over long periods of time.

Kauffman's Type II complexity catastrophe is more complex and most closely resembles what Eric Smith and J. Doyne Farmer describes as "first order efficiency" in financial markets with very thin arbitrage margins for technical traders. To earn "extraordinary returns" traders are forced to undertake "wide searches", equivalent to highly leveraged positions [4]. A third type of complexity catastrophe is explained by Bill McKelvey, in the opening of one of his best known works, where he uses the

methodology of statistical mechanics to provide scalar values for Michael Porter's value chain in order to explain standard models of strategic positioning and microeconomic competition in a more rigorous scientific fashion than the standard model allows. [5]

The biologist Stuart Kauffman suggests a theory of complexity catastrophe offering universal principles explaining phenomena normally attributed to Darwinian natural selection theory. Kauffman's complexity theory seems to apply equally well to firms in coevolutionary pockets. Based on complexity theory, four kinds of complexity are identified. Kauffman's "NK[C] model" is positioned "at the edge of chaos" between complexity driven by "Newtonian" simple rules and rule driven deterministic chaos. Kauffman's insight, which is the basis of the findings in this paper, is that complexity is both a consequence and a cause. Multicoevolutionary complexity in firms is defined by moving natural selection processes inside firms and down to a "parts" level of analysis, in this instance Porter's value chain level, to focus on microstate activities by agents.

3 The Windrum-Birchenhall Model

Paul Windrum and Chris Birchenhall have developed another type of complex adaptive systems model for studying the dynamics of evolutionary economics using a computational simulation based on the performance of quasi-heterogeneous agents under conditions of both "normal" exchange and economic change caused by a technology shock. They explain their model (again for an extended mathematical treatment see [3]) as a "...simulation techniques on an agent-based model containing heterogeneous populations of adaptive users and suppliers that co-evolve over time. In the spirit of Nelson and Winter (1982), producers employ various adjustment rules to their production routines, while simultaneously innovating through a combination of imitation and internal R&D. Whereas Nelson and Winter modeled these using a replicator dynamic algorithm, the current paper employs a modified genetic algorithm in which imitation is conducted via a process of selective transfer (one-way crossover) and internal R&D is conducted via selective mutation." [6]

In a major advance over previous research, where many of the elements of the evolutionary mechanisms of economic change were "black boxed", Windrum and Birchenhall explain that "The key question addressed by the model is whether (a) the young consumer type will treat quality and installed user networks as substitutes and, hence, select the later technology (which is de facto assumed to be of higher quality) or (b) alternatively treat them as complements, in which case they will select the old technology."

In a very general sense, Windrum and Birchenhall account, for the first time, in with an explanation which maps the internal evolutionary dynamics for why, when new technologies enter the marketplace, in some cases (Type I technology shocks) all users switch to the new technology while in other cases (Type II technology shocks) some existing users retain the old technology while virtually all new users adopt the

new technology. This is a situation particularly common in the software industry as well as the broader computer and consumer electronics industries and we have addressed the details of this question ourselves at substantial length [7].

One of the more interesting results of the Windrum-Birchenhall study is that first mover advantages play a crucial role in technology substitution, but that they are “emergent” and not discernible below a certain threshold of market penetration, a point which is also made in earlier analysis by physicist turned economist Theodore Modis. [8] However, both the Windrum Birchenhall technology replacement model and the combinatorial market landscape approach suggest that markets and consumers need to be “tolerant” of new product entrants or new product categories if they expect to raise overall welfare, particularly if the expected mechanism of national prosperity is characterized as a “punctuated equilibrium”, the subject of much of Kauffman’s work as well as economic policy work by Masahiko Aoki [9]

4 Conclusion

The results of the foregoing models suggest that while new technologies may offer potentially high returns to scale and scope, the operating environment at the firm level needs to be flexible and capable of rapid adaptation in order to capture the gains which a high degree of innovation can provide.[10] In this sense, one might argue generically that in order to optimize returns, the organization must imitate the product. Michael Porter argues convincingly that for many industries, corporate strategy needs a time-line of a decade or more in order to establish a unique strategic position based on internal cross subsidization. However, in fields where the product life cycle runs from six to eighteen months (as it does in the case of microprocessors and many other high technology, high value-added products) a different kind of model than the traditional “five forces” or “value cluster” model may be required.

Moreover, the conventional neoclassical micro-economic model of technology, which draws its principles of the firm largely from the “Chicago School” of consumer oriented economics and its principles of market behavior largely from the “Austrian School” of economics, is generally insufficient for characterizing modern relationships between governmental regulation, the production functions of the firm and the emergent role of technology in markets. Indeed this kind of analysis is far better suited to treatments of relatively homogenous consumer preferences, which can then be aggregated as an overall welfare function, but which have decreasing relevance to modern markets where technology and aggregations or networks of technology play an increasing role in economic exchange and the generation of value.

On the other hand, the policy message of the non-linear models discussed above (primarily the NK fitness model, as applied through evolutionary walks on a hypercube of competitive product and state spaces as represented by replicator dynamics) argues that if government policy doesn’t support superior technologies and leading edge sectors, then the country’s entire technology base may ultimately be at risk in the long run. [11] This conclusion is a relatively strong rejection of the efficient market hypothesis, insofar as the empirical level demonstrates rather large

information asymmetries across buyers, sellers, consumers, producers and inventors in the area of new technology.

At the firm level, management in general and top management in particular, needs to exercise an especially sensitive degree of restraint before sidelining or dropping new technology products [8]. Another broad recommendation which comes out of this research is that to be competitive in future markets, large organizations, including large multinational corporations will need to become less hierarchical, less vertically integrated and to adopt more flexible organizational structures if they are to avoid becoming trapped on local fitness landscape maxima. In recent years, a new subfield of organizational behavior, perhaps best described as “organizational complexity” which focuses on just such problems.

Again, one of the most important conclusions of this group of researchers is that in the 21st century, organizations will need to decentralize and move away from more traditional divisional structures and hierarchical control if they are to survive on the emerging technology landscape. A number of new techniques have been designed to address this problem, including “simulated annealing”, “organizational patches” and NK fitness measures of organizational interconnectedness. Firms which cannot adapt their internal structure to the new dynamics of technological competition are not likely to prosper, nor indeed, even to survive in the turbulent years to come.

Appendix: Internal Structure of the Genetic Algorithm¹

One thing I found, well ahead of Koza and other researchers, through my experiments in 1975-1977, at the University of Massachusetts at Amherst, where I beta-tested John Holland's book "Complexity in Natural and Artificial Systems" by coding the Genetic Algorithm into APL and running evolution of software was as follows:

The evolving software must implicitly determine HOW rugged the fitness landscape is, and adapt its mutation rate, cross-over rate, and inversion rate accordingly. My insight beyond that notion was to explicitly add genes that set mutation rate, cross-over rate, and inversion rate right at the end of (as it turned out, location didn't much matter) the existing genes. That is, I put meta-variables which coded for parameters of the Genetic Algorithm itself in among the variables coded for the underlying evolving system.

I then ran the Genetic Algorithm with the extended "chromosomes" on landscapes of different ruggedness. As I'd hoped, the 3 types of mutation rates themselves evolved to good rates that fit the rates optimum for adaptation on that degree and style of ruggedness.

This proved, at least to my satisfaction, that the Genetic Algorithm was not only parallel as explicitly obvious, and parallel in its operation on the higher-dimensional superspace of possible gene-sequences, as Holland demonstrated (in his example where a binary string of 0-1 alleles was part of the subspace of trinary strings of 0-1-"don't care" so that spaces of dimension 2-to-the-power-of-N in which evolution occurred were faithfully sampling and implicitly evolving in superspaces of dimension 3-to-the-power-of-N, where N is the bit-length of the evolving "chromosome"), but parallel at yet a higher level, namely that the Genetic Algorithm worked at simultaneously evolving the parameters of its own operation in rugged landscapes while evolving the simulated organisms that had their fitness determined by that same landscape. My analogy was to "hypervariable" genes in the immune system.

With the infinitely greater computational power and speeds available today, this experiment should, in principle, be repeatable in a multi-generational context which should then allow for the testing of emergent order for global evaluation functions. Until now, evolutionary simulations have been based either on the genetic algorithm or similar structures or else using assumptions that finesse the questions of how global evaluation emerges at all and simply proceeds to use global criteria in a purely local environment.

¹ This appendix was prepared by Jonathan Vos Post, with the intention of clarifying both the mathematical sections of the longer version of this chapter, referenced in [3] as well as for the purpose of addressing the question of what controls the kernel rate, or speed of evolution in an emergent dynamical system, and what endogenous variables can encompass the relationship between local and global maxima on a dynamic fitness landscape, both topics of considerable interest and discussion at the 5th International Conference on Complex Systems.

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Chapter 15

Complex Dynamics of the Cardiac Rhythms

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Many biological systems which appear complex both in space and time and result still not understood, require new theoretical approaches for their nonlinear dynamics. In particular we focus here on the theoretical analysis of the underlying mechanisms of heart dynamics. This could clarify the (apparently) chaotic behavior of the normal heart-beat and especially the control of the bifurcations of dynamics arising in situations of disease. The principal target is to find a possible clear distinction between normal and pathological regimes. A discussion of Complex Ginzburg-Landau equation can give useful hints to this aim.

1.1 Introduction

Complex systems, as observed in Nature and modelled by mechanical or electrical approximations, manifest the property that their dynamics depends on many competing effects. Nevertheless a complex system is composed by many subsystems, so that there can be recognized more or less clearly, depending on the system itself, a hierarchy of structures over a wide range of time and/or length scales and the presence of some form of coherent structures. The description of such interrelated structures with reciprocal influence and peculiar individual behaviors requires mathematical models based on non linear equations. Spiral

waves are a form of self-organization observed in various excitable chemical and biological systems. In particular in heart pathologies such as arrhythmias and fibrillation, the wave of excitation are moving spirals in two dimensions and scroll waves on three dimensional domains. The simplest class of mathematical models generating spiral waves is of reaction-diffusion type. The study in two dimensions of the generation of stable and self-sustained spiral waves is believed to be a preliminary step towards the comprehension of the high-complexity of three dimensional patterns. In cardiac tissue models, the transmembrane voltage and the various gating variables "react" while the role of the diffusion is played by intercellular conductivity. Additional deformation and temperature variations effect can be included to enrich the modellization of the phenomenon (see as an example [1, 2, 3] and references therein). The article is organized as follows. In Sec. 1.2 considerations concerning features and behavior of the cardiac rhythms are presented. In Sec. 1.3, we focus on a phenomenological way to approach the study of travelling waves in an excitable media. In Sec. 1.4 we explain the importance of Landau-Ginzburg theory in physics. Finally in Sec. 1.5 some ideas are exposed in the context of field theory applied to excitable systems.

1.2 The Cardiac Rhythms

The heart is primarily composed of muscle tissue over which a network of nerve fibers coordinates the contraction and relaxation of the whole muscle tissue to obtain an efficient, wave-like pumping action. The sinuatrial node (SA) is the natural pacemaker for the heart. In the upper area of the right atrium, it sends the electrical impulse that triggers each heartbeat. The impulse spreads through the atria, prompting the cardiac muscle tissue to contract.

The impulse that originates from the SA node strikes the atrioventricular (AV) node which is situated in the lower portion of the right atrium. The AV node in turn sends an impulse through the nerve network to the ventricles, initiating then the same contraction of the ventricles.

The electrical network serving the ventricles leaves the atrioventricular node through the right and left bundle branches. These nerve fibers send impulses that cause the cardiac muscle tissue to contract. Even the simplest theoretical model shows the enormous complexity that can arise from periodic stimulation of non-linear oscillations. In fact many different effects can arise from the specific kinds of stimulations and responses. In principle there can be evident a periodic synchronized rhythm, in which appears some "regularity", but most frequently in biological systems one encounters: a) aperiodic rhythms (whose oscillation frequency is not measurable univocally); b) quasi-periodic rhythms (when two rhythms with different frequencies march through each other with little interaction) and c) the most general case of chaotic ones[4].

It is known that some features of normal heart rate (NHR) variability are related to chaotic dynamics. In this view, the long-range correlations in NHR serve as organizing principle for highly complex, nonlinear processes that generate fluctuations on a wide range of time scales involved in the cardiac rhythm.

In fact, the lack of a characteristic scale prevents excessive mode-locking that restrict the functional plasticity of the living system.

For instance in the case of fibrillation, the beating becomes highly regular, manifesting thus the breakdown of long-range correlations which were characterizing the multi-system interrelation. This fact has to be interpreted as the emergence of a dominant frequency mode leading to a highly periodic behavior, so that rather than being a chaotic process, cardiac fibrillation involves an unexpected amount of spatial and temporal patterning and order [5, 6].

1.3 Waves in Excitable Media.

A phenomenological way to approach the evolution of the cardiac muscle lies in the direct study of travelling waves in an excitable media (as the heart tissue has to be considered) and in finding models in order to mimic such excitable media as systems in which a wave propagates. The complexity of the signals which are involved in any heart-beat has lead to inquire about the effect of a very general kind of wave propagating over the heart. It has been shown that spiral waves provide one of the most striking examples of pattern formation in nonlinear active media and have attracted attention since their description in the Belousov-Zhabotinsky (BZ) chemical reaction medium (see Ref.[7] for an experimental survey). Successively they have been described in many other systems and models, coming soon under study for what regards the cardiac activity, being of potentially vital interest, as they underly some lethal pathologies. The construction of models for complex systems spatially extended requires also to take care of the strong irregularity which is found both in space and time for a complex dynamical systems such as heart tissue. Depending on the scales considered, in the fibers' detail or in the whole heart as for few milliseconds (chemical chain reactions) up to minutes and days (typical duration of global rhythmic analysis), new behaviors are always found. In Figure 1, as an example, we present a typical regime present in mathematical models of cardiac tissues, specifically Aliev-Panfilov one (see Ref. [3] for details). To this purpose, the identification of the dynamical degrees of freedom and the instability mechanisms leading to disorder are of great importance.

1.4 Landau-Ginzburg equations

Analogies between bifurcations in dynamical regimes of complex systems and the phenomenology of phase transitions suggest to investigate more deeply the reasons of interest for the Landau-Ginzburg equation in the context of the heart dynamics. Usually LG formulation is introduced in field theory in the context of the ferromagnetic systems of statistical mechanics [8, 9].

In the microscopic scale, one typically starts the discussion presenting an Ising-like ferromagnetic system described by a certain d -dimensional lattice with an attractive, translation invariant, short range two body interaction. The spin

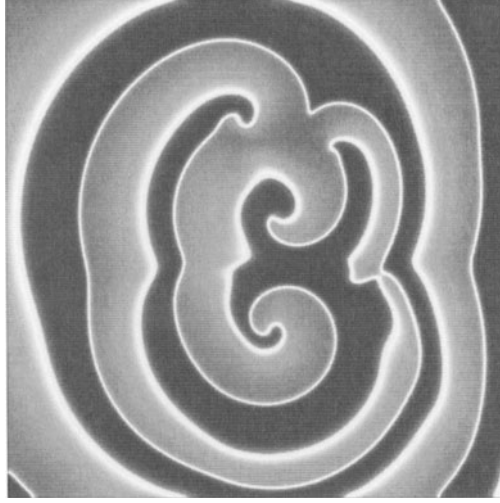


Figure 1.1: Spiral waves in Aliev-Panfilov ionic model of cardiac activity.

variable on the i -th site is defined as S_i , with the additional symmetry $S \rightarrow -S$. Defining $\mathcal{H}$ as the energy of a spin configuration, $d\rho(S)$ the one spin configuration which weights the spin configuration at each site, we can define a partition function whose energy will be given by

$$\mathcal{H}(S) = - \sum_{ij} V_{ij} S_i S_j - \sum_i H_i S_i. \quad (1.1)$$

The first term couples the various spins, and the second one instead represents the coupling with an external magnetic field H whose application will favor or not one of the possible states of magnetization. In particular, if we require a short range ferromagnetic interaction with two possible states of magnetization only (up and down), and we choose $d = 3$, we can approximate the theory close to the phase transition (at temperature $T = T_C$) with a spin density $s(\vec{x})$ whose integral furnishes the magnetization M , i.e. $M = \int d^3x s(\vec{x})$. The dynamics is entirely codified in the Gibbs free energy

$$\int d^3x \left[\frac{1}{2} (\nabla s)^2 + V(s) - Hs \right], \quad V(s) = b(T - T_C)s^2 + cs^4 \quad (1.2)$$

where $b > 0, c > 0$ and H is again the external magnetic field. The variation of G furnishes the well know (real) LG equation

$$-\nabla^2 s + 2b(T - T_C)s + 4cs^3 - H(\vec{x}) = 0. \quad (1.3)$$

We point out that, depending by the fact that $T > T_C$ or $T < T_C$, the potential $V(s)$ has completely different behaviors, manifesting a phase transition. Above

the critical temperature $T > T_C$, the non linear partial derivative equation is approximated by the linear one because the macroscopic magnetization must vanish, i.e.

$$-\nabla^2 s + 2b(T - T_C)s = H(\vec{x}). \quad (1.4)$$

We assume to turn the magnetic field in a point, i.e. $H(\vec{x}) = H_0 \delta^{(3)}(\vec{x})$ and we compute the Green function (zero field spin-spin correlation function)

$$D(\vec{x}) = \langle s(\vec{x})s(\vec{0}) \rangle = \frac{H_0}{4\pi r} e^{-r/\xi}, \quad \xi = [2b(T - T_C)]^{-1/2}. \quad (1.5)$$

The quantity ξ is known as the correlation length (the range of correlated spin fluctuations) which becomes infinite on the transition temperature. If one wants to improve these results, it is necessary to adopt the methods of Euclidean quantum field theory. Clearly there will be additional counter-terms which will furnish a more complicated effective equation than the LG one. In general, adopting such theoretical framework, one will obtain that every computed physical quantity will be related to the phase transition by certain power laws (critical exponents) which result more precise than the one computed using the standard LG theory. For the magnetization for example one will have $M \propto (T_C - T)^\beta$. The interesting result will be that these indices will take a fixed value for all systems in a given universality class. For both single-axis magnets and for fluids $\beta = 0.313$ for example. This is the universality in the critical exponents, which links totally (apparently) different systems using a unique theory. We stress that the reason why such a miraculous thing happens is because the basic idea of the LG theory is that the Gibbs energy of the different physical system can be always expanded in powers of an order parameter (in our ferromagnetic case this is the temperature) [8, 9]. One could generalize the previous discussion introducing a temporal dependence on the equations and requiring complex quantities¹, tending in this way to problems typical of non equilibrium statistical mechanics. In this case one obtains the complex Landau-Ginzburg equation (CGLE)

$$\partial_t A = \mu A - (1 + i\alpha)|A|^2 A + (1 + i\beta)\nabla^2 A, \quad (1.6)$$

which describes, skipping here the discussion on the complicated theories leading to this result (see Kuramoto's monograph[10] for an exhaustive discussion), a large quantity of phenomena ranging from nonlinear waves to second-order phase transitions, from superconductivity, superfluidity, and Bose-Einstein condensation to liquid crystals. In cylindrical coordinates, imposing $A = R(r)e^{i\omega t + im\phi + ikz}$ one gets a complex ordinary differential equation for the quantity R . Studying this ODE one can have a clear understanding of some features of spirals[10]. The study of "wave-like solutions" for this equation shows the existence of a characteristic frequency ω_0 which manifests an Hopf bifurcation between two different regimes (a detailed of this and other technical points can be found in ref. [11]). Very general spiral waves solutions of CGLE in oscillatory

¹In Quantum Mechanics as an example one handles complex quantities (the wave function as an example) so important in condensed matter physics.

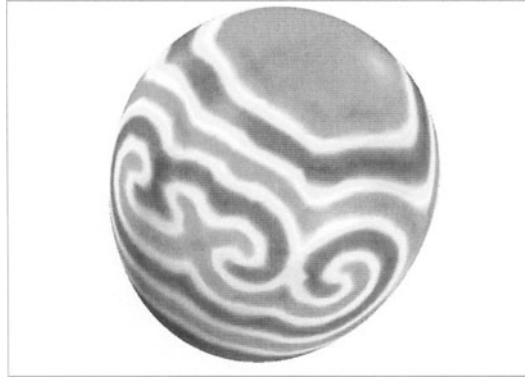


Figure 1.2: Spiral waves in CGLE equation in three dimensions.

media under the effect of inhomogeneity are well studied too[12], taking advantage of the many symmetries underlying this equation. In Figure 2 we present a typical pattern of spirals waves in 3D CGLE equation.

1.5 Field Theory and Heart.

The previous section concerning the Landau-Ginzburg theory suggests some speculations concerning the possible role of field theory ideas in cardiac dynamics:

- The Ising-like structure is quite similar to a cellular automaton in which instead on the magnetizations $\uparrow\downarrow$, there will be two or more different states for the heart cells, i.e. polarized/depolarized.
- We expect that in analogy with the statistical mechanics one could perform the evolution of the model using tools of Field Theory. This is what commonly happens in computational cardiology implementing cellular automata, although a field theory point of view seems to be still absent in the literature, clearly due to the fact that the phenomenon is very complicated.
- In this context one could try to used analog experimental models less complicated than real biological ones. In relation with the previous points, it is well known that a macroscopic non-linear electric circuit can be a model of the heart dynamics. A network of many small non-linear similar electric circuits in interaction could be an approximation of the realistic lattice of

polarizing-depolarizing cells of the exact statistical models. Modern engineering has many tools to simulate this type dynamics both on a computer as well as in a real electronic environment: we think as an example at the chips running *in hardware* the reaction-diffusion equations[13]

It would be a striking result to show that the universality classes of the phase transitions could be extended to biological models too, manifesting in an elegant way the simplicity of Nature.

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Chapter 16

The Ecological Ideal Free Distribution and Distributed Networked Control Systems

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In this paper we first establish an analogy where we view both animals and vehicles as generic agents. We introduce a model of the ecological behavior of a group of agents and establish sufficient conditions for the group to achieve an ideal free distribution (IFD), even when we lift some of the “ideal” and “free” assumptions. Finally, we apply this model to cooperative vehicle control problems and present simulation results that show the benefits of an IFD-based distributed decision-making strategy.

1.1 Introduction

The ideal free distribution concept from ecology characterizes how animals optimally distribute themselves across habitats. The word “ideal” refers to the assumption that animals have perfect sensing capabilities for determining habitat quality. “Free” indicates that they can move from any habitat directly to any other habitat at any time. If an animal perceives one habitat as “better,” via some correlate of fitness such as rate of arrival of nutrients, it will move to

¹This work was supported by the AFRL/VA and AFOSR Collaborative Center of Control Science (Grant F33615-01-2-3154).

it. This movement will, however, reduce the new habitat's desirability, both to itself and other animals in that habitat. The IFD is the equilibrium distribution where all animals achieve equal fitness. This concept was first introduced by Fretwell and Lucas in [4] and independently by Parker in [10].

Many extensions of the IFD have been developed [17]. An important extension to the model takes into account that individuals differ in competitive ability, like in [11],[15]. There, the authors consider different types of interaction between individuals (e.g., unequal competitors and kleptoparasitism), and the modified IFD models predict that individuals should distribute themselves so that the distribution of their competitive abilities matches the quality of the resource sites. Other work that focuses on competitiveness can be found in [8],[16]. The author in [16] introduces the concept of interference as the direct effect caused by the presence of several competitors in the same patch. In [2],[9] the authors discuss the concept of travel cost in IFD models. In [6] the authors consider how the cost of traveling between resource sites might diminish the expected benefits of moving to another site. Other models have incorporated resource dynamics, like in [7],[17]. In [1] the author lifts the ideal assumption and studies the consequences of perceptual constraints on the distribution of individuals. Finally, note that the author in [13] shows that the ideal free distribution is an evolutionary stable strategy (ESS).

The IFD model we introduce here is represented by a directed graph. We build a generic terminology for IFD concepts around this graph, one that is appropriate for biology and engineering. We refer to habitats, food sources, resource sites, etc. as nodes and assume that there are N nodes in the environment. Each node is characterized by its quality, which represents how profitable or suitable the node appears to any agent. Let a directed arc between two nodes represent the travel path for an agent moving from one node to another. The graph topology defines the graph's interconnections between nodes via arcs. It represents which other nodes (habitats) an agent can sense at each node (i.e., "perceptual constraints"), and travel constraints that dictate which nodes (habitats) can be traveled to from a given node (habitat). Hence, the graph topology allows us to represent removal of both the ideal and free restriction to the original IFD model. We assume that each node has a continuous input of tasks that need to be performed by the agents. In biology, tasks could represent animals gathering nutrients, shelter, or mates.

Our model focuses on the agents' motion dynamics across the graph that drive the behavior of the group as a whole. We show how an "invariant set" can represent the IFD. We then use Lyapunov stability analysis of this invariant set to illustrate that there is a wide class of agent strategies (i.e., "proximate" decision-making mechanisms), and resulting agent movement trajectories across nodes (habitats), that still achieve the desired distribution. The results extend the existing theory of the IFD by showing the impact of a class of perceptual constraints, travel constraints, movement trajectories, and animal strategies on achievement of the distribution.

We then apply the IFD model to cooperative vehicle control problems where

there are spatially-distributed tasks which we associate to different regions [3]. We refer to these regions as nodes. Again, we assume that there is a continuous input of tasks to the nodes that need to be processed, and arcs between nodes represent the travel path of vehicles. Tasks represent targets that “pop up” in different regions. By implementing an IFD based strategy we can guarantee that the number of targets in each region stays within an invariant set. While related problems on cooperative control of vehicles to cope with pop up targets have been studied [14],[5] ours is a new formulation for task arrivals and we conduct a stability analysis of the overall behavior of the system. Finally, via simulations we show how a group of autonomous vehicles using such a strategy achieves an IFD-like distribution.

1.2 Stability Analysis

We mathematically quantify the quality of node i via a function defined as

$$S_i = f_i(x_i) \quad (1.1)$$

All parameters that the function f_i depends on will be stored in x_i . Here, we assume $x_i \geq 0$ is a scalar that represents the agent density at node i . Hence, each node i is associated with an area which we denote by A_i . We also assume that f_i is a strictly decreasing positive function. For convenience, we assume that the nodes are numbered so that $f_1(0) \geq f_2(0) \geq \dots \geq f_N(0)$.

We will consider a general network topology to model interconnections between nodes. The nodes, $H = \{1, 2, \dots, N\}$, are all connected to a network which defines if agents can move from one node to another. The network of nodes is described by a directed graph, (H, A) , where $A \subset H \times H$. For every $i \in H$, there must exist $(i, j) \in A$ in order to assure that every node is connected to the network, and if $(i, j) \in A$ then $(j, i) \in A$. An agent at node i can only move to node j if $(i, j) \in A$. If $(i, j) \in A$, then $i \neq j$.

1.2.1 Continuous Case

We use the discrete event system modeling methodology from [12]. Let $\mathcal{X} = \mathbb{R}^N$ be the set of states. Let $x(k) = [x_1(k), x_2(k), \dots, x_N(k)]^\top \in \mathcal{X}$ be the state vector, with $x_i(k)$ the density of agents in node i at time $k \geq 0$. Let $\mathcal{E}$ be a set of events which we define next. Let $e_{\alpha(i)}^{i,p(i)}$ represent the event that possibly multiple agents from node $i \in H$ move to *neighboring* nodes $m \in p(i)$, where $p(i) = \{j : (i, j) \in A\}$. Let the list $\alpha(i) = (\alpha_j(i), \alpha_{j'}(i), \dots, \alpha_{j''}(i))$ such that $j < j' < \dots < j''$ and $j, j', \dots, j'' \in p(i)$ and $\alpha_j \geq 0$ for all $j \in p(i)$; the size of the list $\alpha(i)$ is $|p(i)|$. For convenience, we will denote this list by $\alpha(i) = (\alpha_j(i) : j \in p(i))$. Let $\alpha_m(i)$ denote the number of agents that move from node $i \in H$ to node $m \in p(i)$. Let $\{e_{\alpha(i)}^{i,p(i)}\}$ denote the set of all possible combinations how agents can move between nodes. Let the set of events be described by $\mathcal{E} = \mathcal{P}(\{e_{\alpha(i)}^{i,p(i)}\}) - \{\emptyset\}$ ($\mathcal{P}(Q)$ denotes the power set of the set Q).

Notice that each event $e(k) \in \mathcal{E}$ is defined as a set, with each element of $e(k)$ representing the transition of possibly multiple agents from some node $i \in H$ to neighboring nodes in the network. An event, e , may only occur if it is in the set defined by the enable function, $g : \mathcal{X} \rightarrow \mathcal{P}(\mathcal{E}) - \{\emptyset\}$. State transitions are defined by the operators $f_e : \mathcal{X} \rightarrow \mathcal{X}$, where $e \in \mathcal{E}$.

Let $\gamma_{ij} \in (0, 1)$ for $(i, j) \in A$ represent the proportion of imbalance in nodes' quality that is *sometimes* guaranteed to be reduced when agents move from node i to node j . We now specify g and f_e for $e(k) \in g(x(k))$:

- Event $e(k) \in g(x(k))$ if both (a) and (b) below hold:

(a) For all $e_{\alpha(i)}^{i,p(i)} \in e(k)$, where $\alpha(i) = (\alpha_j(i) : j \in p(i))$ it is the case that:

- (i) $\alpha_j(i) = 0$ if $f_i(x_i) \geq f_j(x_j)$, where $j \in p(i)$,
- (ii) $0 \leq f_i \left(x_i - \sum_{m \in p(i)} \frac{\alpha_m(i)}{A_i} \right) \leq f_j \left(x_j + \frac{\alpha_j(i)}{A_j} \right)$, for all $j \in p(i)$, such that $f_i(x_i) < f_j(x_j)$, and
- (iii) $f_{j^*} \left(x_{j^*} + \frac{\alpha_{j^*}(i)}{A_{j^*}} \right) \leq f_{j^*}(x_{j^*}) - \gamma_{ij^*}(f_{j^*}(x_{j^*}) - f_i(x_i))$
for some $j^* \in \{j : f_j(x_j) \geq f_m(x_m), \text{ for all } m \in p(i)\}$.

Condition (i) prevents agents from moving from node i to node j if the quality of node i is higher than the quality of node j . Condition (ii) implies that after agents move from node i to other nodes, the quality of node i due to some agents leaving does not exceed the node with best quality before agents started moving. Condition (iii) implies that if the quality of node i differs from any of its neighboring nodes by more than M , so that some agents move from that node to another, then some agents must move to the node with best quality. Note that condition (iii) lifts to a certain extent the “ideal” IFD assumption stated above, since it allows some agents to move to nodes that do not necessarily correspond to a best quality choice, as long as at least one individual does.

- (b) If $e_{\alpha(i)}^{i,p(i)} \in e(k)$, where $\alpha(i) = (\alpha_j(i) : j \in p(i))$, then $e_{\delta(i)}^{i,p(i)} \notin e(k)$, where $\delta(i) = (\delta_j(i) : j \in p(i))$ if $\alpha_j(i) \neq \delta_j(i)$ for some $j \in p(i)$. Hence, in each valid event $e(k)$, there must be a consistent definition of agents moving from any node i to any other node j , $\alpha_j(i)$.

- If $e(k) \in g(x(k))$ and $e_{\alpha(i)}^{i,p(i)} \in e(k)$, then $f_{e(k)}(x(k)) = x(k+1)$, where

$$x_i(k+1) = x_i(k) - \frac{1}{A_i} \sum_{\{j : j \in p(i)\}} \alpha_j(i) + \frac{1}{A_i} \sum_{\{j : i \in p(j), e_{\alpha(j)}^{j,p(j)} \in e(k)\}} \alpha_i(j).$$

The density of agents in node i at time $k + 1$, $x_i(k + 1)$, is the density of agents at node i at time k , minus the total number of agents leaving node i at time k over the area of node i , plus the total number of agents reaching node i at time k over the area of node i .

Let $E_v \subset \mathcal{E}^{\mathbb{N}}$ (the set of all sequences of events) be the set of valid event trajectories (i.e., ones that are physically possible). We must further specify the sets of “allowed” event trajectories. Define a *partial event of type i* to represent the movement of $\alpha(i)$ agents from node $i \in H$ to its neighbors $p(i)$. A partial event of type i will be denoted by $e^{i,p(i)}$ and the occurrence of $e^{i,p(i)}$ indicates that some agents located over node $i \in H$ attempt to further move to other nodes. Event $e(k) \in g(x(k))$ is composed of a set of partial events. Next, we define two possibilities for the allowed event trajectories E_a : (i) for $E_i \subset E_v$, assume that each type of partial event occurs infinitely often on each $E \in E_i$, and (ii) for $E_B \subset E_v$, assume that there exists $B > 0$, such that for every event trajectory $E \in E_B$, in every substring $e_{k'}, e_{k'+1}, e_{k'+2}, \dots, e_{k'+(B-1)}$ of E there is the occurrence of every type of partial event (i.e. for every $i \in H$ partial event $e^{i,p(i)} \in e(k)$, for some $k, k' \leq k \leq k' + B - 1$). Clearly,

$$\begin{aligned} \mathcal{X}_b = \{ & x(k) \in \mathcal{X} : f_i(x_i) = f_j(x_j), \text{ for all } (i, j) \in A \text{ such that } i, j \leq N_I \\ & \text{for some } N_I \in \mathbb{N} \text{ and } f_\ell(x_\ell) = f_\ell(0) \text{ for all } \ell, N_I < \ell \leq N \} \end{aligned}$$

is an invariant set that represents a distribution of agents x_i such that the resulting quality at N_I nodes is the same. It represents an IFD distribution since $S_1 = \dots = S_i = S_{i+1} = \dots = S_{N_I}$. The remaining $N - N_I$ nodes have relatively low quality in the sense that no agent at node i , $1 \leq i \leq N_I$, can move to a better quality node j , $N_I \leq j \leq N$, even if it were the only agent at node j . Hence, as $t \rightarrow \infty$ no agents will be at $N_I, \dots, N$. If all nodes are occupied when an IFD distribution is achieved, then $N_I = N$. Notice that the only $e(k) \in g(x(k))$, when $x(k) \in \mathcal{X}_b$, are ones such that all $e_{\alpha(i)}^{i,p(i)} \in e(k)$ have $\alpha(i) = (0, 0, \dots, 0)$.

Theorem 1 Given (H, A) and conditions $a(i) - a(iii)$, the invariant set $\mathcal{X}_b$ is exponentially stable in the large with respect to E_B .

Note that: (i) it is necessary that agents located at node i not only have knowledge of x_j , but also know f_j for all $j \in p(i)$, (ii) if in the statement of Theorem 1 you replace E_B with E_i , $\mathcal{X}_b$ is asymptotically stable in the large with respect to E_i and (iii) Theorem 1 and 2 are an extension of the load balancing theorems in [12] for the case when the virtual load is a nonlinear function of the state. Contact the authors for the proof.

1.2.2 Discrete Case

Originally, the IFD was introduced as in the previous section as a density-dependent model, so that S_i represented a continuous function [4]. Here, however, we use a discrete model by letting S_i be a discrete function. We define the

agent density of node i , x_i , to be a discrete variable, so the quality function associated with node i is also discrete (i.e., quantized). Consequently, the quality levels in the system are partitioned into blocks. The largest block in the network has size $M > 0$, and the smallest block in the network has size m , $M \geq m > 0$. In contrast to the continuous IFD where $S_1 = \dots = S_i = S_{i+1} = \dots = S_{N_I}$, the best we can generally hope to do with only local information in the discrete IFD is to balance each node to node connection to within M . In other words, we can guarantee that $|S_i - S_j| < M$ for all $(i, j) \in A$ and $i, j \leq N_I$. Note that the value of M depends on the quality functions of the nodes. Moreover, M also depends on the competitive capabilities of the agents.

Next, we specify g and $f_{e(k)}$ for $e(k) \in g(x(k))$:

- Event $e(k) \in g(x(k))$ if both (a) and (b) below hold:

(a) For all $e_{\alpha(i)}^{i,p(i)} \in e(k)$, where $\alpha(i) = (\alpha_j(i) : j \in p(i))$:

- (i) $\alpha_j(i) = 0$ if $|f_j(x_j) - f_i(x_i)| \leq M$, where $j \in p(i)$,
- (ii) $f_i \left(x_i - \sum_{m \in p(i)} \alpha_m(i) \right) < \max_j \{f_j(x_j) : j \in p(i)\}$
- (iii) If $\alpha_j(i) > 0$, for some $j \in p(i)$, then $\alpha_{j^*}(i) \geq m$,
for some $j^* \in \{j : f_j(x_j) \geq f_m(x_m) \text{ for all } m \in p(i)\}$.

Condition (i) prevents agents from moving from node i to node j if the profitability of both nodes differ by less than M . Condition (ii) implies that after agents move from node i to other nodes, the benefit for node i due to some agents leaving, does not exceed the most profitable node before agents started moving. Condition (iii) implies that if the quality of node i differs by more than M with some of its neighboring nodes, then at least one agent must move to the node with highest quality.

- (b) For each valid event $e(k)$, there must be a consistent definition of agents moving between nodes as in the continuous case.

Note that $f_{e(k)}(x(k)) = x(k+1)$ is also defined as in the continuous case. The invariant set of interest in this case is

$$\begin{aligned} \mathcal{X}_d = \{ & x(k) \in \mathcal{X} : |f_i(x_i) - f_j(x_j)| \leq M, \text{ for all } (i, j) \in A \text{ such that } i, j \leq N_I \\ & \text{for some } N_I \in \mathbb{N} \text{ and } f_\ell(x_\ell) = f_\ell(0) \text{ for all } \ell, N_I < \ell \leq N \} \end{aligned}$$

Theorem 2: Given (H, A) and conditions (a) – (iii), the invariant set $\mathcal{X}_d$ is exponentially stable in the large with respect to E_B .

1.3 Application: Cooperative Vehicle Control

Here we assume a fully connected topology and that vehicles travel at a constant velocity. We also assume that vehicles have complete knowledge about the loca-

tion of all targets in every region and the rate at which targets appear (e.g., the corresponding task arrival rate for each region). We compare a strategy where agents pursue the region with the highest number of targets (see Figure 1.1) to a strategy based on conditions $a(i) - a(iii)$ (see Figure 1.2). The cooperative IFD based strategy allocates vehicles so that the total number of targets per region is close to each other for all four regions.

The rate at which vehicles reach targets (e.g., the task completion rate) depends on the number of vehicles available for a mission, their turn radii, and their velocity. For the plots we show here, we use an overall task arrival rate which is larger than the overall rate at which tasks are completed. Therefore, in this case targets accumulate during the mission. On the other hand, if vehicles travel fast enough so that their task completion rate is larger than the rate at which tasks arrive, then the number of tasks decreases to zero. If we assume that vehicles can change velocity during the mission, the simulation results suggest that there is an optimal speed to complete the mission in the sense that vehicles should not travel too fast in order to minimize fuel consumption, but fast enough to “keep up” with the arrival rate of tasks. For this case, the invariant set remains constant.

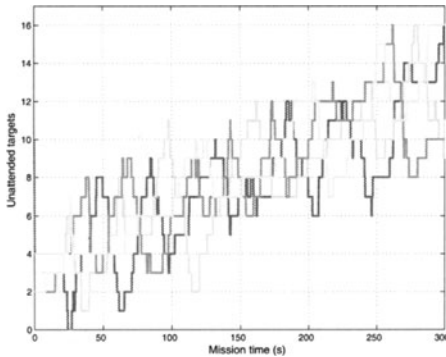


Figure 1.1: Node dynamics when agents pursue the node with highest quality.

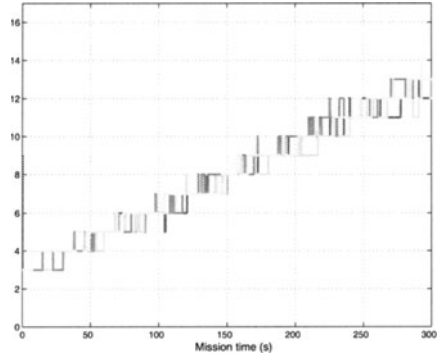


Figure 1.2: Node dynamics when agents satisfy conditions $a(i) - a(iii)$.

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Chapter 17

Protocol Requirements for Self-organizing Artifacts: Towards an Ambient Intelligence

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We discuss¹ which properties common-use artifacts should have to collaborate without human intervention. We conceive how devices, such as mobile phones, PDAs, and home appliances, could be seamlessly integrated to provide an “ambient intelligence” that responds to the user’s desires without requiring explicit programming or commands. While the hardware and software technology to build such systems already exists, as yet there is no standard protocol that can learn new meanings. We propose the first steps in the development of such a protocol, which would need to be adaptive, extensible, and open to the community, while promoting self-organization. We argue that devices, interacting through “game-like” moves, can learn to agree about how to communicate, with whom to cooperate, and how to delegate and coordinate specialized tasks. Thus, they may evolve a distributed cognition or collective intelligence capable of tackling complex tasks.

¹An extended version of this paper can be found at <http://uk.arxiv.org/abs/nlin.AO/0404004>. Related work can be found in [4]

1.1 A Scenario

The diversity and capabilities of devices we use at home, school, or work, are increasing constantly. The functions of different devices often overlap (e.g. a portable computer and a mobile phone have agendas; a radio-clock and a PDA have alarms), but most often we cannot combine their capabilities automatically (e.g. the PDA cannot tell the radio to set its alarm for the early Tuesday's appointment), and users need to repeat the same tasks for different devices (e.g. setting up an address book in different devices). Moreover, using the functionality of some devices in combination with others would be convenient (e.g. if my computer has an Intelligent User Interface, I would like to use it to ask for coffee, without the need of having speech recognition in the coffee machine: The computer should be able to ask the coffee machine for cappuccino).

Could we build devices so that they would *automatically coordinate*, combining their functions, and possibly producing new, "emergent" ones? The technology to achieve this is already at hand. What we lack is a proper design methodology, able to tackle the problems posed by autonomously communicating artifacts in a constantly changing technosphere. In this paper we try to delineate the requirements that such a design paradigm should fulfill. The scenario we imagine considers a nearby future where technological artifacts *self-organize*, in the sense that they are able to communicate and perform desirable tasks with minimal human intervention.

This vision is closely related to the concept of "Ambient Intelligence" (AmI)[11], which envisages a future where people are surrounded by "smart" and "sensitive" devices. AmI would be the result of the integration of three technologies: Ubiquitous Computing [14], Ubiquitous Communication, and Intelligent User Friendly Interfaces. The first one conceives of a seamless integration of computation processes taking place in the variety of artifacts that surround us, being part of "The Grid", the network that would allow anyone anywhere to access the required computing power. The present paper focuses on the aspect of Ubiquitous Communication that attempts to obtain seamless information exchange between devices. Intelligent User Friendly Interfaces should enable an intuitive, effortless interaction between users and devices.

1.2 Requirements for self-organizing artifacts

We see self-organization as a paradigm for designing, controlling, and understanding systems [5, 4]. A key characteristic of a self-organizing system is that structure and function of the system "emerge" from interactions between the elements. The purpose should not be explicitly designed, programmed, or controlled. The components should *interact* freely with each other and with the environment, mutually adapting to reach an intrinsically "preferable" or "fit" configuration (attractor), thus defining an emergent purpose for the system [9]. By "self-organizing artifacts" we mean a setup where different devices, with different fabrications and functionalities, and moving in and out of different

configurations, can communicate and integrate information to produce novel functionalities that the devices by themselves could not achieve.

A first requirement for such communication is cross-platform compatibility. This is already achieved for programming with Java, and for documents with XML. Another requirement is wireless communication, which is offered by technologies such as IR, Bluetooth and WiFi. Near Field Communications (NFC) is a newly envisioned standard, proposed by a consortium headed by Sony, Nokia, and Philips, which would allow information to be transmitted between devices that come in close spatial proximity (“touching”).

Even with such a standard, the problem remains that the user generally would need to specifically request such communication between devices (e.g. “transfer this file from here to there”). Ideally, the devices would *know* what we want them to do and how to do it. User Interfaces already help us to tell them our wishes. Still, one device cannot tell *another* device what we want, especially if they are produced by different manufacturers. This is a general problem of communication between artifacts: they can recognize standard messages, but they do not “know” what the messages *mean*. To avoid endless debates, we can say that the meaning of a message is determined by its *use* [15]: if a device has received a message, and does “the right thing” (for the user), then it has “understood” the meaning of the message. Thus, the user’s satisfaction is the ultimate measure of the effectiveness of the artifacts’ performance.

Another issue is how to deal with changes in technology. We do not want to reconfigure every artifact each time a new device arrives. Moreover, we want the old devices to be able at least to cope with the functionality of new ones. New devices should configure themselves as automatically as possible. Older ones may require user intervention at first (as they cannot know beforehand which functions will be required), but they should be able to cope with new technology being added to the network. The overall system must be *adaptive*, *extensible*, and *open*.

An adaptive system can cope with unexpected changes in its environment, as exemplified by the constantly changing technology. Having flexibility built into our systems is desirable: they should at least be able to tolerate events they were not designed for without breaking down, but preferably try to find adapted solutions, or at least ask assistance from the user. For example, home appliances have a limited set of functions. To have them self-organize (e.g. the alarm clock coordinating with the microwave oven, and the oven with the kettle), their functions could be easily programmed to respond to unknown messages. If a new device arrives, and an old one does not know what to do when it receives a message, it can check what the user wants, thus learning how to respond appropriately. The possibility to add more devices to an existing configuration may be called *extensibility*.

Suppose that a company develops adaptable and extensible devices that interact seamlessly with each other. This would still leave the problem that customers cannot add devices from other companies, as these would follow their own standards, thus creating compatibility problems. We believe that the solution

is to have *open* technologies, in the spirit of GNU. Open means that everyone has free access to their specifications. The advantage is that they can develop much faster, meeting the requirements of more people, because they are developed by a global community that can try out many more approaches than any single company. Still, a company can benefit in promoting an open technology, since this would provide them with free publicity while everyone is using their protocol (e.g. Sun's Java).

1.3 Achieving self-organization

We can divide the problem of self-organizing integration into three subproblems: 1) devices should learn to *communicate* with each other, even when they have no a priori shared understanding of what a particular message or function means; 2) devices should learn which other devices they can trust to *cooperate*, avoiding the others; 3) devices should develop an efficient *division of labour* and workflow, so that each performs that part of the overall task that it is most competent at, at the right moment, while delegating the remaining functions to the others.

These issues are all part of *collective intelligence* [7] or *distributed cognition* [10]: a complex problem cannot be tackled by a single device or agent, but must be solved by them working together, in an efficiently coordinated, yet spatially distributed, system, where information flows from the one agent to the other according to well-adapted rules. Until now, distributed cognition has been studied mostly in existing systems, such as human organizations [10] or animal “swarms” [2], that have evolved over many generations to develop workable rules. Having the rules self-organize from scratch is a much bigger challenge, which has been addressed to some degree in distributed AI and multi-agent simulations of social systems. Inspired by these first explorations, we will propose a number of general mechanisms that could probably tackle the three subproblems. However, extensive simulation will clearly be needed to test and elaborate these mechanisms.

1.4 Learning to communicate

To communicate effectively, different agents must use the same concepts or categories. To achieve effective coordination, agents must reach a shared understanding of a concept, so that they agree about which situations and actions belong to that category, and which do not. A group of agents negotiating such a consensus may self-organize, so that a globally shared categorisation emerges out of local interactions between agents.

Such self-organization has been shown in different simulations of the evolution of language [13]. Here, interacting software agents or robots try to develop a shared lexicon, so that they interpret the same expressions, symbols, or “words” in the same way. In these simulations agents interact according to a protocol called a “language game”. There are many varieties of such games, but the

general principle is that two agents “meet” in virtual space, which means that through their sensors they experience the same situation at the same time. Then they try to achieve a consensus on how to designate one of the components of their shared experience by each in turn performing elementary *moves*.

In a typical move, the first agent produces an “utterance” referring to a phenomenon that belongs to one of its inbuilt or previously learned categories, and the second one finds the best fitting category for that phenomenon in its knowledge base. The second agent then indicates a phenomenon belonging to that same category. If this phenomenon also belongs to the same category for the first agent, both categorisations are reinforced, otherwise they are reduced in strength. In the next move of the “game”, another phenomenon is indicated, which may or may not belong to the category. The corresponding categorisation is strengthened or weakened depending on the degree of agreement. After a number of moves the game is stopped, each agent maintaining the mutually adjusted categories. Each agent in turn is coupled to another agent in the system, to play a new game using different phenomena. After some games a stable and coherent system of categories shared by all agents is likely to emerge through self-organization.

If for some reason devices are not able to communicate, they should be able to notify the user, and ask for the correct interpretation of the message. This is easy, since devices have a limited functionality. It would be possible to “teach” a device what to do if it receives a particular message, and the device should “learn” the meaning of the message.

1.5 Learning to cooperate

Integrated devices should not only communicate, but cooperate. Cooperation may seem self-evident in preprogramed systems, where the components are explicitly designed to respond appropriately to requests made by other components. However, this is no longer the case in open, extensible configurations.

There exists an extensive literature on the evolution of cooperation between initially “selfish” agents, inspired by the seminal work of Axelrod [1] that compared different strategies for playing a repeated “Prisoners’ Dilemma” game. However, this game does not seem directly applicable to information exchanging devices. Moreover, the chief result, while sensible, may seem trivial: the most effective strategy to achieve robust cooperation appears to be *tit for tat*, i.e. cooperate with agents that reciprocate the cooperation, stop cooperating with those that do not. More recent, tag-based models (e.g. [12, 6] start from a simpler situation than the Prisoners’ Dilemma, in which one agent “donates” a service to another one, at a small cost to the donor but a larger benefit to the recipient. The main idea is that agents are identified by “tags”, and that they cooperate with those agents whose tags are similar to their own. The rationale is that agents with the same type of tag belong to the same group, “family” or “culture”, following the same rules, so that they can be trusted to reciprocate.

For artifacts, a tag may include such markers as brand, model, and protocols understood. This would show that a device is capable and willing to lend particular services to another one, thus obviating the need for a repeated, “tit-for-tat-like” interaction probing the willingness to reciprocate. Yet extensible environments should allow the addition of very dissimilar devices, made by different companies using different standards and functionalities. Therefore, we propose a different approach, combining some advantages of tags and tit-for-tat strategies.

1.6 Learning to coordinate

After having ascertained that our devices can communicate and cooperate, we still need to make sure that the functions they perform satisfy the user. This desired functionality can be viewed as a complex of tasks that need to be executed.

Assume that the user regularly expresses his/her overall satisfaction with the ambient intelligence environment (e.g. explicitly by clicking on a scale from one to ten, or implicitly by facial or physiological cues that express happiness/unhappiness). This score can be used as a feedback signal to the network of devices, allowing it to reinforce the more successful rules, while weakening the less effective ones. We will assume that the agent who delegated a task will increase its trust in the competence of the agent that performed that task, and thus increase its probability to delegate a similar task to the same agent in the future. Otherwise, it will reduce its trust. As demonstrated by the simulation of Gaines [3], this assumption is sufficient to evolve a self-reinforcing division of labour where tasks are delegated to the most “expert” agents.

However, when the tasks are mutually dependent, selecting the right specialist to carry out a task is not sufficient: First the preparatory tasks have to be done by the right agents, in the right order. When the agents do not know a priori what the right order is, they can randomly attempt to execute or delegate a task, and, if this fails, pick out another task. Eventually they will find a task they can execute, either because it requires no preparation, or because a preparatory task has already been accomplished by another agent. Each completed task enables the accomplishment of a series of directly dependent tasks. In this way the overall problem will eventually be solved. In each problem cycle, agents will learn better when to take on which task by themselves, or when to delegate it to a specific other agent.

We expect that this learned organisation will eventually stabilise into a system of efficient, coordinated actions, adapted to the task structure. When new devices are added to the system, system and device should mutually adapt, producing a new organization. While no single agent knows how to tackle the entire problem, the knowledge has been “distributed” across the system. The “tags” that identify agents, and the learned associations between a tag and the competence for a particular task, play the role of a mediator [8], delegating tasks to the right agents and coordinating their interactions so that the problem is

tackled as efficiently as possible.

1.7 Conclusions

We cannot keep on adding functions to personal computers. They serve as text editors, game consoles, televisions, home cinemas, radios, agendas, music players, gateway to the Internet, etc. Such general devices will never produce the same quality as specialized appliances. Our PCs are like ducks: they can swim, but not as well as fish; fly, but not as well as hawks; and walk, but not as well as cats. Rather than integrate so many functions in a single device, it seems preferable to entrust them to an ever expanding network of specialized devices that is kept coordinated through an ongoing process of self-organization. We have described a number of general requirements and approaches that may enable our artifacts to learn the most effective way of cooperation.

In our overall scenario, we have assumed that standard functions and interaction rules are preprogrammed by a global community to handle the most common, default situations, but that the system is moreover ready to extend its own capabilities, adapting to newly encountered tasks, situations, or devices. This ability to adapt should be already present in the interaction rules. The adaptation may be achieved through the self-organization of the system of agents, using recurrent, “game-like” interactions, in which the agents learn what messages mean and who they can trust to perform which task. Most of this can happen outside of, or in parallel with, their normal “work”, using idle processing power to explore many different communication and collaboration configurations. Thus, we can imagine that our future, intelligent devices, like young animals or children, will learn to become more skilful by exploring, “playing games” with each other, and practising uncommon routines, so as to be prepared whenever the need for this kind of coordinated action appears.

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Chapter 18

Modeling Social Structure as Network Effects: Rewards for Learning Improves Performance

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A theoretical representation of social structure in agent-based organizations is developed. To test the model we generated a hypothesis from organizational learning theory and tested it using computational experiments. We found that emergent social structure associated with rewarding agent learning increased collective output over and above pay for performance.

1.1. Introduction

Important questions in the social sciences often defy analysis due to their complexity. Not only is it difficult to specify the nonlinear operation of the underlying social mechanisms, it can be impossible to control for numerous interacting variables. Computational methods offer a promising approach to address these concerns. However, computational models are often used without clear linkage to theory, or if

theoretically grounded, they address a single aspect of a complex system. As a result, they often fail to adequately address practical concerns.

This article reports progress on ongoing research intended to bridge the gap between computational organization theory, computational modeling, and real-world organizations. We address the modeling of social structures inherent in computational organization theory [Holland 1995], in particular, the implication to outcomes of rewarding learning as well as performance. To do this we describe an agent-based model and perform computational experiments in artificial organizations as a methodology for theory building [Holland 1995].

2.1. Network Theory For Organizations of Computational Agents

We begin with the axiomatic framework of Carley and Prietula [1994a] where “organizations are viewed as collections of intelligent agents who are cognitively restricted, task oriented, and socially situated” [p. 56], and adopt a description of an organization as a connected network linking persons, resources, tasks and knowledge [Holland 1995]. The agent intelligence mechanism is defined as the agent’s local network connections. These simultaneously constrain agent action and enable the agent to change its local network--its social, task, resource, and knowledge situation for future time steps [Holland 1995]. The outcome of this process at each time step, N , is the agent’s “method”.

The intelligence mechanism treats the agent and its capabilities as being defined by its location in the network. Thus, an agent’s social situation has duality analogous to Giddens’ [1984] duality of structure in structuration theory. An agent’s position in the network constrains its ability to act, just as in structuration theory, social structure is said to “produce” behavior. And action by an agent can make persistent changes to the network that impact its ability, and possibly that of other agents, to act in the future. In structuration, an individual’s actions are said to “reproduce” behavior by creating social structure that persists across time and space [Holland 1995].

2.1.2. Definition of Computational Structuration

When two agents interact, their methods could also interact. For this analysis, we assume that methods from different agents are additive; each change is made on top of the previous one. Method ordering is assumed to occur randomly. As such, at a given time step, boundary interaction for the organization is the aggregate “methods” of all boundary-spanning agents after all agent “methods” are completed. In this theoretical framework, we define the totality of mutual impact, both of the network on the agents and the agents on the network, as computational structuration. In an example from prior research, computational structuration was modeled such that once a new knowledge connection was made, an agent assigned itself to a new task,

performed the task and gathered incremental reward for the initiative [Holland 1995]. A permanent change to social structure was thus created.

2.1.3. Structuration, Organizational Learning and Differentiated Rewards

The organizational learning research used to frame macro effects of computational structuration is built upon the foundational theories of social structure [Holland 1995] and Giddens' [1984] structuration theory. Consistent with this systems theory approach to organizational learning, in their organizational learning system model (OLSM), Schwandt and Marquardt [2000] define organizational learning as "a system of actions, actors, symbols and processes that enables an organization to transform information into valued knowledge which in turn increases its long-run adaptive capacity" [p. 8]. We focus on the environmental interface and flow of information across the boundary [Holland 1995] and the integration and dissemination of resulting knowledge throughout the organization via structuration [Giddens 1984].

The research described here further explores structuration from a specific perspective: the impact of differentiated rewards on social structure and collective outcomes. To do this, we first demonstrate that differentiated rewards are examples of structuration. Our thesis is that agent-level micro interactions related to differentiated rewards give rise to emergent macro relationships at the social and institutional levels.

Giddens [1984], in an effort to integrate agency and structure in his theory of structuration, defines structure as rules and resources, existing outside of time and space, which provide guidance for agency actions. He defines this duality of structure as "the essential recursiveness of social life, as constituted in social practices: structure is both medium and outcome of reproduction of practice" [p. 5]. This duality of structure provides a theoretical platform to formulate and interpret the relationships among differentiated rewards, performance, and interactions of agents.

2.1.4. A Specific Structuration Phenomenon—Distribution of Rewards

In this study, we specifically address the question of how different logic for distributing rewards impacts not only the agent, but also its social situation. As described above, social theory research asserts that differentiated rewards are a structuring variable, that is, they impact the social structures inherent in the system. Variations in logic thus manifest themselves along differing path dependent trajectories toward different outcomes. In particular, social theory argues that distributing rewards based on learning as well as performance promotes better collective outcomes because such a system enables the absorption of new information and the diffusion of knowledge [Holland 1995]. We study the effects of different reward distribution logic first on computational structuration and then on organizational outcomes in artificial organizations. We test the hypothesis:

HYPOTHESIS: When differential rewards are applied to learning contributions over and above performance contributions, collective success, as measured by output and number of surviving agents, improves.

3.1. Methods: Use of An Agent-Based Model to Test Theory

To test our hypothesis in the context of theory, we built upon an agent-based model, described and validated elsewhere [Holland 1995], that was consistent with computational structuration. We then used this model to create artificial organizations on which to run computational experiments. In all, sixty organizations were created in this way, and although each is unique and not replicable, in the aggregate statistically significant differences among various scenarios could be identified. These were used to infer support or refutation of the hypothesis.

All activities within the model could in principle be decomposed into the primitives defined theoretically above, such that at each time step the organization's state could be represented as a network consistent with the meta-matrix representation of persons, tasks, resources, and knowledge [Holland 1995]. Thus social structure and structuration was represented theoretically as network effects.

3.1.1 Value Chain Model

The model selected was chosen because it was organizationally realistic for a broad range of economic entities [Holland 1995]. The task, knowledge and resource environment was structured around value chain [Holland 1995]. Resources were transformed at various stages of value creation by the action of agents with appropriate task assignment and knowledge. Agents consumed energy with each step, and energy was replenished for agents only when the collective goal was achieved. Failure to continually achieve this collective goal would lead to the death of individual agents and, eventually, to the end of the collective.

In this artificial organization, the concept of knowledge and knowledge transfer was also modeled. To produce an output an agent had to be connected to relevant knowledge. Agents accumulated knowledge by interacting with other knowledge-bearing agents. When knowledge was acquired, the agent could change the social structure by performing a task it previously could not, an example of computational structuration [Holland 1995]. Knowledge was refreshed by interaction with other members and with outsider agents bearing more current new information.

Agents are not motivated by the rewards. Rather, this study looks only at the structural effects of differentiated rewards. For each time step, agent action is random, except that it is constrained by the agent's network connections at that point in time and its internal but unchanging method rules.

We look at two distinct structure approaches that could be used to drive differential rewards: 1) rewards to agents based upon direct contribution to successful production only (i.e., performance driven by existing social structures), and 2) rewards to agents based upon contribution to the exchange of knowledge that informs successful production (i.e., learning and the creation of new social structures) as well as contribution to production.

4.1. Computational Results and Analysis

To test the hypothesis, two scenarios, each consisting of thirty organizations, were run. Each represented a different structuring decision. In the first scenario, only an agent's direct contribution to performance was rewarded. In the second, both direct performance and contribution to knowledge diffusion resulted in rewards. All other parameters were identical in both scenarios.

For each scenario, thirty new model runs were completed with identical initial conditions. A particular scenario, therefore, represented the aggregate of thirty possible outcomes, many quite different. The differences among individual model runs resulted from path dependence in the emergent computational structuration patterns inherent in the stochastic nature of agent interactions. As such, the outcome of a particular run could not be predicted or replicated. To identify significant differences that could not be explained by random chance, we used independent sample T-tests to compare scenarios.

4.1.1 Rewarding Performance Only

In the first scenario, agents were rewarded individually when they contributed to the production of the final product. Five tasks were identified in the value chain. Therefore, when the final product was produced, at most five agents, those that were structurally connected to the resources, knowledge and tasks involved in production, participated in the distribution of reward when the output was exchanged for energy. Output value was independent of the number of agents involved in production but was dependent upon the currency of the knowledge used by the agents to produce the product. This reflected the fact that more recent knowledge about the market translates into high-value production. To show the relationship between output and structuration activity, output as a function of knowledge diffusion events (representing structuration events) is shown as the hollow points in Figure 1.

These results indicate that more knowledge diffusion implies more capable agents that produce a more valuable product and thus create the opportunity for greater collective rewards. In this scenario, neither knowledge diffusion nor information transfer was rewarded, yet successful production still occurred. In the next scenario, these activities were rewarded, with significant effect.

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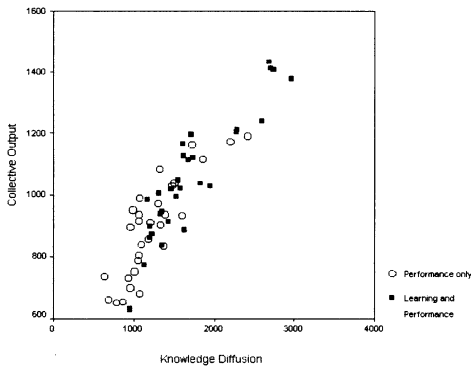


Figure 1. Output Relative to Knowledge Diffusion for 60 Artificial Organizations

4.1.2. Rewarding Contribution to Collective Learning

In the second scenario, agents were rewarded individually when they either contributed directly to the production of the final product or contributed knowledge used in the production, that is, the creation of a knowledge connection was also rewarded if and only if that knowledge contributed to production. In this scenario, many agents contributed to production and shared equally in the value created when the final product was produced. Again, output value was determined by the payoff function and was independent of the number of agents involved in production. The payoff function was identical to that in the performance-only scenario except that the distribution of rewards was changed. The output as a function of knowledge diffusion events is shown in Figure 1 as the solid points.

4.1.4. Rewarding Learning and Performance Versus Performance Only

To test the hypothesis, we compared the differentiated reward scenarios to determine significant differences. Both the number of living agents and the total output of the collective were significantly greater ($\alpha = 0.05$) when learning as well as performance was rewarded (Table 1). Also significantly greater were the levels of knowledge diffusion and information transfer, indicating that more new information was entering the system and more knowledge diffusion was occurring when learning was rewarded. The above results support our hypothesis.

(To test whether the effects observed could be explained simply by the number of agents rewarded rather than by the specific agents rewarded for their contributions to learning and performance, we ran a scenario where we randomly rewarded, with like reward, the same number of agents that would have been rewarded in the direct

contribution scenarios. When the reward-for-performance scenario and reward-for-learning-and-performance scenario were compared with this scenario, a significant difference was observed. Thus the effects of differential rewards on outcomes is independent of the number of agents rewarded.)

It is interesting to note that average payoff per agent (PAY in Table 1) was significantly lower when learning was rewarded as well as performance. In effect, performing agents sacrificed individual reward (and survival potential) in return for rewarding the “teaching behaviors” of other agents that had relevant knowledge.

As shown in Figure 1, when all sixty artificial organizations (thirty in each scenario) were considered, a positive relationship exists between collective output and knowledge diffusion. Also, the two scenarios diverge in a statistically significant way. Rewarding both learning and performance tended to imply higher collective output than rewarding performance alone, thus supporting the hypothesis.

TABLE 1
T-TESTS BETWEEN PERFORMANCE ONLY AND LEARNING AND PERFORMANCE SCENARIOS

	Reward Learning	N	Mean	Std. Dev.	Statistical Significance ($\alpha = 0.05$)
LIVING	False	30	38.5000	7.8773	Yes
	True	30	46.9333	9.3879	$P = 0.000$
OUTPUT	False	30	893.9333	159.5684	Yes
	True	30	1056.6667	196.2437	$P = 0.001$
KNOWDIFF	False	30	1243.7000	408.4304	Yes
	True	30	1729.6333	549.1897	$P = 0.000$
INFOTRAN	False	30	2447.1000	584.8274	Yes
	True	30	3086.1000	676.5974	$P = 0.000$
PAY	False	30	171.2333	34.7361	Yes
	True	30	67.8667	11.4432	$P = 0.000$

NOTE—Living indicates the number of living agents at the end of the run; KnowDiff, the amount of knowledge diffusion (number of agent interactions that resulted in knowledge exchange); and InfoTran the number of agent interactions outside of the organization that resulted in new information.

5.1. Discussion

To explore the relationship between structuration and network effects in organizations this study looked at pay for performance versus for learning and performance. Reward attribution is an key area in complex adaptive systems research [Holland 1995]. It is also an important social structuring variable [Holland 1995]. Thus it is an appropriate area to test computational models.

The results demonstrate that at least for these artificial organizations, aggregate

effects of localized agent-level interactions can be studied in the context of system-level variables. We demonstrated through computational experiments that differences in social structures related to rewards can have a significant effect on organization-level outcomes and that these effects devolve from the particularities of the underlying network structure and how it changes over time. Our model shows for artificial organizations that, as predicted by the OLSM [Schwandt & Marquardt 2000] for real world organizations, rewarding teaching and learning behaviors enhances organizational outcomes over and above rewards for performance. Importantly, the agents did not learn from the rewards and were not motivated by the rewards. Thus, these results demonstrated structural effects that relate to social context, rather than agent talent, skill or motivation, as a measure of collective fitness.

There are several approaches to future research. For example, the implications of differential access to resources and thus social power could be studied. In addition to broadening the organization-level approach, defining and then modeling a more complex micro interaction environment might be useful. This model assumed no differences among agent decision rules. These rules could evolve through variation and differential selection processes [Holland 1995]. Finally, more completely specified social structures could move this approach to practical applications.

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Chapter 19

Permeable Boundaries in Organizational Learning

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The nature of the organizational boundary is investigated in the context of organizational learning. Boundary permeability is defined and hypotheses relating it to performance are tested computationally using data from 5,500 artificial organizations. We find that matching boundary permeability to the environment predicts both agent and organization survival.

1.1. Introduction

The acceleration of global business highlights the importance of being in tune with the environment. In the context of organizational learning research [Schwandt & Marquardt 2000], we examine information flow through an organization's boundary and its impact

on an organization's survivability. Computational modeling is used to explore the impact of boundary permeability on organizational outcomes and to test whether "boundary permeability" as a measure of the collective's ability to sense its environment—that is, gather information external to the organization and diffuse it internally—is a robust and cohesive construct at the organizational level. We do this by describing *boundary permeability* in the context of an agent-based view of organizations [Carley & Prietula 1994] and by varying aspects of agent-level interaction at the boundary. Virtual experiments measure the impact of boundary permeability on organizational learning and outcome variables.

1.2. Organizational Learning and Computational Organization Theory

Organizational learning literature has highlighted the importance of boundaries [Daft & Weick 1984; Schwandt & Marquardt 2000]. In addition, the literature has supported organizational learning as a real, measurable phenomenon at the collective level [Schwandt & Marquardt 2000]. Consistent with systems theory [March & Olsen 1988/1975] Schwandt and Marquardt [2000] in describing their organizational learning systems model (OLSM) defined organizational learning as "a system of actions, actors, symbols and processes that enables an organization to transform information into valued knowledge which in turn increases its long-run adaptive capacity" [p. 8]. This study focuses on the system's environmental interface as a means to gather new information, and its ability to diffuse the information effectively to become usable knowledge is a form of changed social structure, a process called structuration [Giddens 1984]. Carley and Prietula [1994] have said, "organizations are viewed as collections of intelligent agents who are cognitively restricted, task oriented, and socially situated" [p. 56]. With this beginning, we adopt a precise description of an *organization* as a connected network linking persons, resources, tasks, and knowledge to one another [Krackhardt & Carley, 1998]. Also, agents are assumed to have an intelligence mechanism [Hazy & Tivnan 2003] that is determined by their local network connections and also enables the agents to change their local network (social, task, resource, and knowledge situation) over time.

1.2.1. Boundaries and Boundary Spanning

Considerable research has explored the notion of organizational or firm boundaries in the context of environmental change. In many of these accounts, the organization boundary is considered in the context of contractual relationships [Williamson 1985], a particularly

concrete social structure; other research has considered boundaries as socially constructed [Giddens 1984]. Considerable research has explored the nature of boundary-spanning roles [Starbuck 1976]. Aldrich and Herder [1977] identified two distinct functions of boundary-spanning roles: information processing and external representation of the organization to outsiders. In a longitudinal study, Friedman and Podolny [1992] found that representation and gatekeeper roles became differentiated in different individuals over time. It is thus reasonable to assume that the information-processing function of boundary spanning can be studied separately.

2.1. Boundary Permeability

To define *boundary permeability* we look at the collective's need to perceive the environment, interpret information, and pass the benefit of the interpreted information deep into the collective to enhance future collective activities [Daft & Weick 1984].

As a collective level construct, the organizational boundary represents the distinction between "outside" and "inside" and, by default, functions as the organ through which agents inside the collective (participating in collective activities) sense their collective's environment. At the same time, note that it is boundary-spanning agents that cross the organization's boundary to seek and bring back new information. Thus, to be meaningful as an organization-level construct, boundary permeability must capture more than simply the number of boundary crossings. It also has to take into account the efficiency with which new information is gathered outside the boundary and the effectiveness with which the new information is integrated or diffused within the organization as knowledge relevant to collective activities and potential benefit.

To capture these relationships, we define boundary permeability as the ratio between relevant interaction activity outside the organization (actual exploration learning activity) and interaction activity inside the organization that could diffuse knowledge. When two agents interact, an information transfer event or a knowledge diffusion event may or may not occur. An event is counted only when one agent gets new information from another agent. If the agent already has access to the other agent's information, no information transfer event occurs. If both agents gain new information or knowledge, two events are counted in a single interaction.

An organization that has little appetite for learning, that is, low absorptive capacity [Cohen & Levinthal 1990], is unlikely to benefit from new information. At the same time, if the amount of new information that crosses the boundary is limited, the amount of knowledge diffusion events inside is limited, regardless of the organization’s appetite for new knowledge. Therefore, boundary permeability is defined as the ratio of new information gained compared to the organization’s appetite for knowledge. In equation form, we say,

Boundary Permeability

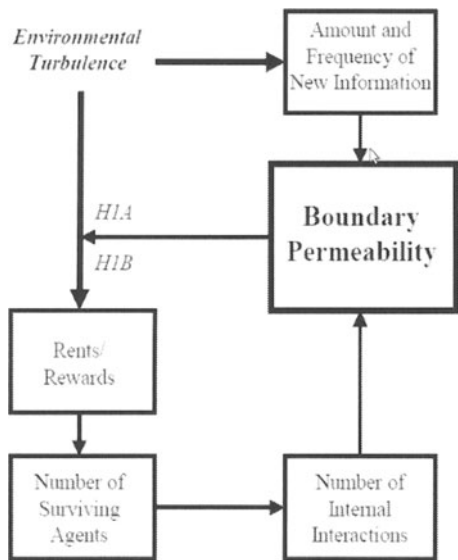
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of Information Transfer Events Outside

of Total Agent Interactions Inside

2.1.1. Hypotheses

Figure. 1. Boundary permeability moderates the effect of environmental turbulence on agent survival level in collective activities.



As Figure 1 shows, boundary permeability is assumed to moderate the impact of environmental turbulence on rents and rewards collected by the system—and thus the number of surviving agents.

The boundary permeability ratio says something about the efficiency of agent search, its intensity, and its effectiveness inside the organization. Given the principle of requisite variety, one may reasonably suspect that the appropriate level of boundary permeability, and therefore internal complexity, depends upon the level of turbulence in the environment, greater turbulence implying greater boundary permeability. Also, results from Hazy, Tivnan, and Schwandt [2002] implied that turbulence increases the impact of boundary spanning on collective outcomes. As the boundary permeability ratio increases significantly beyond one—much more information is being gathered than the organization can consume—the relationship is reversed. Thus as Figure 1 shows, we tested the following:

Hypothesis 1: *High* environmental turbulence implies that *boundary permeability* will be positively related to the number of surviving agents so long as the boundary permeability ratio is not significantly greater than one.

Hypothesis 2: *Low* environmental turbulence implies that *boundary permeability* will be negatively related to the number of surviving agents.

3.1. Research Design and Methods

To test the above hypotheses, many possible scenarios must be observed to determine statistically significant trends across many organizations. It is also important to look at comparable scenarios, at least those where differences can be adequately measured. The nature of these questions would require hundreds of samples—an impractical situation for field research. Instead, computational simulation was selected. Further, our interest in the cumulative, organization-level effects of agent- or individual-level boundary-spanning interactions made agent-based modeling a logical selection.

To do this, we created an artificial organization that included the following: agents (or persons), some members of an organization, and some outsiders; a habitat, defined as a spatial grid with resources scattered randomly across it; and a time-stepping process that allowed agents to move, interact, and either prosper or die over a defined period of time [Epstein & Axtell 1996]. By manipulating characteristics of this artificial organization and then watching it over time, we ran computational experiments that would have been difficult or impractical to duplicate in the real world.

3.1.1 Value Chain Model

To make the artificial world organizationally realistic, we took as a subject an economic entity that survives by producing a product for the market. Thus, we selected a model described and validated elsewhere [Hazy, Tivnan, & Schwandt 2003], wherein, the task and resource environment was structured around the value chain [Porter 1985]. Resources were transformed at various stages of value creation by the action of agents with appropriate task assignment and knowledge. Agents consumed energy with each step, and energy was replenished for agents only when the collective goal was achieved. Failure to continually achieve this collective goal led to the death of individual agents and, eventually, to the end of the collective.

In this model there were N independent tasks, each transforming one resource, R_j , in the value chain into the next resource, R_{j+1} . When any agent that was connected to task T_j became connected to resource R_j by random movement, resource R_j was transformed into R_{j+1} . Production efficiency depended on the currency of the agent's task knowledge. This "production process" continued until the completion of final task, T_N , wherein a final product, R_F , was created and a payoff function exercised. This payoff function added energy to appropriate agents and added new raw resource, R_1 , to re-initiate the production process. In this way, the collective could sustain itself and individual agents could survive by benefiting from collective success.

To produce an output from a resource input and thus complete a task, an agent had to be connected to knowledge relevant for the agent-task pairing. In addition, depending on environmental turbulence (here defined as frequency of change in knowledge generation), the payout value of an agent's knowledge decreased over time. The consequence of knowledge-value decrease was a decline in production efficiency. Agents accumulated knowledge by interacting with other knowledge-bearing agents. Knowledge was refreshed with new generations of knowledge through interaction with other member and outsider agents bearing information that was more current. The number of surviving agents was chosen as the measure of collective outcomes. The level of agent interaction to create product is random. Thus each surviving agent would produce, on average, the same level of output, so there is a positive relationship between individual production and organizational outcomes in the aggregate. It follows that the number of surviving agents positively predicts output.

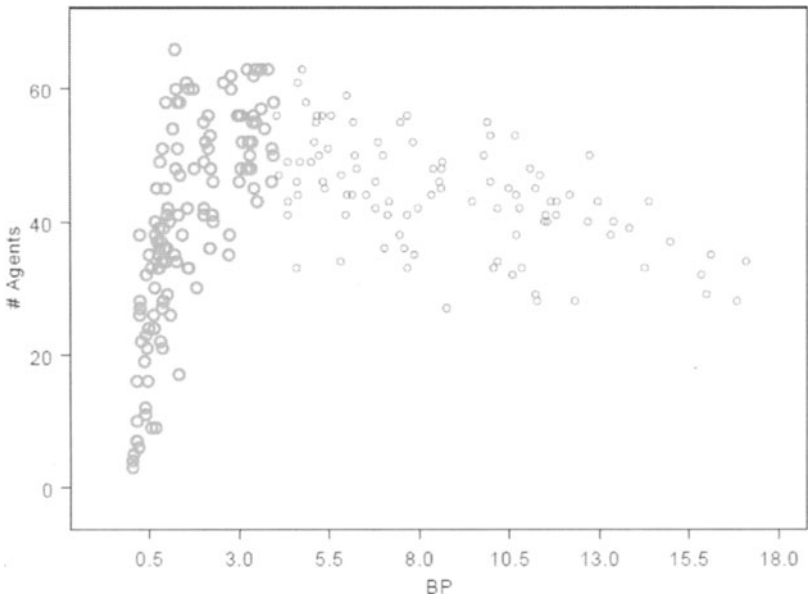
3.2. Virtual Experiments and Analysis

Because the variables that make up boundary permeability interact dynamically, we chose to create many artificial organizations in which the initial conditions were controlled, certain parameters were varied in known ways, and the organizations developed stochastically over time. In particular, for these virtual experiments, only the turbulence in the environment and the number of boundary spanners was varied. All other aspects were identical as the models were initiated. The data set described 5,500 artificial organizations that developed under varied environmental states and with varying levels of boundary permeability. Examining the variables describing the organizations after the model runs, we looked for patterns to support or refute the hypotheses. These results were plotted and statistical analysis performed.

4.1. Results and Analysis

First, 5,500 artificial organizations were created. Each began with similar initial conditions, except for environmental turbulence and number of boundary-spanners at initialization. Thus, a large sample of comparable artificial organizations, each having survived 3,650 time steps (approximating ten years), was available. To test for hypothesized relationships, the number of surviving agents in each scenario was compared with the boundary permeability variables that characterized the scenario. As Figure 2 shows, when the number of surviving agents (#Agents) was compared with boundary permeability (BP) in a high-turbulence environment (i.e., where new information was introduced ever 50 time steps), as expected, for $BP < 1$, #Agents was positively correlated ($r = 0.73$, $r^2 = 0.53$) with BP. As BP increased beyond one, this relationship turned negative ($r = -0.41$, $r^2 = 0.16$). These results imply the benefit of increasing BP reaches an upper limit. These results strongly support Hypothesis 1.

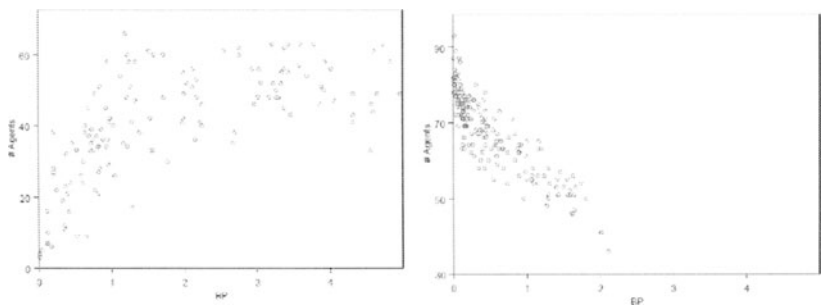
Figure 2. Number of surviving agents (#Agents) versus boundary permeability (BP) in high turbulence environments.



Note. Large points indicate positive gradient for low BP, and small points indicate negative gradient for high BP.

When the number of surviving agents (#Agents) was compared with boundary permeability (BP) in a low-turbulence or stable environment (i.e., cases where new information was introduced every 1050 to 1095 time steps), we found that, as expected, for $BP < 1$, #Agents was negatively correlated ($r = -0.74$, $r^2 = 0.55$) with BP—that is, as BP increased, #Agents decreased. As BP increased beyond one, this relationship continued ($r = -0.76$, $r^2 = 0.58$). For all values of BP, the negative relationship was strongly supported ($r = -0.87$, $r^2 = 0.76$). These results strongly support Hypothesis 2. As Figure 3 shows, increasing BP (up to a point) has a positive effect in turbulent environments but a negative effect in stable ones.

Figure 3. Number of surviving agents (#Agents) versus boundary permeability (BP) for environments with high turbulence (left) and low turbulence (right).



5.1. Discussion

This research investigated the permeable nature of the organizational boundary. We defined boundary permeability with respect to the amount of new information obtained in the environment and the number of agent interactions inside the organization’s boundary. Hypotheses were developed and tested based upon 5,500 artificial organizations that randomly evolved under controlled conditions.

Our results showed that the number of agents surviving in an artificial organization is related to the characteristics of the organization’s boundary. Further, the nature of this relationship depends upon the level of turbulence in the external environment. As expected, in stable environments, although some permeability is necessary for survival, increasing permeability is generally always bad for survival. As turbulence increases, however, increased permeability helps survival of agents up to a point, after which survival potential declines. In effect, increasing permeability beyond a critical point allows too many agents to “leak out” and escape productive activity while providing little incremental benefit from learning.

By its nature, computational analysis has inherent limitations. In this

case we modeled an organization as a system of adaptive agents but not an adaptive system. Agents learn and improve their ability to produce collective output, and thus the system improves its exploitation of its existing capabilities. It does not adapt in the sense that the system cannot adjust its boundary permeability in response to the environment.

The results support the possibility that boundary permeability can be a useful construct for organizational learning research. A next step would involve unpacking boundary permeability to understand the agent level interactions that impact it. In addition, the assumption that agent interaction leads to information and knowledge transfer in every case—while helpful in simplifying the analysis—may have contributed to the strong result. Future research that makes knowledge exchange contingent may highlight the importance of knowledge diffusion effectiveness metrics to organizational learning. Further exploration of these factors is therefore warranted.

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Chapter 20

Mobility of Innovators and Prosperity of Geographical Technology Clusters:

**A longitudinal examination of innovator networks
in telecommunications industry**

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Abstract

Knowledge spillovers have long been considered a critical element for development of technology clusters by facilitating innovations. Based on patent co-authorship data, we construct inventor networks for two geographical telecom clusters – New Jersey and Texas – and investigate how the networks evolved longitudinally as the

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technology clusters were undergoing different stages of their lifecycles. The telecom industry in the former state had encountered a significant unfavorable environmental change, which was largely due to the breakup of the Bell System and evolution of the telecom industry. Meanwhile, the telecom cluster of Texas has been demonstrating a growing trend in terms of innovation output and is gradually replacing New Jersey's leadership in telecom innovation as measured by number of patents per year. We examine differences and similarities in dynamics of the innovator networks for the two geographical clusters over different time periods. The results show that TX's innovator networks became significantly better connected and less centralized than the ones of NJ in the later years of the time series while the two clusters were experiencing different stages of lifecycle. By using network visualization tools, we find the overwhelming power of Bell System's entities in maintaining the NJ innovator network to be lasting a very long time after the breakup of the company. In contrast the central hubs of TX's networks are much less important in maintaining the networks.

Key words: Social network, Technology clusters, Innovation, Telecommunications R&D

1. Introduction

Clustering has become one of the key drivers of regional economic growth by promoting local competition and cooperation. The impact of clustering on business competitiveness and regional prosperity has been well documented (Porter, 1998). The paper is to identify the extent to which technology spillovers are associated with regional economic growth. This is an area of active research.

In this study, the authors provide a new approach of monitoring cluster evolution by conducting a longitudinal analysis of the dynamics of inventor networks. The paper focuses on the telecom sectors of New Jersey and Texas. For almost a century, New Jersey has been the leader in telecommunications innovation, due to the presence of Bell Laboratories. With the break-up of AT&T and passage of 1996 Telecommunications Act that drove the de-regulation of US telecommunications market, New Jersey's telecom sector went through a period of rapid change. However, since the industry downturn of 2000, the NJ's telecommunications sector has been experiencing a hard time. While NJ is struggling to recover from the downturn, we've observed that some other states, such as Texas, have been able to pull ahead and show greater growth (He and Fallah, 2005) as measured by the number of telecom patents. It seems that New Jersey's telecommunications cluster is currently stuck in a stagnant state. The analysis of inventor networks within the telecom industry can provide further insight into the evolution of NJ's telecom cluster and the influence of such networks on performance of the cluster.

2. Inventors Networks

Complex networks are often quantified by three attributes: clustering coefficient, average path length, and degree distribution. The clustering coefficient measures the cliquishness of a network, which is conceptualized by the likelihood that any two nodes that are connected to the same node are connected with each other. The average path length measures the typical separation between any two nodes. Degree distribution maps the probability of finding a node with a given number of edges. Following the discovery of “small world” network phenomenon, which is characterized by short average path length and high degree of clustering properties (Watts and Strogatz, 1998), many empirical studies proved that small-world properties are prevalent in many actual networks such as airline transportation networks and patent citation networks. The dense and clustered relationships encourage trust and close collaboration, whereas distant ties act as bridge for fresh and non-redundant information to flow (Fleming et al., 2004). There is evidence that the rate of knowledge diffusion is highest in small-world networks (Bala and Goyal, 1998; Cowan and Jonard, 2003; Morone and Taylor, 2004).

In order to test the relationship between knowledge transfer network and regional innovation output, Fleming et. al (2004) analyzed co-authorship network data from US patents of the period between 1975 and 2002. Their results are inconsistent with the generally believed proposition that “small world” networks are associated with high level of innovation. It appeared that decreased path length and component agglomeration are positively related to future innovation output; however clustering, in that study, has a negative impact on subsequent patenting. In fact, the existing empirical literature is not rich enough to illustrate the role of knowledge spillovers, created by inventors’ mobility or/and collaboration, in promoting the development of clusters. In this study, we will investigate the evolution of telecom inventor networks of New Jersey versus Texas, and examine their significant differences which may explain the differences in innovation growth and cluster development of the two states.

3. Data and analysis approach

In this study we map the network of telecom innovators using patent co-authorship data. We believe patent co-authorship data is a good quantitative indicator for knowledge exchange. As majority of patents are delivered by teams instead of independent individuals, it is reasonable to assume that co-authors know each other and technical information exchange occurs in the process of innovation. Secondly, patent data can reflect the mobility of the inventors as long as they create patents in different firms or organizations. Cooper’s study (2001) suggests that a higher rate of job mobility corresponds to greater innovation progress because parts of the knowledge generated by a mobile worker can be utilized by both firms involved.

The data for this study was originally collected from the United States Patent and Trademark Office (USPTO) and organized by Jaffe, et. al. (2002). This dataset provided us with categorized patent information covering the period between 1975 and 1999. The objective of our study is to analyze the dynamics of inventor networks for different geographical clusters over time. For this study, we selected the telecom

patents granted to inventors in New Jersey and Texas between 1986 and 1999 for analysis. We consider a patent belongs to either New Jersey or Texas, as long as one or more inventors of the patent were located within that state. Those patents belonging to both states were deleted for this initial study (accounts for 0.9% of the total number of patents).

For each state, we investigated how the inventor network evolved over time by moving a 3-year window. The patent dataset enables us to develop a bipartite network (upper portion of Fig. 1) which consists of two sets of vertices---patent assignees and patent inventors. This type of affiliation network connects inventors to assignees, not assignees to assignees or inventors to inventors, at least not directly. The bipartite networks are difficult to interpret as network parameters such as degree distribution have different meanings for different sets of vertices. In order to make the bipartite network more meaningful, we transform the bipartite network to two one-mode networks. Figure 1 illustrates an example of this transformation from bipartite to one-mode networks. The network analysis tool Pajek was used to explore the patent network and visualize the analysis results.

For the one-mode network of assignees, a link between two nodes means that the two organizations share at least one common inventor. In this network, a link indicates that one or more inventors have created patents for both of the organizations during that time frame. In practice this happens when an inventor who creates a patent for company A joins a team in company B or moves to company B and creates a new patent that is assigned to company B. In either of the scenarios, one can assume there would be a knowledge spillover due to R&D collaboration or job movement.

4. Findings and interpretation

As described, using Pajek software package, we constructed two sets of one-mode networks for each geographical cluster with a longitudinal approach. This paper focuses on the one-mode networks which consist of organizations, in which a tie between any two nodes indicates at least one patent inventor is shared by both assignees during the window period.

Before proceeding to examine the network structures and level of inventors' mobility, we had noticed from the original patent dataset that some assignees indeed represent entities which are associated with a large organization. The Bell System's multiple entities form linkages between their innovators via patent co-authorship and those linkages could account for a considerable portion of linkages over the whole network (He and Fallah, 2006). Since this kind of linkage is not directly associated with the spontaneous job mobility of innovators, which is the focus of our study, we regarded them as noise for our interpretation and therefore treated multiple entities of an organization as one unit by reassigning a new unique name to them.

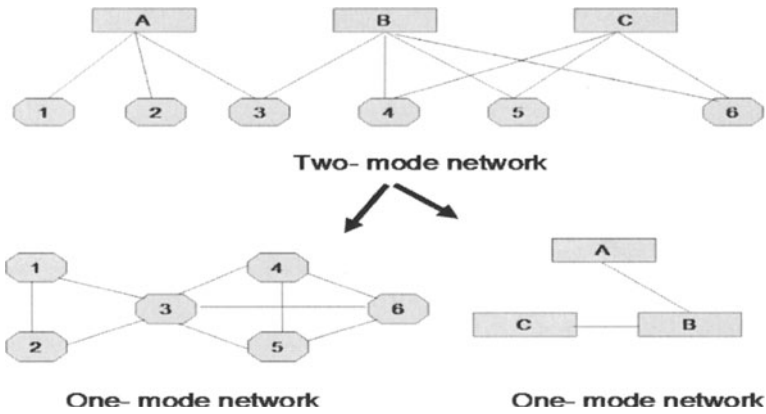


Figure 1: Transformation of a two-mode network to one-mode networks

Figure 2 shows the average node degree of all vertices for each state over different three year window periods. A higher degree of vertices implies a denser network, which in this case indicates inventors are more likely to move from one organization to multiple other ones. Based on this figure, it appears the NJ network was better connected in the earlier years, but the advantage was lessened gradually as the time window moves ahead and NJ finally fell behind of TX in the last period of observation. The situation of NJ in patent network connectedness during the early years may correspond to the regulatory adjustment of the telecom industry. The *1984 Bell System Divestiture* broke up the monopoly of AT&T which led to some redistribution of employees including some of the R&D people. The Telecom deregulation created a substantial undeveloped new market which could be exploited with new technologies. As new starts-ups emerge in a cluster, the job mobility among organizations can be expected to grow also. As can be seen in Figure 2, the connectedness of NJ's patent network had experienced a dynamic change during the period between 1986 and 1993. The network of TX maintained a low level of connectedness in that period because there was very little telecom R&D work in that state. Starting from 1993, the networks in both NJ and TX demonstrated a significant growing trend in connectedness. Indeed, largely due to the further openness of telecom market, that was also a period in which the total patent output for both states was growing rapidly (Figure 3).

In terms of network structure, the major difference between the NJ network and the TX one is the level of degree centralization². We observe that the NJ network is more centralized than that of TX, especially for the later period of observation (Figure 4). Based on our analysis, we noticed that, compared with the counterpart of TX, the main component of the NJ network always accounts for a larger portion of

² Degree centralization is defined as the variation in the degree of vertices divided by the maximum degree variation which is possible in a network of the same size (De Nooy, 2005). Put it differently, a network is more centralized when the vertices vary more with respect to their centrality; a star topology network is an extreme with degree centralization equals one.

the total connectivity, and the difference becomes more significant in the later periods. This may correspond to the disappearance of many of the start-ups that emerged in mid to late 1990s. Based on the network measurement in overall connectedness, though the NJ network also shows a growing trend after 1993, we conclude that the growth was largely corresponding to the size growth of the main component rather than a balanced growing network.

Figure 5 and 7 visualize the one-mode network of assignees for NJ and TX, respectively (window period of 1997-1999). Figure 6 and 8 correspondingly demonstrate the main components extracted from the parent networks. Interestingly, we notice that the “Bell Replace” which represents the entities of the old Bell System is the key hub maintaining the main component of the NJ network (Figure 6).

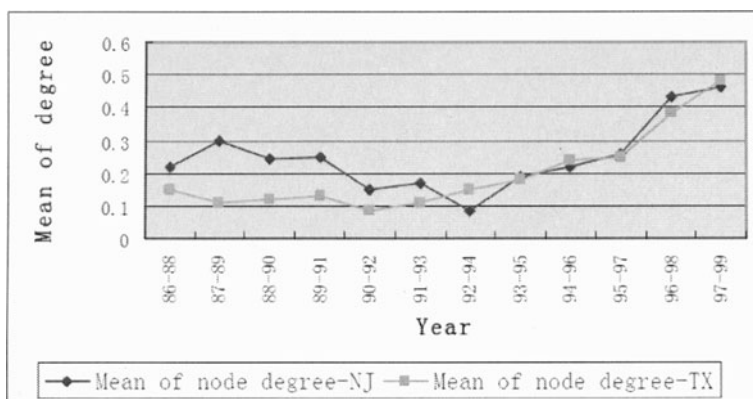


Figure 2: Mean of Degree – NJ vs. TX

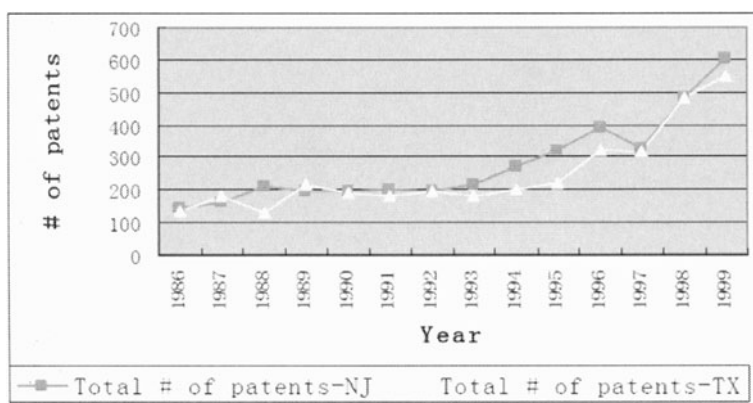


Figure 3: Total number of telecom patents – NJ vs. TX

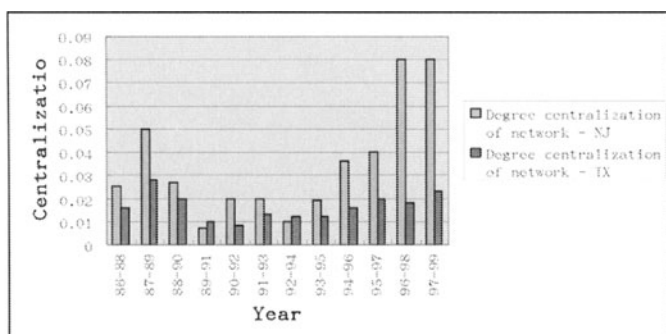


Figure 4: Network Centralization – NJ vs. TX

Consistent with above-mentioned findings, the visualization of TX network demonstrates a decentralized pattern, in which most of the network connection would still exist even if the most connected hub is removed (Figure 7, 8).



Figure 5: NJ's one-mode network of assignees – 1997-1999



Figure 6: Main component extracted from Fig. 5



Figure 7: TX's one-mode network of assignees – 1997-1999

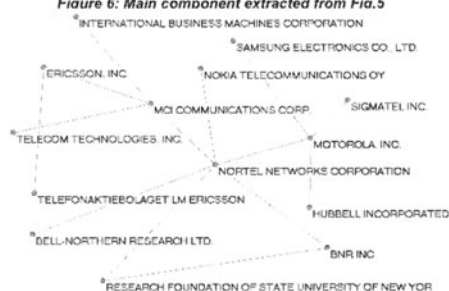


Figure 8: Main component extracted from Fig. 7

We interpret the highly centralized network structure as a weakness of NJ's telecom industry which may explain the cluster's performance in innovation output. As a majority of job movements in the cluster originate from a common source, the diversity of the knowledge transferred in such a network is limited if compared to a network in which innovators move around more frequently with a variety of random routes. Also, considering the history and background of AT&T and the change of regulatory environment, there is a good possibility that the AT&T-hubbed patent

network may, to a large extent, correspond to a firm- level adjustment resulting from the corporate fragmentation, rather than the macro-dynamics of labor market; while the latter scenario is a more desirable attribute for encouraging cluster development.

5. Conclusions and future work

Our results illustrates that patterns of job mobility may be predictive of the trend in cluster development. The study suggests, compared with New Jersey, Texas telecom inventors were more frequently changing their employers, starting their own business or/and joining others teams from different organizations. The latter scenario may often result from formal collaborations between organizations, such as contracted R&D projects. Either way these types of ties increase the possibility of technical information flowing within the industry cluster, though the two classifications of ties may vary in their capability for knowledge transfer. One limitation of the network analysis is that, based on the patent dataset itself, the proportion of connections corresponding to each type of ties cannot be explicitly measured, so future researches may benefit from interviewing those inventors to further investigate their motivations or duties involved with the connected patents.

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Towards Computing the Battle for Hearts and Minds: Lessons from the Vendée

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For Charles Tilly (1929 – 2008)

We analyze the conditions and processes that spawned a historic case of insurgency in the context of regime change. The analysis is an early step in the development of formal models that capture the complex dynamics of insurgencies, resistance and other conflicts that are often characterized as “battles for hearts and minds” (henceforth BHAM). The characterization, however, flattens the complexities of the conflict. It suggests bloodless engagements where victories come from public relations and demonstration projects that foster positive attitudes among a subject population. Officials conducting these battles sometimes use the label to mask their ignorance of the complexities and sometimes with the intention of minimizing their difficulties in dealing with them. Modeling can therefore be a constructive step in overcoming their impoverished thinking.

1 Introduction

American government officials have described the struggle of United States and Iraqi government forces against insurgents in Iraq as a “battle for hearts and minds.” The description flattens the complex dynamics, which fuel this conflict and similarly described ones. It suggests that either side can gain victory by fostering positive attitudes toward it among a relatively inert population through

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good public relations and demonstration projects. Since that has hardly been the case, models of “battles for hearts and minds” (henceforth BHAM) should include both the dynamics that generate such insurgencies and those accounting for their progress. By examining a historic insurgency, especially one that occurred within the context of regime change, we can appreciate the complexities in BHAM’s and be prepared to build more adequate models of them.

A useful historic case is the Vendée, a peasant-based insurgency or counter-revolution during the French Revolution in 1793. The insurgency spread through the lower Loire region, on the west coast of France, beneath Brittany, with one of its principal sites being the department of Vendée, hence the name. After achieving some initial success, the insurgency was suppressed by troops that the revolutionary government sent into the area, but the rest of the decade witnessed occasional and sizeable outbursts of violence. As many as 150,000 people died as a result of the Vendée, the overwhelming majority of whom were executed by the victorious government for being insurgents or their suspected supporters[Schama, 1989]. The dead numbered at least 10% of the region’s indigenous population and, despite the Reign of Terror occurring elsewhere in France, especially in Paris, accounted for the bulk of killing by the Revolution in 1789 – 1795. The legacy of the Vendée was a deep emotional rift between the political right and left in France that persisted well into the 20th century.

2 Reasons for Making it the Case

The Vendée was a rural revolt in a pre-modern, early capitalist society; consequently, it is not directly comparable to urban based insurgencies in developing countries. Nevertheless, there are several good reasons for studying its dynamics. First, it appears the foremost instance where the French Revolution lost a BHAM. Here *liberté, égalité et fraternité* were not welcomed with shouts of joy, but with cries of *monarché et clergé* and shots of anger. Second, the case permits a look at the links of an insurgency to “regime change;” in respect to having this context, it resembles the insurgency in Iraq. In both cases, the regime change involves more than the replacement of one ruler by another; the process creates new institutions and empowers a new set of groups, while suppressing some groups formerly in power and continuing to exclude others. This has some implications for insurgency, since the excluded have reason to resist their exclusion, violently if need be, as even American officials and media have begun to understand in the case of Iraq. Third, the Vendée is a historically distant episode, at least for American audiences, so theories, interpretations and data about it can be discussed with some dispassion. In France, where the Vendée is part of historical legacy, discussions of its significance and moral accountability remain contentious, though less so

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than, say, those on the Algerian war. Finally, the emergence of the Vendée is the subject of a classic study that drew on numerous demographic, social and political data. [Tilly, 1964] casts this account in terms of change in social organization, economic opportunities and frustrations, social alliances and their connections with political control. His work gives perspective to the role of attitude and opportunism in explaining a BHAM.

Moreover, Tilly's methods of building the social and material worlds of the insurgents from the ground up, highlight conditions which support complex social dynamics, e.g., accumulated grievances surpassing thresholds for action, social relations that spur or inhibit emergence of large, mobilized groups. model of insurgency. These methods indeed suggest a particular dynamic model for explaining the outbreak of insurgency, but we do not intend in examining them to produce a master pattern or analogy that explains or predicts the unfolding situation in Iraq and insurgencies elsewhere. Rather we believe that a guided, methodologically rigorous review of a past situation can expand our thinking about current and future ones. We can learn that situations, which appear simple at first sight, might prove very complex.

2.1 The Principal Findings according to Tilly

Tilly uses a comparative method to probe the character of the Vendée. He identifies two adjacent districts, Mauges and Saumurois in the lower Loire, whose populations supported and opposed the insurgency, respectively. He compares the socio-economic conditions in each district and the consequences in each of measures that the revolutionary government in Paris initiated, such as the sale of church lands and military conscription. To broadly summarize his principal finding, peasants and workers rose against the French Revolution because it primarily benefited the bourgeois, at their expense, and excluded them from participation in the management of local affairs. Thus the insurgents' first acts were to drive out or kill the revolutionary cadres – bourgeois local officials, their supporters and the local militias. Then in scattered skirmishes they engaged the soldiers sent in relief of the officials. Only after their initial successes and with a need for better organization did the insurgents turn for leadership to some nobles and ex-soldiers in the area.

2.2 The Reasons for the Results

Class conflicts fueled the violence. These were latent in 1789, but the revolution created conditions and processes that in turn exacerbated and actualized them. First, in Mauges bourgeois were squeezing peasants, mostly subsistence farmers with few ties to the towns and their markets. Some bourgeois had acquired land

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and proved more effective than the nobles in collecting rents from peasant tenants. The bourgeois also invariably outbid peasants when church lands in the district were put up for sale in 1791. Second, workers in the fairly extensive textile industry, which was controlled by the bourgeoisie, became increasingly unemployed during the revolution. This was partly due to the loss of some foreign markets in the late 1780s, but the situation worsened when foreign armies invaded France to quash the revolution and disrupted the export trade. These structural conflicts were not balanced by a need for peasants and bourgeois to collaborate in struggle against the local nobility, because almost all the nobles were absentees. The few who lived in the area either emigrated or withdrew from public affairs in the first years of the revolution. (Note this same factor undermines a theory that the peasants resisted the revolution out of loyalty to the nobles, developed through frequent interactions with them.) Saumurois, in contrast, provided fewer grounds for class conflict. First, the peasants there were principally occupied in growing grapes and wine making for commercial markets. That brought them into the towns and frequent cooperative contacts with the bourgeois. Second, the percent of textile workers in the district was much lower.

2.3 Influences on Tilly's Theoretical Framework

Tilly's method has several influences of particular relevance for students of complex systems: the *Annales* school of French historiography, Marx's theory of socio-economic development and American theorists of change in social organization, notably Lewis Mumford, C. Wright Mills and Eric Wolf. These theorists were influenced by sociologist Max Weber as well as by Marx.

The *Annales* school was founded at the end of the 1920s, by French historians Marc Bloch and Lucien Febvre, and built on the considerable archival work in the late nineteenth and early centuries. The *Annales* approach integrated economic, social and cultural history with the political history that had previously dominated accounts of the past. It emphasized the importance of local conditions in differentiating the receptions, adaptations and development of institutions and practices. Its practitioners were generally suspicious of grand syntheses of history that were not rooted in careful, data-rich examinations of the material life and social realities of their subjects. Influenced by Marx, the approach can be characterized as "history from the bottom up," in contrast to the "top down" Hegelian histories that sought to define and describe a period in terms of a multi-faceted, unifying "spirit."

Marx himself can easily be claimed as a theorist of complex, dynamic, self-organizing, living systems. According to him, people create their history, though the outcomes of their actions seldom match the intentions, often because of systemic constraints and the mutual interference of actions. On his view, a

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new mode of production, e.g., industrial production, the classes associated with it and their conflicts emerge within the context of the current, dominant mode. The new mode expands and is iterated over different locales; the efforts of diverse individuals and groups amount to a process of organizing all production under this new mode. Eventually political revolution sweeps away the legal and political structures that block its progress. Thus, quantitative change in the system becomes qualitative, but the seeds for the next new mode are being sown. In terms of complexity theory, the social system is far from equilibrium and its transformations are path dependent.

This theory, however, does not entirely fit a program of “history from the bottom up.” In his later writings, which were best known to the historians he influenced, Marx tended to reify social structure, especially class. Classes are treated as cohesive groups, with memberships and interests determined unambiguously by peoples’ places and degree of control in production systems, rather than as conceptual handles for actual social networks that form and change among individuals and groups, on a variety of bases.¹ This treatment creates a gap between the level of individuals and their collective actions.² Tilly [2002; 2003] in more recent writings acknowledges this tendency on his part in the Vendée study. As a result, he might have minimized the importance of networking among local opponents to the revolution in the two years preceding the outbreak of violence and presented those outbreaks as more spontaneous than they probably were.

Ironically, Marx offers little help in understanding an agrarian insurgency, since he considered the peasants politically inert or, as he famously dismissed them, “a sack of potatoes.” [Marx, 1852]. Tilly shares some of this opinion. In discounting the notion that some ideology or vision of restored monarchy motivated the Vendée, he approvingly quotes the Marxist theorist Karl Kautsky to the effect that the French peasant’s horizons were limited to the nearby village and the world beyond it was a shadowy place. This point is probably correct; it would help explain why the insurgents sought out nobles to lead them and why they later failed to coordinate effectively the goals and activities of their several “armies.” However, it does not clarify the context in which events spurred the formation of those armies. With respect to that question, Tilly finds the American of social change more helpful.

On their basis, he describes eighteenth century as undergoing urbanization or a set of changes associated with “the appearance and expansion of large-scale coordinated activities in a society” [Tilly, 1964, p. 16]. In addition to the re-emergence of the city as a center of population, activity and control, these processes include social differentiation, standardization in production and shifts

¹ [Marx & Engels, 1848] do see both the bourgeoisie and proletariat in these terms, as do some Marxist historians, like [Thompson, 1991].

² Reference is to processes of recruitment and collective will formation, rather than the [Olson, 1971] problematic of collective action for public goods among rational actors, addressed by [Axelrod, 1984] and other models of social dilemmas.

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toward instrumental social relationships. These developments occurred in rural as well as urban France, but their occurrence was uneven. For example, on the eve of the Revolution, urbanization was much farther advanced in the Saumurois countryside than in the *bocage* lands of Mauges and other districts. As previously noted, the Saumurois peasants were engaged in monoculture; they had links to the towns and thoughts about nameless consumers and distant markets. The peasants in Mauges lived on their own produce and came to town only when they needed to sell livestock for money to pay taxes or rents. However, the urbanization of rural Mauges accelerated with the revolution. More effective tax collection and measures, reviewed in the next section, that reorganized social institutions increasingly chained the peasants to the towns and increased their hostility toward them.

2.4 The Strengths of Tilly's Method

The above influences help shape Tilly's comparative, "class conscious," process oriented approach that is alert to instantiations of broad social changes in particular locales. His theoretical structures and the historical evidence he uses to support them undercut attributions of the Vendée to the peasants' change of heart as the result of a single event or to the hold of the old regime on their collective mentality. To rephrase a principal finding, not all the peasants in the region demanded a return to the old regime. Those who did voiced their demand only after several years of the revolution and out of hostility toward the bourgeois who implemented and supported the revolution in their locales. The finding similarly rebuts an explanation of the insurgency based on opportunism. This is the argument that where rough or distant areas make policing difficult or government authority is weak, gangs will form and use violence for their own private gain. Such opportunism is evident in kidnappings or looting in countries that have low capacities for internal control and/ or inaccessible areas, e.g., Columbia. Indeed, the hedged fields (*bocages*) in Mauges and elsewhere in the lower Loire were to give the insurgents some tactical advantages over the soldiers, who were sent to suppress them. But in some ways the terrain in Saumurois was as difficult, and there was little difference between the districts in government control before the outbreak of the Vendée. Moreover, while some opportunistic looting accompanied the Vendée, its violence was more coordinated and destructive than those of small groups seeking private gains.

From the perspective of formal modeling, particularly agent based modeling, this comparative method has constructed two different systems or populations that will be differentially perturbed by the same events. Each of the systems is composed of heterogeneous agents, that is, agents with different instruction sets based here on occupational categories. More, however, is involved than just different distributions of the various agent types in each system, because the agents are "wired together" differently. The interaction patterns of agents of the

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same type – the *who* with *whom* about *what* in *what manner* and *how frequently* – are likely to differ over the two systems. These patterns have ramifications for the agents' instruction sets. As we have seen, although both wine growers and *hocage* farmers can be labeled peasants, their mentalities, interests and, consequently, responses to events differed. On the other hand, we would not expect significant differences in the instruction sets of textile workers over the systems.

3 The Emergence of the Vendée Insurgency

3.1 Events Driving the Emergence

Important measures taken by the French authorities in the early 1790s included a) the administrative reorganization of France into departments, cantons and communes; b) the forced sale of lands owned by churches and monasteries; c) the requirement that priests swear allegiance to the French state and the dismissal of those priests who refused; d) the military conscription of 1793. The implementation of these measures brought conflicts originally based on competing economic interests into political space. [Tilly, 1964] notes “all important events...between 1790 and the outbreak of the counter-revolution found two parties opposed to each other.” But these parties were chiefly class based: the bourgeois Patriots, who supported, implemented and personally benefited from the measures, and the peasants and workers, who resisted or tried to circumvent them. Politicization intensified the latent economic conflict and with each new measure the social distance between the sides increased, even as their members came into more frequent contact.

The administrative reorganization enhanced the power and reach of the central government in Paris and the efficiency of tax collection. At the local level, it combined small villages into larger communes, and changed locations of government offices from one town to another, according to the preferences of local supporters of the revolution. Many village mayors, usually parish priests, lost their offices. An additional measure excluded poorer peasants and workers from voting in the new councils, by basing this traditional right on the amount of taxes paid. The bourgeois quickly dominated these councils, which had power over the distribution of some local tax burden, the organization of labor for public works, and meeting military conscription quotas. The affected peasants and textile workers resented these moves. Most lost their individual status as commune members, many saw their villages lose prestige, some lost their link in the village mayor to the outside world, and all the subsistence peasants now had to monetize more of their activities to meet the rising tax and rent bills. (Many peasants thought at first that the revolution had cancelled land rents in money, but found to their dismay that it had only cancelled rents in service, most of which had already been commuted to money payments before

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the revolution.)

The breakup and sale of the ecclesiastical estates in 1791-1792 did not benefit the *hocage* peasants who were eager to acquire land. Some in the Mauges tried to overcome their limited liquidity by forming buyer groups, but in each case bourgeois buyers outbid these groups. In Saumurois, however, some winegrowers built upon their existing relationships with bourgeois merchants to form successful land buying syndicates.

To compensate for the clergy for the loss of income following the confiscation and sale of the church land, the state offered to pay their salaries, providing they would swear allegiance to the state. Most priests regarded that demand as a means to put them under state control, a particularly loathsome position at a time when the revolutionary government itself was promoting a "religion of reason," with its own rituals and celebrations, in direct opposition to Christianity and its rites. Faced with this choice or the prospect of dismissal that was tantamount to abandoning their parishioners, most priests refused to swear. The state soon closed the churches of some and replaced other with clergy, who swore allegiance, were often related to prominent Patriots and sometimes foreign to the region. Many disposed priests celebrated mass and other rites in secret and almost all parishioners joined with them to the point that local officials occasionally conducted sweeps of peasant and worker houses to drag newly born to the government priests for baptism. The struggle over the clergy was political and social as well as religious, since the village priest was often the hub in the community (very much in the network sense) for the peasants and workers. However it did provide a distinctly Catholic dimension to mobilizing and articulating hostility to the bourgeoisie. Support for the Vendée would be strongest in those areas of the region where the rate of refusal had been highest.

In early 1793, the National Assembly in Paris, faced with the invasion of France by foreign armies, order a national conscription. The bourgeois who controlled the local communal councils in the lower Loire quite logically decided to draft first young peasants and workers, since the bourgeoisie and their affiliates were needed at home to administer the revolution. There were too few of them to spare. Peasants and workers, most not having a vote in council, took exception to these decisions. In mid-March, in several communes, angry crowds, braced by drink, drove out the local officials and later disarmed the few militiamen who faced them.

3.2 The Government's Failure to Understand the Insurgency

One might wonder what the bourgeois both in Paris and the lower Loire were thinking during this contentious run-up to the Vendée. Did they not realize their actions were lighting a powder keg upon which they happened to be sitting?

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Apparently not. Because of their structural conflict with peasants and workers, the bourgeois neither had sympathy for their grievances nor were prepared to deal with them politically. They believed their polity should include only men of property. In the same vein, they would later contemptuously dismiss the insurgents as “brigands and beggars,” who were motivated by greed and took advantage of a weak government and hostile terrain.³ It would therefore have to be suppressed by military means. Moreover, the Patriots were too distracted by conflicts within their own camp between the Girondins and the Jacobins and by the pressure of external war to spare much thought on the Vendée. At least none of them at the time seems to have characterized it as a “battle of hearts and minds.”

4 Concluding Lessons and Applicability

The emergence of insurgency appears to be an epigenetic development from latent economic conflict through ideologically tinged political conflict to violence. This development is accompanied at the local level by increasing arousal and cohesion among the future insurgents, but there is scant development of a more extensive network. The disposed priest, if he remains in the parish, provides much of this cohesion. He serves as a hub for the aggrieved peasants and workers. His saying mass with these parishioners constitutes a collective transgression of the state's authority. A major point in this development is the exclusion of the peasants and workers from the institutionalized political arena, at a time when the regime assumes greater control over the allocation of opportunities and burdens. Since the regime would not let the peasants withdraw to their former state of relative isolation, they resort to violence to try to block its power.

How applicable are the dynamics of an agrarian insurgency to contemporary situations? Some lessons are almost certainly relevant. First, economic hardship or the failure of economic promise is a pre-condition for a group's turn to insurgency. So winning the battle for bellies might prevent the need to fight a battle for hearts and minds. Second, insurgency is a probable response by a group to its exclusion from a political order that controls all the economic opportunities. So while military power might win a battle for hearts and minds, a political solution can probably do it with fewer lives lost.

³ Such explanations are typical of elite mentalities. Social movement research finds that people who are well embedded in social networks are more likely to join social movements than marginal or isolated “outlaw” types (Diani & McAdam, 2003).

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Chapter 22

The Structure of Algal Population in the Presence of Toxicants

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1.1. Introduction

Algal bioassays are routinely employed as part of a battery of toxicity tests to assess the environmental impacts of contaminants on aquatic ecosystems. This estimation is an essential component of the ecological risk assessment.

From an ecotoxicological point of view, analysis of the dose - effect relationship between toxic substances and biota reaction plays a key role in the understanding of experimental data and its quantitative assessment. However, the statistically and biologically significant responses (hormesis and paradoxical, three-phase curves) frequently occur below the NOAEL. It supports the nonrandom nature of such responses and need to transform the phenomena to an accepted for risk assessment. Low-dose effects deal with homeostasis disruptions that are mediated by agonist concentration gradients with different affinities for stimulatory and inhibitory regulatory pathways. The response of biological systems to low levels of exposure has been challenged especially for the hormesis and large implication for the safety standards for health and environment have been indicated [Calabrese 2003].

Water pollution is altering ecosystem, community, population, organism, cell, subcell, molecular – level processes. It are causing structural-functional alteration in populations and communities and decreasing a biodiversity. Chromium is one of the contaminants, which is extensively used in industry and high levels of chromium contamination of both terrestrial and aquatic habitats occur. Pesticides which are used to protect agricultural crops can be detected in aquatic environments, too.

The aim of our research was to reveal the general rules of microalgal population response on toxic action of the pesticide (fungicide) and chromium according to changes in dimensional-age and functional population structure.

1.2. Materials and Methods

The culture of green chlorococcal alga *Scenedesmus quadricauda* (Turp.) Breb. (strain S-3) was grown in Uspenskii medium N1 (composition, g/l: 0.025 KNO₃, 0.025 MgSO₄, 0.1 KH₂PO₄, 0.025 Ca(NO₃)₂, 0.0345 K₂CO₃, 0.002 Fe₂(SO₄)₃; pH 7.0-7.3) in conical flasks in luminostat under periodic illumination (12:12 h). The culture contained two- and four-cellular coenobia. Cells were counted with a Goryaev's hemocytometer under a light microscope. Cell width was measured with a calibrated ocular micrometer. Cells were grouped according to their width into classes at 0.5 μm steps. And the cell size distribution was plotted as a percentage of the total cell number. Number of alive, dead and dying cells was counted with luminescent microscope Axioskop 2FS (Carl Zeiss, Germany). The functional state of the photosynthetic apparatus of the alga was characterized by *in vivo* measuring of delayed fluorescence (DF) of chlorophyll *a*. The amplitude of the DF decay phase during photosynthetic induction in dark pre-adapted samples was used to characterize the photosynthetic efficiency (PE, η). We investigated the toxic action of potassium dichromate (K₂Cr₂O₇, PD), fungicide imazalil sulfate (1-[2-(2,4-dichlorophenyl)-2(2-propenyloxy)ethyl]-1H-imidazole sulfate, IS) in the long-term experiments up to 30-36 days in three assays.

1.3. Results and Discussion

In the culture exposed to the toxicants for 4-7 days, cell number changed in a complicated pattern (fig. 1). At low and high concentrations of IS and PD the number of cells was less than in the control culture, whereas at moderate concentrations had no effect. Such concentration-response dependence we could observe during long-term experiment. This type of the population number changes (so called “paradoxical reaction”) is a usual behavior of biological systems in increasing of damaging factors intensity. We have shown earlier that nonlinear concentration response curve of cell survival reflects of hierarchy of cell responses to increasing concentration of IS: cell division inhibition in low doses, stress and adaptive tolerance increasing in moderate doses and immature cell division and death in high doses [Prokhotskaya 2003]. The number of dead cells increased only at high toxicant concentration (fig. 1). Therefore, the change in the relative cell number at low IS and PD concentrations cannot be explained by the summing of the process of cell division and death.

It was supposed to be existence of certain principles of intrapopulation responses to the toxic exposure, which does not depend on chemical nature of acting factor. These principles reflect the changes of structural and functional characteristics of algal population. We investigated the changes of population structure and average functional characteristics of cells of *S. quadricauda* in the control cultures and in the presence of various concentrations of the toxic substances.

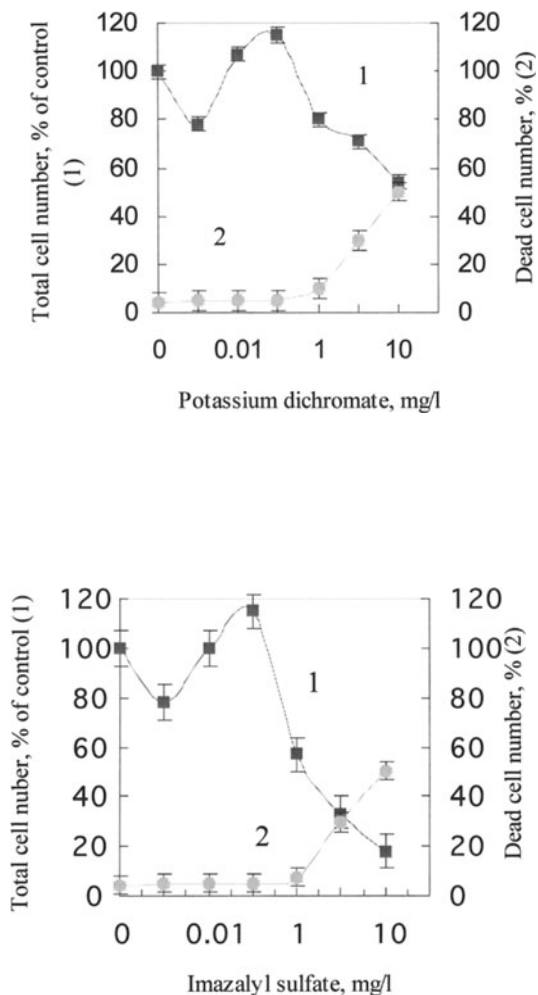


Figure. 1. Changes of the total cell number (1) and dead cell number (2) in the *S. quadricauda* culture as a function of PD and IS concentrations on the 4th – 7th days of treatment.

1.3.1. Size-age distribution, coenobial composition and functional characteristics of the control culture *S. quadricauda*

The growth curve of the control culture had a stepwise shape apparently due to a partly synchronization of cell division under continuous light-dark periods. We can observe the simultaneous presence of two cell groups differing in size (large and small cells).

That fact agrees completely with model previously described for population structure of chlorococcal alga *Chlorella* and *Scenedesmus* [Tamiya 1966, Senger 1986].

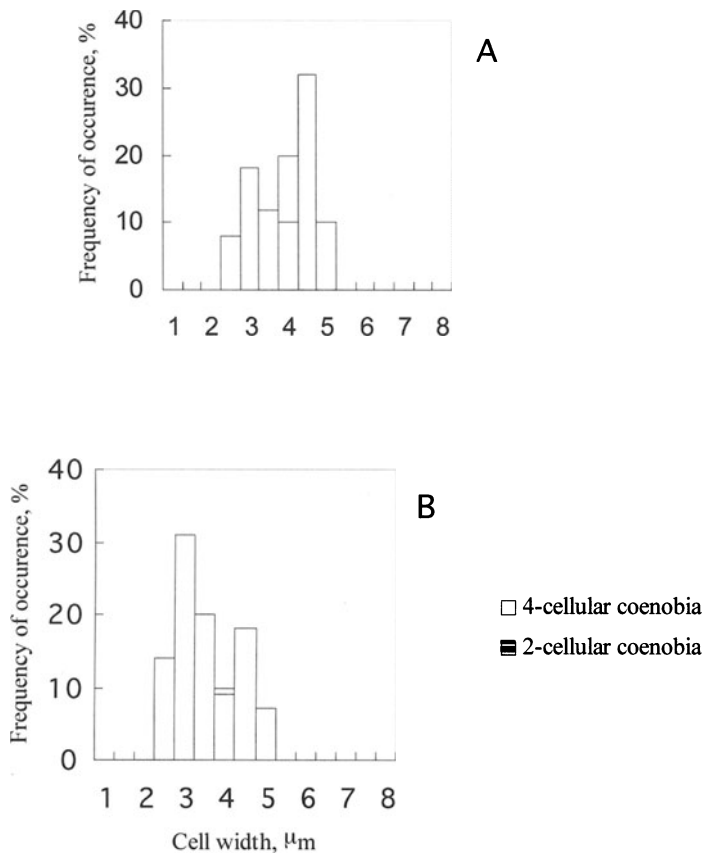


Figure. 2. Cell width distribution in the control culture of *S. quadricauda*. A – before and B – after increasing of cell number.

Figures 2 shows changes in the cell size distribution during growth of the control culture. Large cells (4.5 μm in width) composing 2-cellular coenobia dominated before the cell number increasing; the share of small cells in 4-cellular coenobia (3.0-3.5 μm) was less, than the share of large cells. The increase of the cell number was accompanied by mirror changes in bimodal distribution with “large” maximum for small-sized cells and “lower” maximum for large-sized cells. The volumes of large and small cells differed by a factor of two. Hence, it seems likely that large cells are ready for division and small cells are daughter young cells.

The sedimented isolation of young cells from the various-aged culture revealed the functional differences between mature and young cells. The PE was slightly higher in small cells ($\eta=0.86\pm0.02$) than in large cells ($\eta=0.80\pm0.02$). The thermal stability of

thylakoid membranes in small cells was higher than that of large cells (49.5 and 47.5°C, respectively).

1.3.2. Effect of toxicants at low concentrations (0.001 mg/l)

The chromium and IS at concentration of 0.001 mg/l were found have an slight influence upon cell number, cell division rates, photosynthetic efficiency and share of alive cells. We observed slowdown population growth as compared to the control culture starting from 3th – 4th days. Analysis of size-age distribution showed the appearance of large cells (width 4.5-5.5 μm) in 2-cellular coenobia. It was seemingly caused by cell division inhibition. Later, the size of these cells increased to 6.0-6.5 μm , they became single and formed 50 % of population. The size distribution of cells had two maxima: the first wide maximum included proliferating cells, united in 2- and 4-cellular coenobia and the second maximum was comprised by large single cells. By the 25th day of experiment, large cells transformed into single round “giant cells”. The reason of possible population growth delay under low-level toxic exposure was the arrest of proliferation of some cells rather than deceleration of cell cycle in all cells. The other part of the population did not respond to the presence of PD and IS and continued to proliferate. In other words, the respond of the algal population to weak toxic effect can be related with cell heterogeneity. Toxicant had no strong effect on the PE as compared to the control level.

1.3.3. Effect of toxicants at moderate concentrations (0.01-0.1 mg/l)

In the presence of moderate, seemingly inactive concentrations of toxicants cell division was stopped during two days, and size both large and small cells increased. Simultaneously, the share of large cells (4.5-5.0 μm) in 2-cellular coenobia increased. On the third day, cell division was restored synchronously and then cell number was only slightly differed from the control level. The cell population mostly contained small cells organized in 4-cellular coenobia (maximum in the cell size distribution near 3.0-3.5 μm , which is characteristic of the control culture, was restored).

During the cell division arrest the PE decreased only slightly ($\eta=0.70\pm0.02$) as compared to the control culture ($\eta=0.82\pm0.02$), but it was restored within two days to the control level. The thermal stability of large-sized cells became 1.5 °C higher than that for the control culture. After cells are being resumed division, they retained the elevated thermal stability. It was suggested that we observed an adaptive increase in cell resistance to the toxicants.

1.3.4. Effect of toxicants at high concentrations (1.0-3.0 mg/l)

At sublethal concentrations of IS and PD the culture growth was stopped for a long period of time (up to 70% relative cell number decreasing by the 30th day of experiment). Number of dead cells varied from 15 % in the presence of IS to 30 % in the presence of PD. During 4th – 21th days the large cells (width 6.5-7.0 μm) appeared in both 2- and 4-cellular coenobia. They did not divide and had only one nucleus. Later, (21st - 30th days) the changes of the algal population structure depended on the chemical structure of the toxicant. In the presence of PD the cell size distribution became the

same as the control one with maxima 3.5 and 5.0 μm . It means that initial cell division arrest was reversible even under the toxic pressure, and the usual cell cycle was restored.

The response of algal population to IS at sublethal concentration was drastically different. The cell width was 11.0–12.0 μm by the 30th day. The coenobial envelope was disrupted, and only single giant cells were present in the culture. Division of such cells resumed after they had been washed of fungicide and transferred to a toxicant-free medium. 2- and 4-cellular coenobia with control-sized cells reappeared in the culture.

At the concentration 3.0 mg/l of PD the cell number was the same as initial one during the experiment. Analysis of size-age structure and functional characteristics of the cells showed that there were at least two reasons: delay of cell division of one cells and division and death of others. By the 2nd–4th days we observed both undividing large cells (width 6.0 μm) in 2-cellular coenobia and small proliferating cells in 4-cellular coenobia. Then, (4th – 7th days) 2-cellular coenobia with cells (width 3.5–4.0 μm) which were smaller than control ones appeared. It means that toxicants disturbed coenobial wall integrity caused their breakdown. Beginning from 15th day size-age structure was the same as control one again, but a stable increase of relative cell size was observed.

At high PD and IS concentrations (1.0–3.0 mg/l) we can observe long-term cell division inhibition and giant cells forming. Number of dead cells varied from 15 % in the presence of IS (1.0–3.0 mg/l) to 30 % in the presence of PD (1.0–3.0 mg/l). At the concentration 3.0 mg/l of PD the cell number was the same as initial one during the experiment. Analysis of size-age structure and functional characteristics of the cells showed that there were at least two reasons: delay of cell division of one cells and division and death of others. We observed both undividing and proliferating cells.

Sublethal concentrations of IS and PD did not significant inhibit photosynthesis ($\eta=0.72\pm0.03$, as compared to $\eta=0.80\pm0.02$ in the control culture). The thermal stability of thylakoid membranes in giant cells exceeded that of the control by 1.5 °C.

1.3.5. Effect of PD and IS at lethal concentration

At the lethal concentration 10.0 mg/l the cell number decreasing was caused by their death, but during the first day of cultivation the cell number did not change.

The very small cells (width 2.0–2.5 μm) in 2- and 4-cellular coenobia appeared within population (fig. 3, A, B). Therefore, toxicant first initiated cell division in all cells, including those that had not attained the mature cell size. In the normal culture cells divided after attaining about 4.5 μm in diameter, whereas in the presence of toxicant they divided after attaining the size of 3.5 μm . Since the total cell number did not change, it is clear that a certain part of cells died. Therefore, the analysis of size-age population structure can find out the lethal effect earlier than counting of cell number.

Characteristics of DF monotonically changed: the higher the concentrations, the faster they changed. PE was dropped to $\eta=0.50\pm0.05$, as compared to $\eta=0.80\pm0.02$ in the control. The thermal stability of thylakoid membranes decreased to 44–45 °C (48.5°C in the control). These changes accelerated with an increase in IS concentrations within the lethal range (10–20 mg/l) and indicated that cell damage was irreversible.

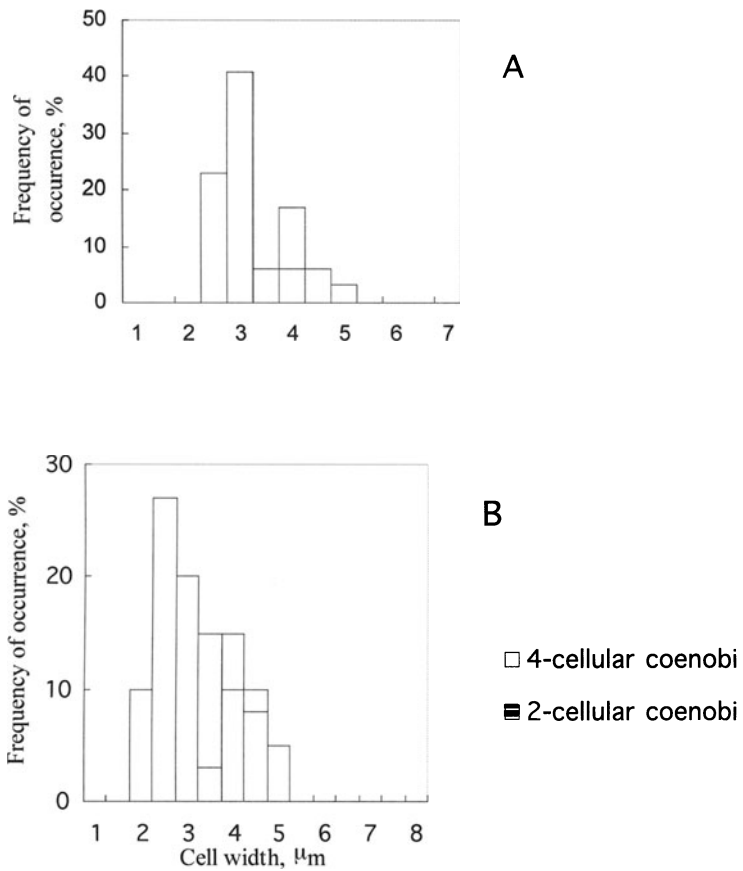


Figure 3. Size-age and coenobial structure of *S. quadricauda* population after PD and IS 10.0 mg/l incubation. A – PD, 1st day of treatment; B – IS, 1st day of treatment.

1.3.6. Long-term effects of PD lethal concentration

With the aim to estimate the share of resistant cells within the heterogeneous algal population we carried out experiment with triple chromium 10.0 mg/l intoxication during 90 days. In spite of the long-term exposition with toxicant some algal cells remained alive. Their number was 5-6 % of initial cell number in the presence of chromium. The cell size spectrum in the presence of PD was rather the same as control one. It indicates that after toxic exposure the normal algal cells remain in population. The photosynthetic activity of these cells was the same as control one, too. The number of these resistant cells corresponds with frequency of mutation for unicellular algae, fungi and bacteria in nature. The presence of resistant cells can be related to their constant presence in population or is the result of selection. It is need of special research for clarification of this phenomenon. The resistant cells cause quick population

restoration after the intoxication. The growth rate of the cells, which were pre-adapted with 3.0 mg/l $K_2Cr_2O_7$ and re-inoculated twice to the medium with 10.0 mg/l $K_2Cr_2O_7$, was ten times as many as that of the control. The maximal resistance of the algae to the toxicants was revealed in spring-summer, the minimal resistance – in winter.

1.4. Conclusion

The concentration-response curve of cell survival reflects a hierarchy of cell responses to increasing concentration of the toxicants. On the base of structural and functional population characteristics analysis we suggest to appropriate the following types of population reaction to the toxicant action: at low PD and IS concentrations, the decreasing of cell number is the result of cell division arrest; at moderate, the absence of effect is caused by renewal of cell division after temporary arrest; at high sublethal concentrations, we can observe long-term cell division inhibition and giant cells forming; at lethal concentration, the cell division is stimulated and the small immature cells predominated at the beginning of intoxication. We offer using described types of reaction to the toxic action for risk assessment and biotesting. The informational value of DF characteristics is most appropriate for recording the responses of algal cultures to lethal concentrations of toxic agents. At low concentrations, DF characteristics are more due to the proportion of various cell types in the population.

In the present research we demonstrated the method of proportion of resistant cells estimation in the heterogeneous algal population. The population heterogeneity ensured the cell number restoration after the removing of toxic pressure due to the minimal amount of the most resistant cells (3-6 % of the initial cell number). Thus, in the long-term intoxication of algal populations experiments we can see the common rules of adaptive and compensation reaction, e. g. elimination of the most sensitive cells and reconstruction the population as a whole system already in the new conditions. By this method we could do qualitative analysis of population reaction to the toxicants: appearance of large and giant cells denotes possible presence of sublethal toxicant concentrations, appearance of very small cells as the result of premature cell division means lethal effect of toxicant. Changes of the population structural and functional characteristics can be special way of survival in unfavourable conditions. Data on the cell number, their photosynthetic characteristics, population structure and share of alive and dead cells will be appropriate for use to predict the most sensitive ecosystem responses and indicate the permissible amount of toxic substances in the environment.

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Chapter 23

Vortex Analogue of Molecules

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Kelvin's theory of vortex atoms, in which Kelvin considered knotted strings as atoms, has been debunked and considered to be a failure. A theory of atoms as vortices is incapable of explaining stability and vibrational properties of atoms. With electrons representing ethereal vortices, the vortex atom theory tries to explain the relation between magnetic field and electrical current. In recent years, this simple Kelvin model has been shown to bear resemblance to the superstring theory. Although the vortex atom theory is considered to be scientifically incorrect (in the sense of its being unable to explain atomic properties), it may still be valid in a dynamical sense as for an example considered in this paper. With atomic potentials of logarithmic type, a dynamically stable vortex buckyball is 'grown' here. If stability is considered only from point of view of Huckel theory and eigenvalues of adjacency matrix, it may not be a sufficient test. It will be shown that such a vortex molecule is stable when Floquet theory of periodic orbits is used as a test of stability.

1.1 Introduction

Buckminsterfullerene, C_{60} , is a perfectly symmetrical molecule made up of 60 carbon atoms arranged in the shape of a soccer ball and resembling a geodesic dome [2]. Hexagonal and pentagonal patches on a soccer ball are sewn together such that there are exactly 60 vertices with 3 edges intersecting at each vertex. In 1996, the Nobel Prize in chemistry was awarded to Smalley, Curl and Kroto for their discovery of this molecule. Structure of C_{60} is a truncated icosahedron with carbon atoms occupying each vertex. Such a structure is obtained from an

icosahedron by truncation of each of its 12 vertices resulting in a 5-membered ring at the location of each vertex and a 6-membered ring corresponding to each icosahedral face. Icosahedral configuration itself is a fixed equilibrium configuration when each of its vertices is replaced by a vortex of strength Γ . C_{60} exhibits an unusually high stability since all its valencies are satisfied by truncated icosahedral structure. Bonding environment of each carbon atom is identical and each carbon atom is located at the intersection of two hexagons and a pentagon.

In a buckyball, double bonds connect the pentagons and each pentagonal ring is made up of single bonds. The bond lengths r_d and r_s are 1.401 and 1.458 Å with cage radius

$$R_c = \frac{1}{2}[g^2(r_d + 2r_s)^2 + r_d^2]^{1/2} \quad (1.1)$$

g is the golden ratio [3].

For point vortex calculations, these points are projected onto a unit sphere.

The molecule is the largest possible symmetric molecule, 60 being the largest number of proper rotations in the icosahedral group which is the largest group in which symmetry operations leave a point fixed. C_{60} is a very stable molecule with a high binding energy. Regular truncated icosahedron has $r_s = r_d$ and a circumscribing (normalized) unit sphere and is one of the Archimedian solids [4]. There are four Archimedian solids with 60 vertices :

solid	v	e	f	configuration
truncated icosahedron	60	90	32	5-6-6
truncated dodecahedron	60	90	32	3-10-10
rhombicosidodecahedron	60	120	62	3-4-5-4
sunb dodecahedron	60	150	92	3-3-3-3-5

Configuration a-b-c is vertex connectivity with a, b and c-sided regular polygon in cyclic order a-b-c. With atomic interactions of the logarithmic type, the governing Hamiltonian is

$$H = - \sum_{i < j} \Gamma_i \Gamma_j \log(l_{ij}^2) \quad (1.2)$$

which is the so-called point-vortex Hamiltonian of N-vortex theory [1]. Here, l_{ij} denotes the chord distance between a particle of strength Γ_i and one with strength Γ_j , which in standard cartesian co-ordinates is

$$l_{ij}^2 = \|\vec{x}_i - \vec{x}_j\|^2 \quad (1.3)$$

The numerical integrations used in this paper were carried out using a symplectic time-splitting method based on 3-vortex integrable subclusters which suppress numerical instabilities [5], then corroborated using variable time-step Runge-Kutta methods.

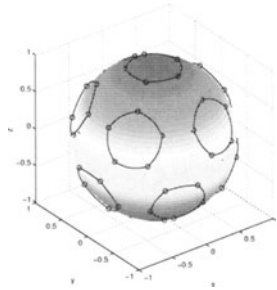


Figure 1.1: The vortex buckyball is made up of 12 clusters of 5 vortices each. A stable icosahedral equilibrium structure is formed by joining the centers of vorticity of each of the 12 clusters.

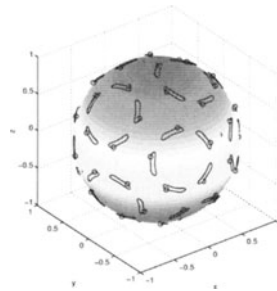


Figure 1.2: Snub Dodecahedron made up of 60 clusters each containing a single vortex.

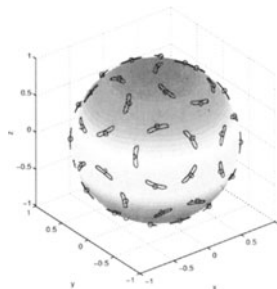


Figure 1.3: Rhombicosidodecahedron made up of 60 clusters each containing a single vortex.

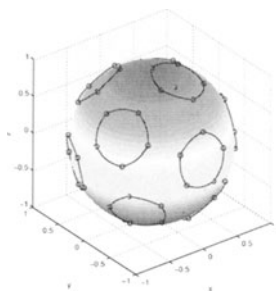


Figure 1.4: Truncated Icosahedron made up of 12 clusters of 5 vortices each.

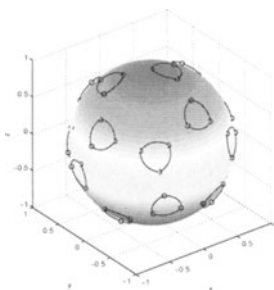


Figure 1.5: Truncated Dodecahedron made up of 20 clusters of 3 vortices each.

1.2 Clustering Dynamics

With a logarithmic Hamiltonian, the $N=60$ point vortex atoms associated with the Archimedean solids undergo spontaneous clustering, with each cluster undergoing periodic motion with characteristic frequencies based on the number of vortices, $m < N$, and the ring radius, r , of each cluster. Shown in figure is the vortex buckyball - 60 equal strength ($\Gamma_i = \Gamma_j=1$) particles are placed initially at the co-ordinates of bucky molecule. The vortices form 12 groups of 5 vortices each which co-orbit in periodic motion. Similar clustering occurs when vortices are placed at the vertices of the four Archimedean solids as shown in figures 2,3,4,5. The snub dodecahedron (SD) and the rhombicosidodecahedron (RI) form 60 individual clusters of one vortex per cluster; the truncated icosahedron (TI) forms 12 clusters of 5 vortices each (like the vortex buckyball); the truncated dodecahedron (TD) forms 20 clusters of 3 vortices per cluster.

Figure 6 shows the genesis of the vortex buckyball as it arises from its associated icosahedral equilibrium structure. Equal strength vortices (say 5Γ) placed at the 12 vertices of an icosahedral Platonic solid are known to form a fixed

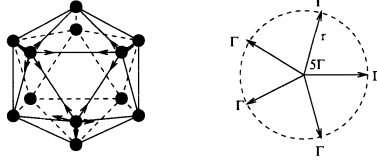


Figure 1.6: The vortex buckyball arises from splitting each of the vortices at the 12 vertices of an icosahedron into 5 equal parts along the adjacent edges. Icosahedral equilibrium structure with arrows denoting the splitting process are shown. Each vortex is split equally among the 5 edges to form a cluster of 5 co-orbiting vortices. The radius r measures the distance from equilibrium and has value $r=0.34$ for the vortex buckyball.

equilibrium structure [5]. Each vertex is then split into 5 equal strength vortices (Γ) along the edges of an icosahedron giving rise to 12 interacting rings of radius r with 5 vortices per ring. The ring parameter r measures the distance from equilibrium and has value $r \approx 0.34$ for the vortex buckyball.

In order to calculate the frequency associated with these periodic orbits, consider an isolated ring of m equal strength evenly spaced point vortices placed on the surface of a unit sphere at co-latitude θ . Frequency of rotation of such a latitudinal ring can be easily calculated to be equal to

$$\omega = \frac{\cos \theta}{\sin^2 \theta} \cdot \frac{(m-1)\Gamma}{2\pi} \quad (1.4)$$

with Γ being the point vortex strength. We know that the co-latitude and ring radius r are related by $\sin \theta = r$, which gives rise to the frequency-radius formula for an isolated ring of m point vortices

$$\omega = k_m \frac{\sqrt{1-r^2}}{r^2} \quad (1.5)$$

Here, k_m is a constant depending only on m . This yields

$$\left(\frac{\omega}{k_m} \right)^2 = \frac{1}{r^4} - \frac{1}{r^2} \quad (1.6)$$

for an isolated ring, shown as the dashed curve in figure 7. Also shown in this figure are the frequencies associated with the interacting clusters, with the rightmost data point representing the vortex buckyball. Assuming these 12 interacting clusters obey a similar scaling law

$$\left(\frac{\omega}{k} \right)^2 = \frac{1}{r^a} - \frac{1}{r^b} \quad a > b \quad (1.7)$$

the 2 scaling exponents can be computed by making the following observation. If the above equation is multiplied by r^b and a new variable is defined

$$\tilde{\omega} = 1 + r^b (\omega/k)^2 \quad (1.8)$$

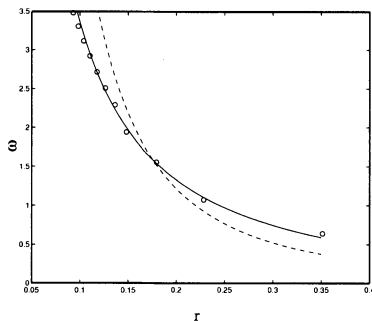


Figure 1.7: Both the dashed and the solid curves obey the formula $(\omega/k)^2 = r^{-a} - r^{-b}$. The dashed curve corresponds to an isolated ring with scaling exponents $a=4$, $b=2$ and $k=0.05$. The solid curve with exponents $a=2.65$, $b=2$ and $k=0.16$ more closely fits the data for cluster-cluster interactions.

then $\tilde{\omega}$ obeys the power law

$$\tilde{\omega} = r^{b-a} \quad (1.9)$$

Thus, if the scaling relation holds, a correct choice for exponent b will force the data (on a log-log plot) to lie with slope s , which is related to the exponents by $s=b-a$. From this, the remaining exponent a can be computed. The curve with exponents $a=2.65$ and $b=2$ is shown (solid) in figure 7 and the fit with the data is excellent.

1.3 Stability Theory

The Huckel molecular orbital formalism allows for quick, albeit crude electronic structure calculations, including information about molecular stability [3]. The theory is based on diagonalizing the Huckel matrix Hm

$$Hm = \beta A + \alpha I \quad (1.10)$$

with co-efficients α being a Coulomb integral and β a resonance integral. The matrix A is the adjacency matrix associated with the configuration, whose eigenvalues for the buckyball are shown in table 2. Eigenvalues of adjacency matrix are one way of characterizing stability of a molecule. An N -vortex graph will have a size N adjacency matrix with a 1 at position (i,j) if vertices of the corresponding solid are joined by an edge, and 0 otherwise. This simple topological Huckel approach focuses on the topology of bonds which incorporates the interaction laws through co-efficients α and β .

Eigenvalues of adjacency matrix			
λ_{TI}	λ_{TD}	λ_{RI}	λ_{SD}
3×1	3×1	4×1	5×1
2.757×3	2.842×3	3.618×3	4.488×3
2.303×5	2.562×5	2.925×5	3.577×5
1.82×3	2.303×4	2.236×4	2.717×4
1.562×4	1.618×4	1.382×3	1.322×3
1×9	1.507×3	1×4	1.071×4
0.618×5	0×10	0.552×5	0.195×5
-0.139×3	-0.507×3	0×6	-0.285×5
-0.382×3	-0.618×4	-0.382×8	-1×6
-1.303×5	-1.303×4	-1×4	-1.252×3
-1.438×3	-1.562×5	-2.236×4	-1.507×4
-1.618×5	-1.842×3	-2.477×5	-2.136×5
-2×4	-2×11	-2.618×8	-2.28×4
-2.562×4			-2.351×5
-2.618×3			-2.558×3

In Huckel theory for molecular stability [2], the eigenvalues of adjacency matrix are arranged in decreasing order and conclusion of stability follows if

$$\frac{2 \sum_{i=1}^{N/2} \lambda_i}{N} > 1 \quad (1.11)$$

Calculation of adjacency matrix for each of the above solids enables us to form a table as above which lists the eigenvalues for these solids in decreasing order. Adjacency matrix and eigenvalues for buckyball and truncated icosahedron are the same. Since N is same for each solid, the factor $h = \sum_{i=1}^{N/2} \lambda_i$ is an indication of how resilient the structure is.

Solid	h	Point Vortex Energy (H)	h/H
SD	55.0	65.2	0.84
RI	49.3	65.2	0.76
Bucky	46.6	65.0	0.72
TI	46.6	65.0	0.72
TD	44.5	63.3	0.70

From the table, it is immediately evident that Hamiltonian of the point vortex motion is directly proportional to the sum of eigenvalues of adjacency matrix for a given N. Moreover, if the solids are arranged in the decreasing order of distance between two adjacent vertices, l_{ij} ,

Solid	l_{ij}
SD	0.46
RI	0.45
Bucky	0.41
TI	0.40
TD	0.34

then too the same arrangement follows.

Stability of such a periodic orbit governed essentially by nonlinear differential equations [6] can be determined by linearizing it about the periodic orbit. For the buckyball, all the eigenvalues of the fundamental matrix lie on a unit circle and the orbit is linearly stable [5]. Thus, adjacency spectrum predicts stability of the truncated icosahedral state and Floquet theory shows stability of periodic orbits in the case of logarithmic interactions.

1.4 Conclusions

With logarithmic interactions, the buckyball configuration leads to periodic orbits of 12 interacting clusters with 5 vortices per cluster. The stability of these orbits is evidenced by their Floquet spectrum. The nonlinear scaling theory accurately predicts the interacting cluster frequencies through the full range of values of ring radii from the icosahedral equilibrium, $r=0$, to the buckyball value $r=0.34$. Periodic or quasi-periodic states that arise via symmetric splitting processes of the type described in this paper are generic objects that can be obtained from other regular structures such as Platonic solid equilibria or relative equilibria [5]. Asymmetric splitting processes give rise to much more complex dynamical states whose properties are not nearly as well understood yet seem rich and well worth pursuing.

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Chapter 24

Handling Resource Oscillations Through Selective Misinformation

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When resource consumers select among competing providers based on delayed information, inefficient oscillations in resource utilization can emerge. This paper describes an approach, based on selective stochastic resource request rejection, for dealing with this emergent dysfunction.

1. The Challenge

The convergence of ubiquitous electronic communications such as the Internet, electronic agents acting as proxies for human consumers, and web/grid service standards such as XML are rapidly ushering in a world where hordes of software agents, acting for humans, can rapidly select among multitudes of competing

providers offering almost every imaginable service. This is inherently an “open” world, a marketplace where the agents operate as peers, neither designed nor operated under central control. Such a world offers the potential for unprecedented speed and efficiency in getting work done.

In such open peer-to-peer systems we face, however, the potential of highly dysfunctional dynamics emerging as the result of many locally reasonable agent decisions [1]. Such “emergent dysfunctions” can take many forms, ranging from inefficient resource allocation [2] to chaotic inventory fluctuations [3] [4]. This problem is exacerbated by the fact that agent societies operate in a realm whose communication and computational costs and capabilities are radically different from those in human society, leading to collective behaviors with which we may have little previous experience. It has been argued, for example, that the 1987 stock crash was due in part to the action of computer-based “program traders” that were able to execute trade decisions at unprecedented speed and volume, leading to unprecedented stock market volatility [5].

Let us focus on one specific example of emergent dysfunctional behavior: resource use oscillation in request-based resource sharing. Imagine that we have a collection of consumer agents faced with a range of competing providers for a given resource (e.g. a piece of information such as a weather report, a sensor or effector, a communication link, a storage or computational capability, or some kind of data analysis). Typically, though not exclusively, the utility offered by a resource is inversely related to how many consumers are using it. Each agent strives to select the resource with the highest utility (e.g. response time or quality), and resources are allocated first-come first-served to those who request them. This is a peer-to-peer mechanism: there is no one ‘in charge’. This kind of resource allocation is widely used in settings that include fixed-price markets, internet routing, and so on. It is simple to implement, makes minimal bandwidth requirements, and - in the absence of delays in resource status information - allows consumers to quickly converge to a near optimal distribution across resources (see figure 1 below).

Consumers, however, will often have a delayed picture of how busy each resource is. Agents could imaginably poll every resource before every request. This would cause, however, a N -fold increase in message traffic (for N servers), and does not eliminate the delays caused by the travel time for status messages. In a realistic open system context, moreover, consumers probably cannot fully rely on resource providers to accurately characterize the utility of their own offerings (in a way that is comparable, moreover, across providers). Resource providers may be self-interested and thus reluctant to release utilization information for fear of compromising their competitive advantage. In that case, agents will need to estimate resource utilization using other criteria such as their own previous experience, consulting reputation services, or watching what other consumers are doing. Such estimates are almost certain to lag at times behind the actual resource utility.

When status information is delayed in some way, we find that resource use oscillations emerge, potentially reducing the utility achieved by the consumer agents far below the optimal value predicted by an equilibrium analysis [6]. What happens is the following. Imagine for simplicity that we have just two equivalent resources, R_1 and R_2 . We can expect that at some point one of the resources, say R_1 , will be

utilized less than the other due to the ebb and flow of demand. Consumer agents at that point will of course tend to select R1. The problem is that, since their image of resource utilization is delayed, they will continue to select R1 even after it is no longer the less utilized resource, leading to an “overshoot” in R1’s utilization. When the agents finally realize that R2 is now the better choice, they will tend to select R2 with the same delay-induced overshoot. The net result is that the utilization of R1 and R2 will oscillate around the optimal equilibrium value. The range of the oscillations, moreover, increases with the delay, to the extent that all the consumers may at times select one server when the other is idle:

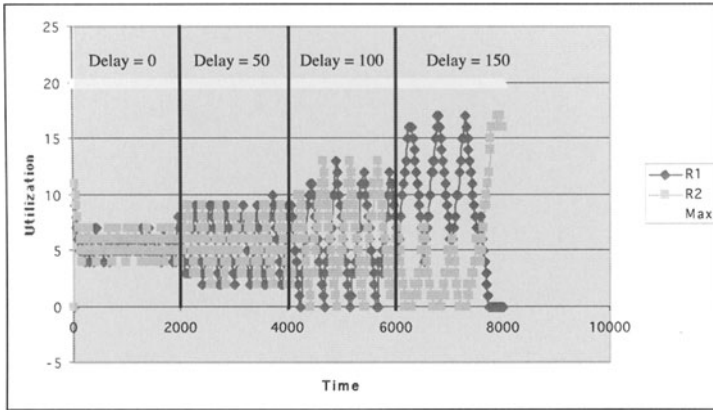


Figure 1: Utilization of two equivalent resources with and without information delays

Oscillations have several undesirable effects. One is that they can reduce the utility received by consumers below optimal values. This can occur, for example, when the oscillations are so severe that some of the resources go idle some of the time, reducing the effective resource availability. The other is that they can increase the variability of the utility achieved by the consumers, which may be significant in domains where consistency is important.

2. Our Approach: Stochastic Request Rejection

We have developed a technique for addressing delay-induced resource inspired by a scheme developed to improve the allocation of network router bandwidth [7]. We call our scheme ‘stochastic request rejection’, or SRR. Imagine that every resource stochastically rejects new requests with a probability proportional to its current load. This can be implemented by the resource itself, or by ‘sentinel’ agents that track the number of consumers each resource is currently serving, and stochastically intercept/reject consumer requests with a probability proportional to that load. When oscillations occur, we would predict that the increased level of rejections from the currently more heavily utilized resource will shift the requests to the less-utilized resource, thereby damping the oscillations and ameliorating their negative impact on the utility and consistency experienced by consumer agents.

3. Experimental Evaluation

Resource use oscillations will only occur if the utility of a resource to a consumer is a *negative* function of its utilization. If the utility of a resource to a consumer increases when the resource is more heavily utilized (e.g. imagine night-clubbers who want to select the club which has the most people there) then all consumers will eventually converge on a single resource. We can divide the remaining cases into two scenarios. One is the “grocery store scenario” where grocery store customers (consumers) choose from two checkout lines (resources). Their utility is inversely related to how long they have to wait, which is a *linear* function the length of a line. The second scenario is the “movie theater”, where the utility of the resource is a *non-linear* function of how many people are already there (assuming that good seats are consumed before poorer ones). We did separate evaluations for these two scenarios.

The Grocery Checkout (Linear) Scenario: There were 20 consumers and 2 resources. Each consumer sends a ‘request’ message to the resource it believes has the smallest backlog, waits until it receives a ‘job completed’ message from the resource, and then after a randomized delay sends the next ‘request’ message. The consumers’ estimate of a resources’ utility may lag the correct value. Resources may either take on requests or reject them. If a consumer receives a ‘reject’ message, it sends the request to the other resource. Messages take 20 units of time to travel, resources require 20 units of time to perform each task, and consumers have a normally distributed delay at 40 ticks, with a standard deviation of 10, between receiving one result and submitting the next request. The aggregate results reported below represent averages over 100 simulation runs, each 4000 ticks long, and all the conclusions we make were statistically significant at $p < 0.01$.

The impact of applying SRR in this scenario can be visualized as follows:

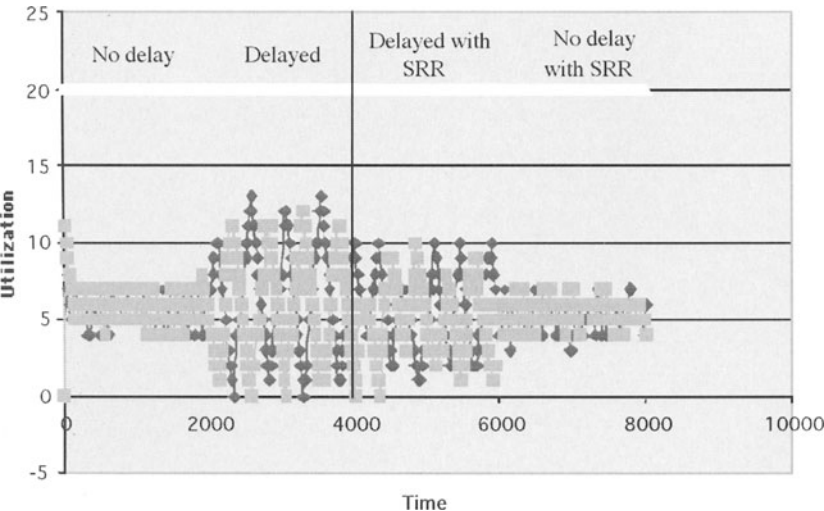


Figure 2: The impact of SRR on resource oscillations.

In this simulation run, the agents initially made their resource requests using current information on the length of each resources' backlog. As we can see, in this case the resource utilization clusters tightly around the optimal distribution of 50-50 across resources. At $T = 2000$, the backlog information provided to the consumers was made 100 time units out of date, rapidly leading to large resource use oscillations. At $T = 4000$, SRR was turned on, resulting in substantial damping in the magnitude of these oscillations. At $T = 6000$, the delay was removed but SRR was left on, whereupon the resource utilization returns to clustering tightly around the optimal distribution. The aggregate results confirm the patterns suggested by this example:

	Null	SRR
No delay	160 +/- 4 0%	160 +/- 6 33%
Short Delay (50)	160 +/- 7 0%	160 +/- 6 34%
Long Delay (100)	167 +/- 8 0%	161 +/- 6 35%

Table 1. Task completion times ± 1 standard deviation, as well as reject rates, for different delays, with and without SRR.

As we would expect for the grocery scenario, the variability in task completion times without SRR increases with the delay in status information, and if the delay is long enough, the average task completion time can increase as well. If we turn on SRR, we find that it significantly reduces the variability in task completion times in the delayed cases, and almost eliminates the increase in task completion times in the long delay case. Rejecting some requests can thus, paradoxically, actually speed up task completion when delay-induced oscillations occur. But this does come at a cost. Message traffic is increased: roughly $1/3^{\text{rd}}$ of the consumer requests elicit a reject message and must be re-sent. The variability of task completion times in the no delay case is also increased by SRR. This is because many resource requests that would otherwise simply have been queued up incur the additional delay of being rejected and re-submitted. The absolute size of these effects, of course, can be expected to vary with the ratio of task and messaging times. Ideally, we would be able to enable SRR only when it is needed, so we can avoid incurring its costs in the no-oscillation contexts where it is not helpful. We will return to this point later.

The Movie Theater (Nonlinear) Scenario: The parameters for these simulations were the same as in the grocery store case, except for the following changes. Resources do not have a waiting line, but instead offer concurrent access to 15 different 'slots' with varying utility (the first slot has value 15, the second has value 14, and so on). Tasks take 160 ticks to perform. The aggregate results are as follows:

	Null	SRR
No delay	9.6 +/- 1.5 0% 331	9.7 +/- 1.2 59% 303
Short Delay (50)	9.1 +/- 1.9 0% 332	9.8 +/- 1.4 60% 303
Long Delay (100)	7.6 +/- 2.1 3% 331	9.6 +/- 1.4 66% 300

Table 2. Average quality +/- 1 standard deviation, as well as reject rates and number of completed requests, for different delays, with and without SRR.

As we can see, SRR is also effective in this scenario. Delay-induced oscillations cause consumers to often select the resource that is actually more heavily utilized and thus lower in quality, resulting in a reduction of the average achieved quality. Using SRR eliminates this problem, but with the cost of increasing message traffic, as well as reducing the rate of task completion (since every time a task is rejected a delay is incurred while the request is re-submitted). As in the “grocery checkout” case, we would ideally prefer to be able to apply SRR selectively, so we do not incur these costs when oscillations are not occurring. Can this be done?

4. Avoiding Needless Rejects Via Selective SRR

It is in fact straightforward to use spectral analysis to determine if persistent oscillations are occurring in resource utilization. In our implementation, each resource periodically (every 20 ticks) sampled its utilization and submitted the last 30 data points to a Fourier analysis. SRR was turned on if above-threshold values were encountered in the power spectrum so determined. The threshold was determined empirically. This approach proved to be successful. In the grocery checkout scenario, selective SRR was as effective as SRR in maintaining throughput and task duration consistency while avoiding increases in message traffic in the no-delay case:

	Null	SRR	Selective SRR
No delay	160 +/- 4 0%	160 +/- 6 33%	160 +/- 4 0%
Short Delay (50)	160 +/- 7 0%	160 +/- 6 34%	160 +/- 6 29%
Long Delay (100)	167 +/- 8 0%	161 +/- 6 35%	161 +/- 6 33%

Table 3. Task completion times +/- 1 standard deviation, as well as reject rates, for different delays, with and without [selective] SRR.

In the movie theatre scenario, selective SRR maintained task quality while almost eliminating increases in message traffic and task time in the no-delay case:

	Null	SRR	Selective SRR
No delay	9.6 +/- 1.5 0% 331	9.7 +/- 1.2 59% 303	9.5 +/- 1.4 6% 327
Short Delay (50)	9.1 +/- 1.9 0% 332	9.8 +/- 1.4 60% 303	9.6 +/- 1.5 41% 311
Long Delay (100)	7.6 +/- 2.1 3% 331	9.6 +/- 1.4 66% 300	9.3 +/- 1.6 54% 305

Table 4. Average quality +/- 1 standard deviation, as well as reject rates and number of completed requests, for different delays, with and without [selective] SRR.

This simple spectral analysis approach can be fooled, of course, into triggering SRR when resource use oscillations are due to variations in aggregate demand rather than status information delays. This problem, however, is easily addressed: whenever a resource detects significant usage oscillations, it analyzes the correlation of its utilization with that of the other resource. Variations in aggregate demand will show a positive correlation, while delay-caused oscillations show a negative one. We have implemented this approach and found that it successfully avoids triggering SRR for aggregate demand variations while remaining effective in responding to delay-induced oscillations.

5. Contributions and Next Steps

The problem of resource use oscillation in request-based systems has been studied in some depth, most notably in the literature on “minority games” [8] [9]. This line of work has investigated how to design agents so that their local decisions no longer interact to produce substantial resource use oscillations. One example involves designing agents that make resource selection decisions using historical resource utilization values [6]. If the agents look an appropriate distance into the past, they will be looking at the resource state one oscillation back in time, which should be a good approximation of the current resource utilization. The agent’s delay parameter is tuned using survival of the fittest: agents with a range of delay factors are created, and the ones that get the highest utility survive and reproduce, while others do not. With this in place the resource utilization, under some conditions, settles down to near-optimal values. Any such approach, however, predicated as it is on the careful design of agent resource selection strategies, faces a fundamental flaw in an open systems context. In open systems, we do not control the design or operation of the consumer agents and can not be assured that they will adopt strategies that avoid emergent dysfunctions. Our challenge, therefore, is to find an approach that moderates or eliminates oscillatory resource utilization dynamics without needing to control the design or operation of the consumer agents. This paper presents such an

approach, based on stochastic load-proportional rejection of resource requests, triggered selectively when spectral and cross-resource correlation analyses reveal that delay-induced oscillations are actually taking place.

Next steps for this work include evaluating the selective SRR approach when there are more than two resources. This research is part of the author's long-standing efforts to develop a systematic enumeration of the different multi-agent system exception types as well as how they can be addressed in open systems contexts [10] [11]. See <http://cci.mit.edu/klein/> for further details.

Acknowledgements

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Chapter 25

On the evolution of structure in ecological networks

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Previous research on simulated ecological networks has often focused on issues such as the distribution of the number of links between species, without generally categorizing the types of inter-species relationships that develop, unless those relationships are of some predesigned form (e.g., food webs). In this work we use a model system to examine general, dynamically-evolved ecological networks that are subject to occasional invasion by novel species. Keeping track of the specific types and numbers of interactions between species over time leads to insight on how these affect network stability, fragility and evolution. We discuss the role that assembly rules play on the evolutionary trajectories of randomly initialized communities. We also investigate the occurrence of certain types of interactions (e.g., cyclic) and quantify their destabilizing effect on the network. In particular, extinctions and secondary extinctions (“avalanches”) are related to these issues.

1.1 Introduction

The structure of an ecological species network is influenced to a large degree by the historical nature of its construction [4]. This contingency effect, wherein the outcome of some event depends on the sequence of events that preceded it, can make the details of network architecture difficult to predict. In addition, there is a high degree of nonlinearity in the system due to the elaborate feedback between different parts of the network. Nevertheless, there is a great deal of regularity in the structure of many networks, both biological and non-biological. What causes this regularity and what are its effects? To what extent is network structure influenced by assembly rules, and how much of it is the result of general organizing principles that are relatively insensitive to the details of the model? There is a tension between the forces of self-organization and species-species interactions that combine to give the network its structure. Species interactions lead to perturbations in the network and the network forms the framework which gives these interactions their meaning. These interactions are never absolute. A species that fares well in one community may be doomed in another.

Real ecological networks have been shown to exhibit clustering and small world organization, and this influences community stability and diversity [6, 9, 5].

Our goal is to simulate ecological networks that are allowed to evolve as freely as possible rather than imposing some *a priori* structure. For example, we do not assume that our networks have food web topologies. It must be acknowledged, of course, that assumptions must be made in any model and these can bias the system. For example, species with negative intrinsic growth rates are obligate predators. Such species tend to have more interactions with other species than do those with positive intrinsic growth rates. It is for this reason, as well as our vast ignorance regarding the detailed interactions in most biological communities, that it is essential to let *in silico* ecological networks evolve on their own rather than simply assigning the interactions at random. Evolution and shared history are hallmarks of real communities.

Although the observations generated by our simulations should be applicable to a large range of ecosystems, we are particularly interested in microbial communities. In such a setting, our knowledge of inter-species interactions in natural and clinical settings is very tenuous. In addition, the number of “species” can be very large; e.g., estimates of 1000 bacterial species in a gram of soil are typical.

Most studies of real ecosystems are based on a snapshot in time and many of the statistics used to study these, as well as model ecosystems, are based on observations at a fixed time. In some cases, historical observations may be available that shed light on the past history of a particular ecosystem. In microbial communities, the time scales are such that “real-time” observations can be made and temporal data on community structure can be collected, although not without considerable effort. Because of the temporal nature of community construction and the state-dependent nature of community dynamics, we suggest that the collection and interpretation of temporal data can lead to a better understanding of complex ecological networks.

Our model ecosystems can be thought of as directed graphs with vertices representing species and edges representing interactions. We explicitly model the directions and strengths of the interactions, so these graphs are both directed and weighted. The sign of the interactions determine the types of pairwise interactions (predator-prey, competitive, mutualistic).

1.1.1 The model

Our simulations are based on simple Lotka–Volterra dynamics with no spatial structure. With $u_i(t)$ denoting the density of species i , the basic equation is

$$\frac{du_i}{dt} = u_i(r_i + \sum_j a_{ij}u_j). \quad (1.1)$$

Here, r_i denotes the intrinsic growth rate of species i and the a_{ij} 's represent interaction strengths. We simulate a discretized version of this model. Interaction strengths in stable communities are typically quite small [6, 8]. It has been observed [7] in similar food web simulations that the addition of nonlinear functional responses does not have a strong effect, at least for certain statistics. For this reason, we chose to treat only the above model. It should be noted, however, that certain types of nonlinear functional response, as well as spatial structure, can strongly influence the outcomes of multi-species associations, leading, for example, to a stabilization of competitive loops [1, 2, 3]. These complications provide fertile ground for future studies of ecological network evolution and suggest that we should not be overly biased by predictions arising from simple Lotka–Volterra models.

Our simulations were set up as follows. The initial ecosystem for each run consisted of 200 species. Each species had a maximum carrying capacity generated randomly (i.e., uniformly) over the range [1000, 10000] and a growth rate generated randomly over $[-0.1, 0.1]$. These values were used to generate a species self-interaction term (a_{ii}). Each species had an initial population size of 1000.

The probability of a given (one-way) link between two species was set at X/N , where N is the number of species in the population. Our experiments used values $X = 2, 3, 4$. The sign of the link (interaction strength) between two species that are connected (in a given direction) is positive or negative with probability $1/2$ each. The strength of such a link was randomly calculated using the formula

$$|a_{ij}| = \alpha R_{ij} \min_i |a_{ii}|,$$

where the R_{ij} 's are independent random numbers uniformly chosen from the range $[0.1, 1]$, and α is a fixed constant. We used values $\alpha = 1.0, 0.75, 0.5, 0.25$ in the simulations. Small values of α correspond to weak interactions.

The maximum total population was fixed at 1,000,000. This global density dependence is necessary to keep the number of species from growing without bound; without it, non-interacting species with positive growth rates keep accumulating. To implement this in the simulation, we trim an overfull ecosystem

as follows. After a given iteration, if the sum of the populations of all species exceeds 1,000,000 by an amount P percent, then we reduce each population by P percent. This brings the total population size back down to 1,000,000 before the next iteration. If the population of a species drops below 1, that species is removed from the ecosystem; it goes extinct.

New species (immigrants) were added (i.e., invade) when the ecosystem had stabilized after the previous migrant addition. Based on preliminary experiments, we say that the ecosystem has *stabilized* if there are 100 consecutive iterations without an extinction. New species are introduced with a population size of 100 and the corresponding parameters are chosen randomly according to the same rules as for the initial species.

In several of the experiments we measured avalanches of extinctions. The *avalanche size* is the number of extinctions between the addition of a new immigrant and re-stabilization of the ecosystem. For example, assume that a new species is added (with a population of 100) during some iteration, and over the course of the next 75 iterations five species go extinct, followed by 100 iterations without any further extinctions. The system is assumed to have stabilized, an avalanche of size five is recorded, and a new immigrant species is added to the ecosystem.

We consider two kinds of statistics: dynamic (time dependent) and static (collected only at the end of a run). Both viewpoints can provide information on community structure and stability.

1.2 Simulations

In the simulations, one typically sees an initial crash as a large number of species go extinct in a short time. This is followed by a gradual build-up in the number of species until some equilibrium level is reached. Throughout this process, extinctions occur, sometimes followed by secondary extinctions, or “avalanches”. We emphasize that our extinction events are dynamically generated, not just artificial removals.

Our first figure illustrates this process and shows the dependence on the parameters X and α . Note that the ecosystem is more stable for low values (roughly, less than 1.5) of the product $X\alpha$ and becomes more unstable as this product increases. In the accompanying tables, we say that an ecosystem is “successful” if it does not lose all its species during the time of the run.

If we let b be the average absolute interaction strength, L the total number of links, and N the number of species, then both empirical and model ecosystems typically have values of $b\sqrt{L/N}$ that are roughly constant as a function of time. This quantity can also be written as $b\sqrt{CN}$, where $C = L/N^2$ is the connectance of the network. In Figure 1.2, we see that as the product $X \cdot \alpha$ increases, the corresponding trajectory (an average of 20 ecosystem runs) has larger values and is more erratic. A large part of the increased variability comes from the fact that increasing $X \cdot \alpha$ tends to decrease the number of species.

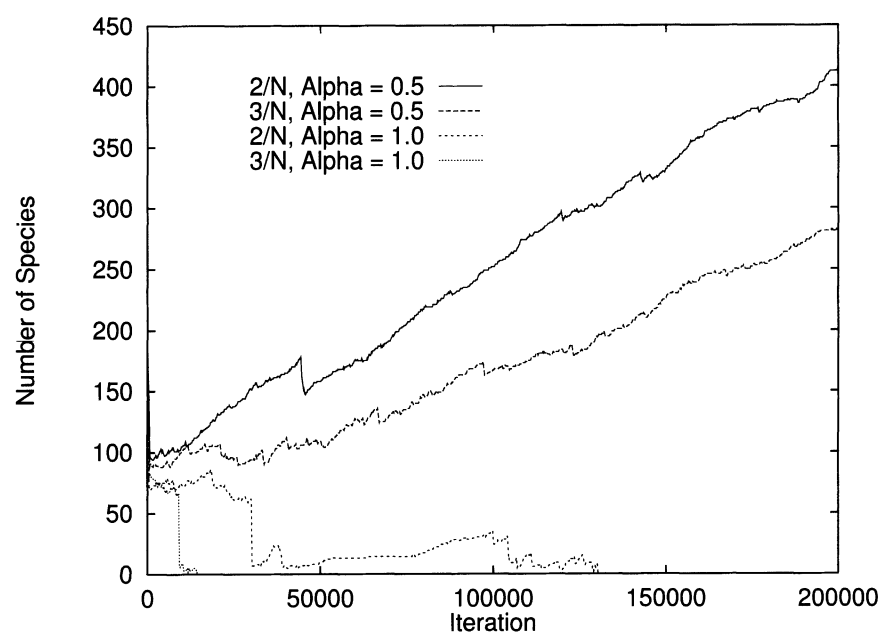


Figure 1.1: Number of species for different parameter settings. Each curve represents an average of 20 runs. Notice that diversity and stability are strongly influenced by the product $X\alpha$.

	2/N	3/N	4/N
alpha = 1.0	1	0 (49,750)	-
alpha = 0.75	16	0 (193,950)	1
alpha = 0.5	20	18	17
alpha = 0.25	-	20	20

Table 1.1: Number of ‘successful’ ecosystems out of 20. Number in parentheses is the iteration in which the last ecosystem failed.

	2/N	3/N	4/N
alpha = 1.0	13.0767 (0)	0	-
alpha = 0.75	75.125 (92.9324)	0	4 (0)
alpha = 0.5	393.5 (98.7666)	117.611 (131.196)	28.882 (48.516)
alpha = 0.25	-	476.65 (17.4822)	409.300 (124.612)

Table 1.2: Average number of species per ecosystem after 200,000 iterations. The number in parenthesis is the standard deviation.

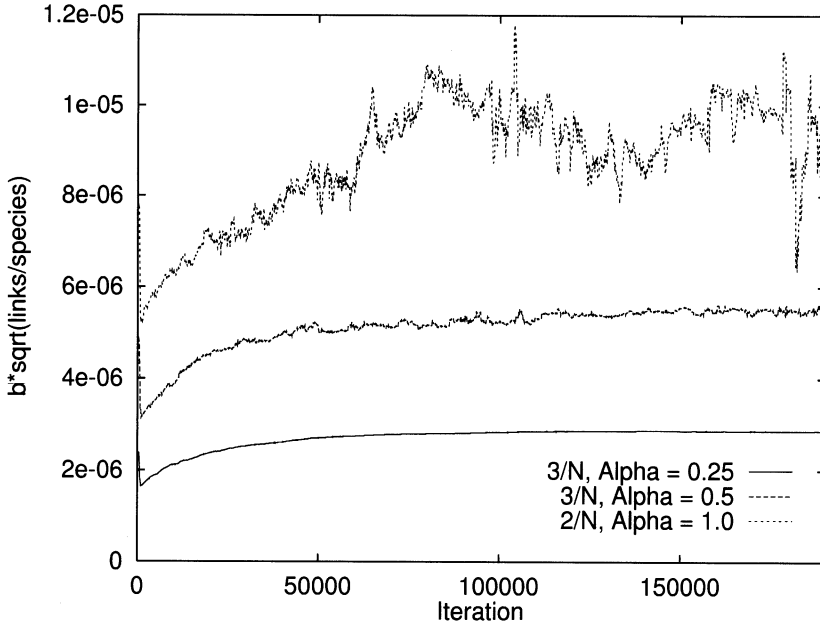


Figure 1.2: A plot of $b\sqrt{L/N}$ as a function of time. See text for parameter definitions.

1.2.1 The effect of loops

Occasionally, a group of species will become connected in a loop. If, going in a particular direction (and independent of what happens in the other direction), we have positive interactions (say $a_{i,i+1} > 0$), then we call this a *positive loop*. The ecosystems often became very unstable after the formation of such a loop. For the final set of experiments we examined the effects of positive loops directly by running a version of the model that does not allow any positive loops to form. For these trials when a new species is added to the ecosystem, it is immediately checked for positive loops that may have been created by the new species. If a positive loop is found then the new species is removed from the ecosystem and another species with different, random connections is added instead. This process is repeated until a new species is added that does not create any positive loops. This technique is also applied in generating the initial ecosystem of 200 species; so the ecosystem will never contain any positive loops.

For ecosystems with parameters that produce unstable conditions the results with no positive loops are significantly different from the results with positive loops. Figure 1.3 shows the effect on diversity and stability by recording the number of species as a function of time.

In the last figure, we show that the avalanche size distribution obeys a power law, $y = \text{const.}x^{-\gamma}$, if we let x represent avalanche size and y the number of avalanches of that size.

We also counted the total number of avalanches for all twenty runs for the

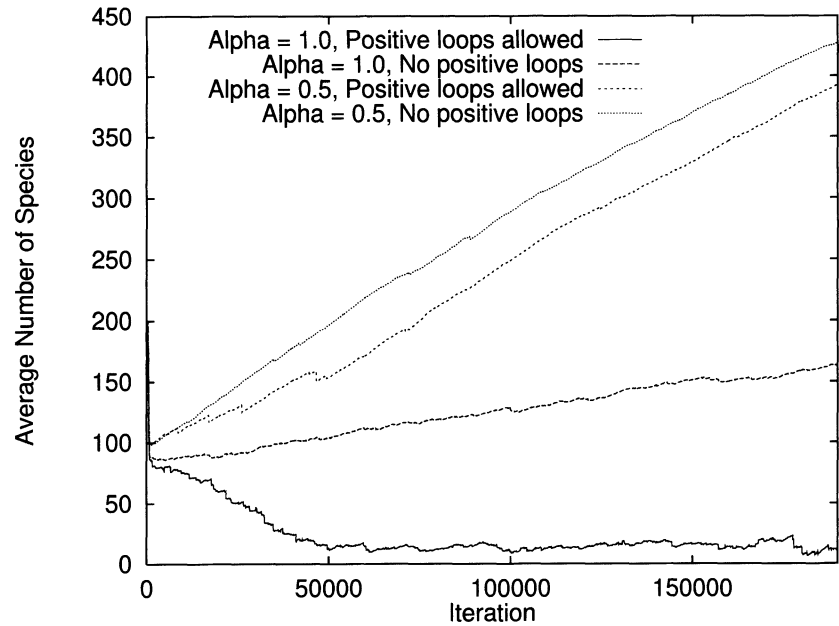


Figure 1.3: The average number of species (averaged over 20 runs, with $X = 2$) as a function of time, both with and without positive loops.

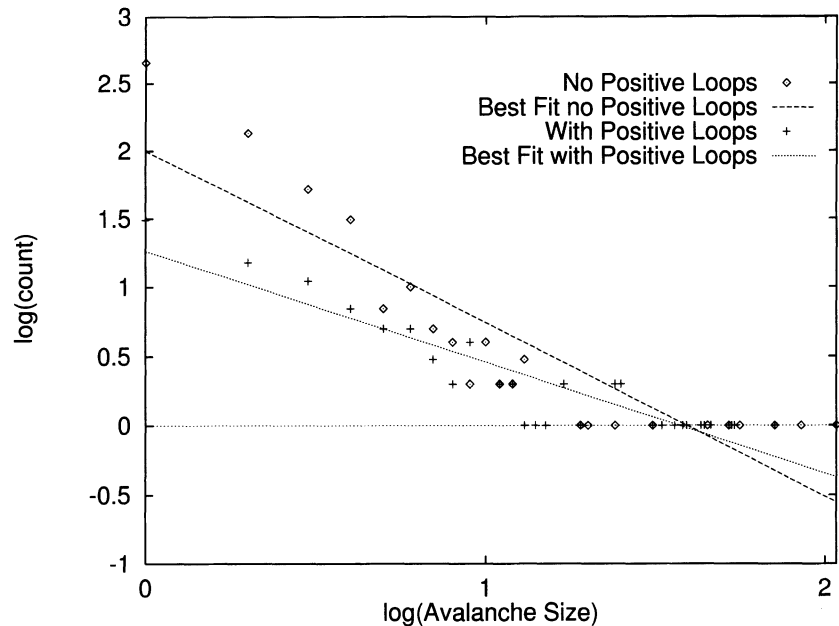


Figure 1.4: Power law behavior for avalanche size distribution, both with and without positive loops. The power law exponents are $\gamma = 0.802$ (loops) and $\gamma = 1.255$ (no loops).

unstable parameters $2/N, \alpha = 1.0$ with positive loops allowed and without positive loops. We did not count the initial species ‘crash’ that occurs in the first few hundred iterations. In both cases the smaller avalanches, those in which 1 to 36 species went extinct, obeyed a similar power law relationship. The smaller avalanches are much more frequent.

However, for avalanches larger than 36, the behaviors were very different. Without positive loops there were no avalanches larger than size 36. With positive loops there were 15 avalanches of size 37 to 100, including two of size 91. There was slightly less than one large avalanche per trial. Note that, in general, the ecosystems can only support one such large avalanche as, after it occurs, the number of species is typically less than 36. Thus, the lower number of species observed in Figure 1.4 with positive loops (parameters $2/N, \alpha = 1.0$) can be attributed to the occurrence of a single large avalanche that does not occur when positive loops are not allowed.

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Chapter 26

Spatio-temporal dynamics in a Turing model

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In this paper we study numerically two-dimensional spatio-temporal pattern formation in a generic Turing model, by investigating the dynamical behavior of a monostable system in the presence of Turing-Hopf bifurcation. In addition, we study the interaction of instabilities in a tristable system. We speculate that the interaction of spatial and temporal instabilities in Turing systems might bring some insight to a recent biological finding of temporal patterns on animal skin.

1.1 Introduction

In 1952 Alan Turing showed mathematically that a system of coupled reaction-diffusion equations could give rise to spatial concentration patterns of a fixed characteristic length from an arbitrary initial configuration due to diffusion-driven instability [1]. A remarkable feature of Turing systems as compared to other instabilities in systems out of equilibrium [2, 3] is that the characteristics of the resulting patterns are not determined by externally imposed length scales or constraints, but by the chemical reaction and diffusion rates intrinsic to the system.

Turing's goal was to model mechanisms behind morphogenesis, i.e., biological growth of form. Although genes play an important role in determining the anatomical structure of the resulting organism, from physical point of view they cannot explain spatial symmetry-breaking, which takes place as the cells start to

differentiate. Turing hypothesized that as soon as the spherical blastula becomes large enough and there are some random deviations from the perfect symmetry, that state becomes unstable and the system is driven to another state defined by spontaneous physico-chemical processes. It has been qualitatively shown that Turing models can indeed imitate biological patterns [4, 5], but the question whether morphogenesis really is a Turing-like process still remains.

The first experimental observation of a Turing pattern in a chemical reactor was due to De Kepper's group, who observed a spotty pattern in a chlorite-iodide-malonic acid (CIMA) reaction [6]. Later the results were confirmed by Ouyang and Swinney, who observed both striped and spotty patterns in extended systems [7]. The experimental observation of Turing patterns renewed the interest in these complex systems and subsequently a lot of research has been carried out employing theoretical [8, 9], computational [10, 11, 12] and experimental approaches [13].

Although Turing instability results in spatially periodic patterns that are stationary in time, in general reaction-diffusion system can also exhibit a variety of spatio-temporal phenomena [14, 15]. Hopf instability results in spatially homogeneous temporal oscillations and its relation to Turing instability is of great interest. This is because both instabilities can be observed experimentally in the CIMA reaction by varying the concentration of the color indicator in the reactor [15, 16]. The interaction between these instabilities [17] may take place either through a co-dimension-two Turing-Hopf bifurcation, when the corresponding bifurcation parameter threshold values are equal [18, 19] or due to different competing bifurcations of multiple stationary states [15, 20]. Both the situations result in interesting spatio-temporal dynamics. In addition, Yang et al. have recently obtained a variety of both stationary and oscillating structures in the numerical simulations of a system with interacting modes [21, 22].

In this article we report a study of Turing pattern formation in a two-species reaction-diffusion model with one or more stationary states. Simultaneous instability of many states results in competition between bifurcating states and the system exhibits spatial, temporal and spatio-temporal pattern formation depending on the system parameters. We are especially interested in the coupling of Turing and Hopf bifurcations, which results in periodic spatial patterns and temporal oscillations. In the next section we introduce and briefly analyze the model that we have used. Then, we present and discuss the results of our numerical simulations, which is followed by conclusions.

1.2 Analysis of the model

In this paper we use the so called generic Turing model [23], where the temporal and spatial variation of normalized concentrations is described by the following reaction-diffusion system [24]

$$\begin{aligned} u_t &= D\nabla^2 u + \nu(u + av - uv^2 - Cuv) \\ v_t &= \nabla^2 v + \nu(bv + hu + uv^2 + Cuv), \end{aligned} \quad (1.1)$$

where the morphogen concentrations have been normalized so that $u = U - U_c$ and $v = V - V_c$, which makes $(u_c, v_c) = (0, 0)$ the trivial stationary solution. The term C adjusts the relative strength of the quadratic and cubic nonlinearities favoring the formation of either linear (2D stripes, 3D lamellae) or radial (2D spots, 3D droplets) Turing structures [23, 25]. D is the ratio of diffusion coefficients, whereas the linear parameters a , b , h and ν adjust the presence and type of instability.

For $h \neq -1$ the system of Eq. (1.1) has two other stationary states in addition to $(0, 0)$. These states are given by $u_c^i = -v_c^i/K$ and $v_c^i = -C + (-1)^i \pm \sqrt{C^2 - 4(h - bK)/2}$ with $K = (1 + h)/(a + b)$ and $i = 1, 2$. One should notice that the values of these stationary states depend also on the nonlinear parameter C . The characteristic equation corresponding to Eq. (1.1) can be written in the form

$$\lambda^2 + [(1 + D)k^2 - f_u - g_v] \lambda + Dk^4 - k^2(f_u + Dg_v) + f_u g_v - f_v g_u = 0, \quad (1.2)$$

where the partial derivatives of the reaction kinetics are given by

$$\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} = \nu \begin{pmatrix} 1 - v_c^2 - C v_c & -2u_c v_c + a - C u_c \\ v_c^2 + h + C v_c & b + 2u_c v_c + C u_c \end{pmatrix}. \quad (1.3)$$

Here u_c and v_c define the stationary state, whose stability we are studying. The dispersion relation $\text{Re}\{\lambda(k)\}$ can be solved from Eq. (1.2). The real and imaginary parts of the eigenvalues corresponding to the single stationary state $(0, 0)$ are shown in Figure 1.1 for two sets of parameters corresponding to a Turing bifurcation (k_c unstable) and a Hopf bifurcation in a monostable system. The parameters used in Fig. 1.1 were $D = 0.122$, $a = 2.513$, $h = -1$, $b = -1.005$ and $\nu = 0.199$ for the Turing instability around $(0, 0)$ with critical wave number $k_c = 0.85$ and the same except $b = -0.8$ for the Hopf instability. For more details of the linear stability and pattern selection in the generic Turing model we refer the reader elsewhere [24].

From Fig. 1.1 one can observe that a Turing bifurcation corresponds to the case, where there is some k_i such that $\text{Re}\{\lambda(k_i)\} > 0$ and $\text{Im}\{\lambda(k_i)\} = 0$. On the other hand, a Hopf bifurcation corresponds to the situation, where a pair of imaginary eigenvalues crosses the real axis, i.e., there is some k_i with $\text{Re}\{\lambda(k_i)\} > 0$ and $\text{Im}\{\lambda(k_i)\} \neq 0$. The parameters can also be adjusted such that $k_c = 0$ for Turing instability or so that there is a combined Turing-Hopf bifurcation from one stationary state. The condition for the Hopf bifurcation in the system of Eq. (1.1) is $b > -1$ and for the Turing bifurcation it is $b < (1 - \sqrt{-4Dah})/D$ [24]. If the parameter $h < -1$ the stationary state $(0, 0)$ goes through a subcritical pitchfork bifurcation [2]. For $h > -1$ a tristability is established, i.e., there are three stationary states.

1.3 Numerical simulations

We have performed extensive numerical simulations of the generic Turing model (Eq. (1.1)) in two-dimensional domains of size 100×100 by using parameter

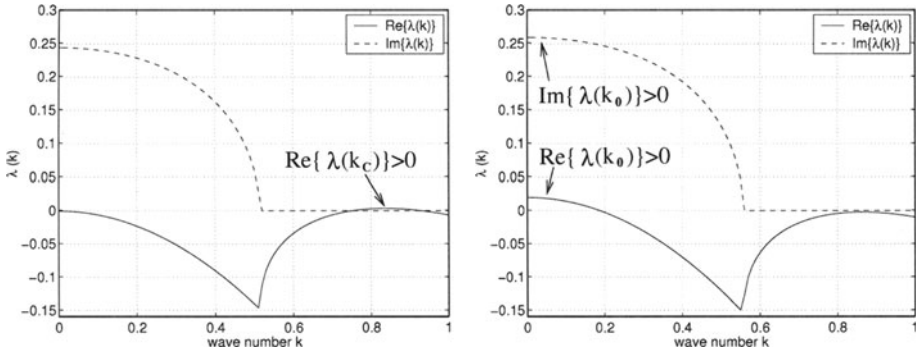


Figure 1.1: The largest eigenvalue of the linearized system corresponding to a Turing (left) and Hopf bifurcation (right). The real and imaginary parts of the eigenvalues correspond to solid and dashed lines, respectively.

values corresponding to different bifurcation and stability scenarios. The time integration of the discretized problem was carried out by using the Euler method ($dx = 1$ and $dt = 0.01$). On one hand, we have studied the interaction of Turing and Hopf bifurcations in a monostable system, and on the other hand, a tristable system with a coupled Turing-Hopf-Turing or Turing-Turing bifurcation. These conditions result in a variety of spatio-temporal dynamics, whose characterization is very challenging.

By using the parameters $D = 0.122$, $a = 2.513$, $h = -1$, $b = -0.95$, $\nu = 0.199$ and $C = 1.57$ one can adjust the system in such a way that there is only one stationary state $(0, 0)$, which is both Turing unstable with $k_c = 0.85$ and characteristic length $L = 2\pi/k_c \approx 7.4$, and Hopf unstable with oscillation period of $T_c = 2\pi/\text{Im}\{\lambda(k_0)\} \approx 25.40 = 2540 \times dt$ ($k_c = 0$). Eventually, the oscillations fade away and a stationary hexagonal spotty pattern is established. Fig. 1.2 shows snapshots of the behavior of the system at arbitrary moments of time. The homogeneous domains changing color correspond to oscillations.

By fixing $h = -0.97 \neq -1$ we admitted two additional stationary states and studied the pattern formation with parameters $D = 0.516$, $a = 1.112$, $b = -0.96$ and $\nu = 0.450$, which correspond to a Turing-Hopf bifurcation of the state $(0, 0)$ with $k_c = 0.46$ and Turing bifurcation of the stationary states $(-2.01, 0.40)$ and $(9.97, -1.97)$, both with $k_c = 0$. The Turing-Hopf modes growing from $(0, 0)$ excite the former of these two states, which results in a coupling between Turing-Hopf and Turing instabilities. From random initial configuration the parameter selection $C = 1.57$, which corresponds to spotty patterns [24] resulted in a hexagonal lattice with a few twinkling spots at dislocation sites. Twinkling hexagonal lattices of spots have previously been obtained in numerical simulations of a four-component Turing model [21] and of a nonlinear optical system [26]. Our results show that "twinkling-eye" behavior can also be observed in a two-component model without any special preparations [27].

Using the same parameters as above, except choosing $b = -1.01$ one still ob-

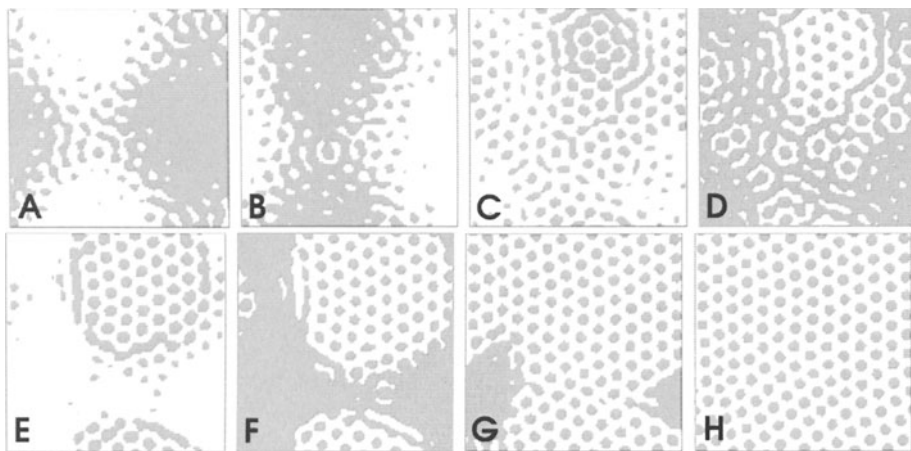


Figure 1.2: A two-dimensional concentration patterns obtained in a system with a coupled Turing-Hopf bifurcation as the simulation is started from a random initial configuration. White and gray domains correspond to areas dominated by chemical u and v , respectively. The time evolution goes from left to right and from top to bottom [27].

tains a tristable system, although the stationary state $(0, 0)$ is no longer Turing-Hopf unstable, but Turing unstable with $k_c = 0.46$. The two other stationary states $(-1.191, 0.350)$ and $(6.529, -1.920)$ are Turing unstable with $k_c = 0$ as in the previous case. Again the Turing modes growing from $(0, 0)$ excite another nearest stationary state, which results in an interesting competition between growing modes. Although there is no straightforward Turing-Hopf bifurcation, the modes growing from the state $(-1.191, 0.350)$ with $\text{Re}\{\lambda(k_0)\} > 0$ are coupled with the damped Hopf modes $\propto e^{i\omega_0 t}$ of the state $(0, 0)$, which results in oscillatory behavior with period $T_c \approx 3765 \times dt$. This dynamics is described by a series of snapshots in Fig. 1.3, where the homogeneous oscillations sweep out spots with period T_c , and then the spots are again nucleated at the centers of concentric target pattern waves. The competition continues for long times of up to $10^6 \times dt$, although the oscillations gradually fade out.

One should mention that for parameter value $C = 0$, which has been shown to correspond to a striped pattern [24], the system showed a straightforward Turing bifurcation of the state $(0, 0)$ without any oscillatory competition. This happened because the Turing modes growing from the state $(0, 0)$ and resulting in stripes did not excite the other stationary states, i.e., the amplitude of the striped concentration pattern was not large enough for the modes to interact with other stationary states. Based on this observation, one can state that in multistable systems the parameter selection might have drastic effects on the dynamical behavior of the system.

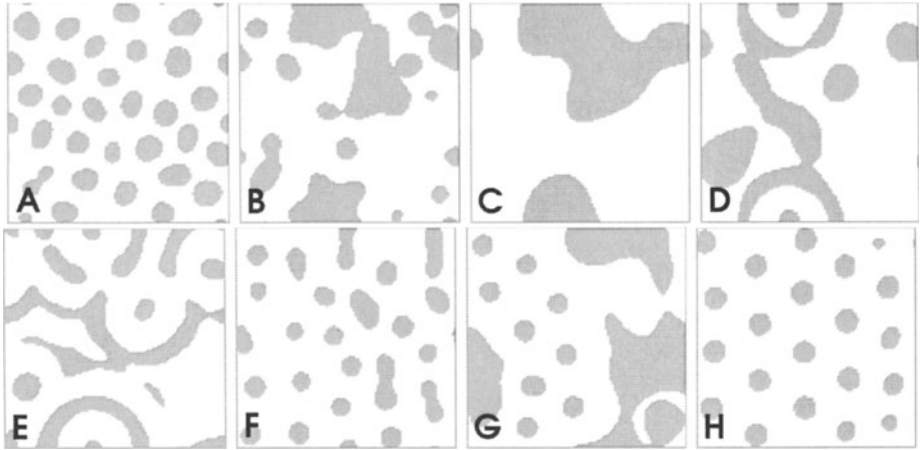


Figure 1.3: The two-dimensional concentration patterns obtained in a tristable system with a coupled Turing-Hopf-Turing bifurcation as the simulation is started from a random initial configuration. The time evolution goes from left to right and from top to bottom [27].

1.4 Conclusions

In this paper we have studied spatio-temporal pattern formation in the generic Turing model. Most of the studies of spatio-temporal dynamics have in general been carried out in one-dimensional systems, since they make it feasible to study the Turing-Hopf interaction by using amplitude equation formalism [15, 18]. In the two-dimensional case (not to talk about three dimensions) the studies of spatio-temporal behavior have typically, although not always [28], been more or less qualitative. By considering stability and bifurcation aspects one can govern and interpret the behavior of the systems to some extent, but otherwise two-dimensional spatio-temporal dynamics is often too complex to be studied analytically.

By using different parameter sets we have studied the Turing-Hopf coupling in a monostable system, which resulted transient oscillatory behavior combined with localized spotty and oscillatory domains. By establishing a tristability in a similar system we obtained a hexagonally arranged spotty pattern with a few twinkling spots, i.e., spots appearing and disappearing at dislocation sites. The tristability without straightforward Turing-Hopf bifurcation resulted in temporal competition since the stable Hopf modes of one stationary state were coupled with the Turing bifurcation of another state, caused by competition between a homogeneous oscillatory wave and a spotty pattern. In addition, we have observed that different parameter values might prevent this coupling and instead pure stationary Turing stripes would settle in.

Turing instability is not relevant only in reaction-diffusion systems, but also in describing other dissipative structures, which can be understood in terms of

diffusion-driven instability. Turing instability has been discussed in relation to gas discharge systems [29], catalytic surface reactions [30], semiconductor nanostructures [31], and surface waves on liquids [32]. The studies of temporal and spatial pattern formation in Turing system are important, since they may be of great interest also in biological context, e.g. skin hair follicle formation, which is closely related to skin pigmentation, occurs in cycles [33]. Recently, spatio-temporal traveling wave pattern has been observed on the skin of a mutant mouse [34], which might perhaps be the result of a misconfigured Turing mechanism with competing instabilities, i.e., the pattern becomes temporal instead of stationary due to a shift in the values of the reaction and diffusion rates of morphogens.

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Chapter 27

Evolution of Money Distribution in a Simple Economic Model

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An analytical approach is utilized to study the money evolution in a simple agent-based economic model, where every agent randomly selects someone else and gives the target one dollar unless he runs out of money. (No one is allowed to go into debt.) If originally no agent is in poverty, for most of time the economy is found to be dominated by a Gaussian money distribution, with a fixed mean and an increasing variance proportional to time. This structure begins to be drifted toward the left when the tail of the Gaussian hits the left boundary, and the drift becomes faster and faster, until a steady state is reached. The steady state generally follows the Boltzmann-Gibbs distribution, except for the points around the origin. Our result shows that, the pdf for the utterly destitute is only half of that predicted by the Boltzmann solution. An implication of this is that the economic structure may be improved through manipulating transaction rules.

1.1 Introduction

Recently there is a surge of interest in applying statistical mechanics laws to study economics[1]. This helps shed light on some aspect of economic phenomena which would otherwise be difficult to see. It has been shown that, for a closed economic system, the equilibrium money distribution often obeys a Boltzmann-Gibbs distribution[2]. This remarkable result follows from an analogy of atoms to agents and energy to money.

Use of the physical equilibrium metaphor, however, should be cautioned. The “invisible force” underlying the market need not be equivalent to a mechanical one, as interactions between agents are due to human activities which are accompanied with unpredictable arbitrariness. As a result, the law of Boltzmann-Gibbs distribution may not be as universal as it appears in physics[1][3][4].

An unfavorable rule of transaction could have it broken. In this paper, we want to use a concrete example to give this problem an illustration.

On the other hand, an economic model mirroring reality faithfully is rarely in equilibrium. In an agent-based model, Carter[5] showed that the time scale for its money distribution to reach a quasi-stationary state is grindingly long. More often than not, observed in the economy might be some distributions on evolution, instead of a final equilibrium. In this sense, transient money states are equally of importance, and more is needed than just the Boltzmann solution.

These two problems, as far as we know, are still not well studied. Particularly lack is a study from analytical point of view, though Monte Carlo simulations with specific problems are not uncommon[1][3]. In this paper, we use an analytical approach to re-examine these problems. We want to demonstrate the applicability limits for the statistical physics laws and, particularly, address through this study the fundamental issue that market rules which may have the Boltzmann distribution assumption violated could be on the other hand utilized to manipulate the economy into a healthier structure. The whole study is limited within the framework of a simple model, which is introduced in the following section. We first derive for this model a master equation, and its corresponding boundary conditions. Asymptotic solution is then sought, and the result analyzed. In Sec. 1.4.2, we give a description of the transient states, and show how the money distribution evolves toward its equilibrium. Sec. 1.4.3 explores the steady state of the probability density function, particularly its structure near the origin. These analyses are then verified in a numerical solution (Sec. 1.5). This work is summarized in Sec. 1.6.

1.2 Master equation

The simple model we are about to use in this study is from Carter[5]. At each time step, every agent randomly selects someone else among a collection of agents and gives the target one dollar. If an agent has no money, the agent waits until someone gives him a dollar (no one is allowed to go into debt.) For convenience, suppose that the amount given out by every agent at a transaction is Δx , in some scaled units. (From now on, money is dimensionless). Note that Everyone has to meet someone, but he is not necessarily met by anyone else. One agent could be visited by many agents. For easy reference, we introduce the following notations:

- N : number of total agents
- M : total money (in some scaled units)
- $n_x(t)$: expected number of agents with money x at time t . Agents in this group hereafter will be referred to as x -agents.

Now consider the increase of $n_x(t)$ during a short interval $[t, t + \Delta t]$. In the following formulation, the fact that everybody has to visit someone at a time has been used (with probability 1). Lying at the heart of this problem is therefore how one in group $n_x(t)$ is visited by others.

Related to the change of $n_x(t)$ at time t are the following events:

- $E_{n_x} = .\text{NOT. } \{x\text{-agent visited only by one nonzero-agent}\}$
- $E_{n_{x+\Delta x}} = \{(x + \Delta x)\text{-agent visited by zero nonzero-agent}\}$
- $E_{n_{x-\Delta x}} = \{(x - \Delta x)\text{-agent visited by two nonzero-agents}\}$
- $E_{n_{x-2\Delta x}} = \{(x - 2\Delta x)\text{-agent visited by three nonzero-agents}\}$
- ...

- $E_{n_{\Delta x}} = \{\Delta x\text{-agent visited by } \frac{x}{\Delta x} \text{ nonzero-agents}\}$
- $E_{n_0} = \{\text{zero-agent visited by } \frac{x}{\Delta x} \text{ nonzero-agents}\}$

The increase in expected number of x -agents are then

$$\begin{aligned} n_x(t + \Delta t) - n_x(t) = & -n_x \times P(E_{n_x}) + n_{x+\Delta x} \times P(E_{n_{x+\Delta x}}) \\ & + n_{x-\Delta x} \times P(E_{n_{x-\Delta x}}) + n_{x-2\Delta x} \times P(E_{n_{x-2\Delta x}}) + \dots \\ & + n_{\Delta x} \times P(E_{n_{\Delta x}}) + n_0 \times P(E_{n_0}). \end{aligned} \quad (1.1)$$

Let $q = \frac{1}{N-1}$, and denote $P_k = P(\text{an agent visited by } k \text{ nonzero-agents})$, which is a binomial for $k \leq N - n_0 - 1$ and zero otherwise,

$$P_k = \begin{cases} C_{N-n_0-1}^k q^k (1-q)^{N-n_0-1-k}, & \text{for } k \leq N - n_0 - 1 \\ 0, & \text{else} \end{cases} \quad (1.2)$$

then the probabilities in (1.1) can be evaluated as:

$$\begin{aligned} P(E_{n_{x+\Delta x}}) = P_0, \quad P(E_{n_x}) = 1 - P_1, \quad P(E_{n_{x-\Delta x}}) = P_2, \quad P(E_{n_{x-2\Delta x}}) = P_3, \\ \dots \quad P(E_{n_{\Delta x}}) = P_{x/\Delta x}, \quad P(E_{n_0}) = P_{x/\Delta x}. \end{aligned}$$

So Eq. (1.1) can be rewritten as

$$\begin{aligned} n_x(t + \Delta t) - n_x(t) &= -n_x(1 - P_1) + n_{x+\Delta x}P_0 + n_{x-\Delta x}P_2 + n_{x-2\Delta x}P_3 + \dots + n_{\Delta x}P_{x/\Delta x} + n_0P_{x/\Delta x} \\ &= -n_x + \sum_{k=0}^{x/\Delta x} n_{x+(1-k)\Delta x}P_k + n_0P_{x/\Delta x} \end{aligned} \quad (1.3)$$

Normalizing n_x with the total number of agents N , we obtain the probability assigned to money x . For analytical convenience, we may approximately understand it to be $\Delta F(x \leq \text{money} < x + \Delta x)$, the probability associated with the interval $[x, x + \Delta)$. ΔF divided by Δx is the probability density function (pdf) f . We hence obtain an equation governing the evolution of the pdf of money x at time t :

$$f(x, t + \Delta t) = \sum_{k=0}^{x/\Delta x} f(x + (1-k)\Delta x, t) P_k + f(0, t) P_{x/\Delta x}, \quad x \in [0, M]. \quad (1.4)$$

This is similar to Einstein's master equation for diffusion[7], but with an expression much more complicated.

In the above formulation, the total number of agents (N) and the total money (M) are preserved. In terms of f , these two conservation laws are expressed as follows:

$$(a) \quad \int_0^M f(x, t) dx = 1, \quad (\text{conservation of } N) \quad (1.5)$$

$$(b) \quad \int_0^M x f(x, t) dx = \frac{M}{N}. \quad (\text{conservation of } M) \quad (1.6)$$

Note (a) and (b) are not constraints in addition to the above formulation. Rather, they are two properties inherently associated Eq. (1.4).

1.3 Boundary conditions

The probability space of (1.4) is not the whole real line. Given a time, f varies on a closed domain $[0, M]$. We therefore need to find boundary conditions for the equation at $x = 0$ and $x = M$.

At the left boundary $x = 0$, the change in number of zero-agents at time t , $n_0(t)$, is due to

- (a) $E_{\Delta x} = \{\Delta x\text{-agent not visited by nonzero-agents}\}$,
- (b) $E_0 = \{\text{zero-agent visited by nonzero-agents}\}$.

Of these two events, (a) is to increase n_0 , while (b) is to decrease the number. Following a similar procedure as above for the master equation,

$$\begin{aligned} n_0(t + \Delta t) - n_0(t) &= n_{\Delta x} P(E_{\Delta x}) - n_0 P(E_0) \\ &= -n_0[1 - (1 - q)^{N-n_0-1}] + n_{\Delta x}(1 - q)^{N-n_0-1}, \end{aligned} \quad (1.7)$$

which reduces to

$$f(0, t + \Delta t) = [f(0, t) + f(\Delta x, t)] (1 - q)^{N-n_0-1}, \quad (1.8)$$

if normalized by N and divided by Δx . Recall that $n_0 = N\Delta x f(0, t)$ and $q = \frac{1}{N-1}$, implying that

$$(1 - q)^{N-n_0-1} = (1 - q)^{1/q - Nf\Delta x} \rightarrow e^{-1+f\Delta x}, \quad \text{as } q \rightarrow 0.$$

The left boundary condition then becomes

$$f(0, t + \Delta t) = [f(0, t) + f(\Delta x, t)] e^{-1+f(0,t)\Delta x} \quad (1.9)$$

At the right boundary, $x = M$, f can only have two choices: $\frac{1}{N\Delta x}$ and 0. The former is unstable, as one transaction will revoke the membership of the M-agent. We may hence safely claim that $f(M, t) = 0$.

1.4 Asymptotic solution

1.4.1 Simplified governing equation

The master equation (1.4) can be simplified in the limit of $\Delta t \rightarrow 0$, $\Delta x \rightarrow 0$. Making Taylor's expansion on both sides, and retaining respectively terms up to $O(\Delta t)$ and $O((\Delta x)^2)$, we get

$$f + \frac{\partial f}{\partial t} \Delta t = \sum_{k=0}^{x/\Delta x} P_k \left[f + \frac{\partial f}{\partial x} (1 - k) \Delta x + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} (1 - k)^2 (\Delta x)^2 \right] + f(0, t) P_{x/\Delta x} + h.o.t. \quad (1.10)$$

The key to the problem now is to evaluate the sum over k .

Suppose for the time being x is away from the origin far enough such that $P_{x/\Delta x}$ is ignorable to some given order. This is not a strict constraint. In fact, from Eq. (1.2),

$$P_k < C_N^k \frac{1}{N^k} < 10^{-6}, \quad \text{for } k > 10, \text{ when } N = 10000.$$

Therefore, the summation limit $k = x/\Delta x$ may be replaced by $k = N - n_0 - 1$ up to a reasonable precision for x on most of its definition domain, viz.

$$f + \frac{\partial f}{\partial t} \Delta t \approx f \sum_{k=0}^{N-1-n_0} P_k + \frac{\partial f}{\partial x} \Delta x \sum_{k=0}^{N-1-n_0} (1 - k) P_k + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} (\Delta x)^2 \sum_{k=0}^{N-1-n_0} (1 - k)^2 P_k. \quad (1.11)$$

We know from binomial distribution $\sum_{k=0}^{N-1-n_0} P_k = 1$, and

$$\sum_{k=0}^{N-1-n_0} k P_k = (N-1-n_0)q = 1-n_0q, \quad (1.12)$$

$$\begin{aligned} \sum_{k=0}^{N-1-n_0} k^2 P_k &= (N-1-n_0)q + (N-1-n_0)(N-2-n_0)q^2 \\ &= (1-n_0q) + (1-n_0q)[1-(n_0+1)q]. \end{aligned} \quad (1.13)$$

Eq. (1.11) then can be simplified as

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x} n_0 q \frac{\Delta x}{\Delta t} + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \frac{(\Delta x)^2}{\Delta t} [1 - (n_0+1)q(1-n_0q)]. \quad (1.14)$$

When N is large,

$$n_0 q = \frac{n_0}{N-1} \rightarrow \frac{n_0}{N} = f(0, t) \Delta x,$$

the first term on the right hand side of (1.14) is of order $O[(\Delta x)^2]$. The second term becomes

$$\frac{1}{2} \frac{\partial^2 f}{\partial x^2} (\Delta x)^2 + O[(\Delta x)^3].$$

These two terms are thence balanced on the order of $(\Delta x)^2$ as $\Delta x \rightarrow 0$. Write $\frac{(\Delta x)^2}{\Delta t}$ as μ . The above equation is reduced to

$$\frac{\partial f}{\partial t} = \mu f_0 \frac{\partial f}{\partial x} + \frac{1}{2} \mu \frac{\partial^2 f}{\partial x^2}, \quad (1.15)$$

where f_0 is the shorthand for $f(0, t)$. This Fokker-Planck-like equation is similar to the nonlinear Boltzmann equation[6] used in [1], but with different coefficients.

1.4.2 Transient states

As mentioned in the introduction, generally it takes a long time for the money to reach its steady distribution. In other words, this economy is rarely in equilibrium. Transient states are therefore of very much importance. In this section, we investigate how the economy is evolved toward its equilibrium, and how long the evolution takes.

Eq. (1.15) is an advection-diffusion equation. When the collection of zero-agents is not empty, $f_0 > 0$, the advection is thence toward the left. If, by any chance, the money distribution is away from the origin, the advection halts, and the solution of f adopts a form of Gaussian. Gaussian dominates the pdf evolution before it hits the left boundary. We will see later in a numerical solution, a non-Gaussian distribution will be adjusted into a normal form very quickly.

During the evolution, the center of the Gaussian keeps fixed if $n_0 = 0$. This is guaranteed by property (1.6) of the master equation. But the variance increases in proportion to t , and sooner or later, the tail of the Gaussian will hit the left boundary at $x = 0$. It is at this time the whole structure begins to be drifted leftward. As f_0 increases, the drift becomes faster and faster, and eventually the Gaussian gives itself away to other structures. The whole evolution scenario is schematized in Fig. 1.1.

We may also estimate the time scale of duration in maintaining f in the shape of Gaussian. From Eq. (1.15), Gaussian form is destroyed when its tail hits the boundary. Let the center sit at x_0 , then

$$t \sim \frac{2x_0^2}{\mu} = \frac{2x_0^2}{(\Delta x)^2} \Delta t,$$

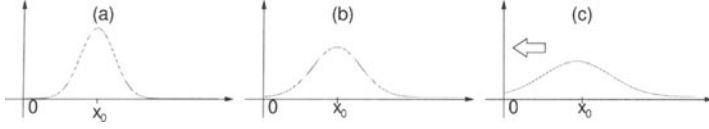


Figure 1.1: A schematic of the transient states of the pdf evolution: Initially a Gaussian centered at x_0 (a) will maintain its form centered at the same location (b), until its left tail hits $x = 0$. Beginning this time, the whole structure is drifted toward the left (c).

i.e., the time scale is of the order of $2 \left(\frac{x_0}{\Delta x} \right)^2$ times the time step Δt . When x_0 is not too small, this scale is usually very large. Therefore, for most of time, the economy is dominated by a Gaussian money distribution. In other words, the economy chooses for the money distribution a Gaussian on its route of evolution toward the equilibrium, which we are now to explore.

1.4.3 Steady state

In the steady state, $\partial/\partial t = 0$, Eq. (1.15) is simplified to an ordinary differential equation

$$\frac{\partial^2 f}{\partial x^2} + 2f_0 \frac{\partial f}{\partial x} = 0. \quad (1.16)$$

Notice that here $f_0 = f(0, \infty)$ is a constant in x . The ODE thus can be easily solved, with a solution in the form

$$f = D e^{-2f_0 x}. \quad (1.17)$$

Constants D and f_0 can be determined by the two conservation properties. When M is large, they are

$$D = 2f_0 \quad (1.18)$$

$$f_0 = \frac{N}{2M}. \quad (1.19)$$

The equilibrium solution is therefore

$$f(x, \infty) = \frac{N}{M} e^{-\frac{N}{M} x}, \quad (1.20)$$

same as the Boltzmann solution obtained from the maximal entropy principle[5].

Note that Eq. (1.20) does not hold near the origin. We emphasized this when we made the assumption in simplifying the master equation. What is of interest is: the pdf at the origin actually has been determined in (1.19). It is equal to $\frac{N}{2M}$, half of the pdf predicted by (1.20), the Boltzmann solution.

We can learn more about the steady probability distribution near the origin through the boundary condition. Using f_k to indicate $f(k\Delta x, \infty)$, the equilibrium form of Eq. (1.9) is:

$$f_0 = [f_0 + f_1] e^{-1+f_0 \Delta x} \quad (1.21)$$

which, when substituted with $\frac{N}{2M}$ for f_0 , gives

$$f_1 = \left[e^{1-\frac{N}{2M} \Delta x} - 1 \right] \frac{N}{2M}. \quad (1.22)$$

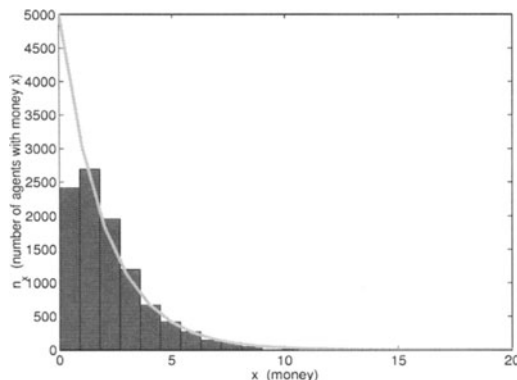


Figure 1.2: Histogram of a Monte Carlo simulation with $N = 10000$, $M = 20000$, and $\Delta x = 1$. The solid curve is the Boltzmann-Gibbs money distribution for this economy. Our estimation, $n_0 = 2500$, $n_1 = 2793$, agrees well with the simulated result near the origin.

As a verification, we have run a Monte Carlo simulation with $M = 20000$, $N = 10000$, $\Delta x = 1$. In this economy, our model predicts that the numbers of zero-agents and Δx -agents are, respectively, $n_0 = N \times \frac{N}{2M} \Delta x = 2500$, $n_{\Delta x} = (e^{1 - \frac{N}{2M} \Delta x} - 1)n_0 = 2793$. The simulated equilibrium state is shown in the histogram Fig. 1.2. Shown also in the figure is the Boltzmann solution, which agrees very well with the simulation except for a small region around the origin. Apparently, n_0 and $n_{\Delta x}$ are very close to our predictions. Particularly, n_0 is approximately half of 5000, the pdf at $x = 0$ given by (1.20).

1.5 Numerical solution

In order to have a better understanding of the evolution scenario described above, we present in this section a numerical solution for the master equation (1.4), with $N = 10000$, $M = 956779$, and $\Delta x = 1$. [The value of M is not essential. It takes this number from the initial beta distribution (see below) we generate numerically.] The result is shown in Fig. 1.3. The initial condition is approximately a beta distribution on $[0, 100]$ (Fig. 1.3a). From the solution, after only ten time steps, it gets adjusted into a Gaussian-like shape, which is centered at $x_0 = \frac{M}{N} = 96$. This state lasts for a long time, and even after it hits the left boundary at about $t = 2000$, most of it still keeps a norm form. The final steady state is like an exponential decay, as predicted by Eq. (1.20). For points near the left boundary, (1.20) is not valid. But the expected numbers of agents at $x = 0, 1$, $n_0 = 52$ and $n_{\Delta x} = 89$, agree well with the prediction with formulas (1.19) and (1.22).

1.6 Summary

With the aid of a master equation, we have investigated the evolution of money distribution in an agent-based simple economic model. If originally no agent is in poverty, for most of time the money is distributed in a Gaussian form, with the mean fixed at x_0 , the arithmetic average of money for the economy, and the variance increasing with time. This geometric structure is very stable, lasting for a time scale proportional to $\left(\frac{x_0}{\Delta x}\right)^2$, with $\frac{x_0}{\Delta x}$ being the ratio of the mean to the minimal amount of money exchange per transaction. After hitting the boundary, the structure

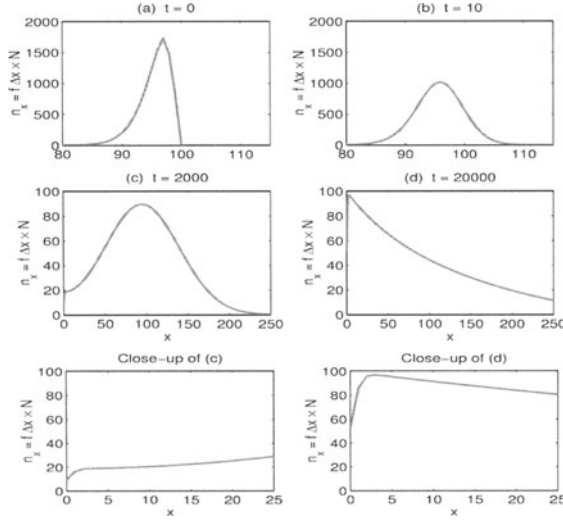


Figure 1.3: A numerical solution of the master equation (1.4) with $N = 10000$, $M = 956779$, and $\Delta x = 1$. The value of M is not essential. It is from the initial beta distribution we generate numerically.

is drifted leftward, faster and faster, until an equilibrium is reached with a completely different structure.

The equilibrium state of the economy has also been explored. The stationary distribution is roughly the same as the Boltzmann solution obtained from the maximal entropy principle, except for points near the origin. By our estimation, the number of agents without any money is only half of the number predicted for the same group from the Boltzmann solution. This estimation has been verified in a Monte Carlo simulation.

We remark that the solution thus obtained has practical implications, though the economy itself is too simple to model the real world. Given the number of total individuals and the total money, by Eqs. (1.19) and (1.22) f_0 is fixed, but f_1 drops with Δx increased. That is to say, in this economy, we may reduce the number of the poor by increasing the amount for one transaction. It is of our interest to explore the possibility of improving the structure of a society through manipulating market rules with a more sophisticated model.

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Chapter 28

Chaos as a Bridge between Determinism and Probability in Quantum Mechanics

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X.1 Introduction

Quantum mechanics is fundamentally a probabilistic science, whereas classical mechanics is deterministic. This dichotomy has led to numerous disputes and confusion, ranging from the Einstein-Bohr debates of the 1930's [Einstein, Podolsky, and Rosen 1935; Bohr 1935], through attempts to establish determinism in quantum mechanics by means of introducing "hidden variables" [de Broglie 1960, 1964; Bohm 1952], to lengthy discussions of epistemological versus ontological interpretations of quantum mechanics [Bohm and Hiley 1993]. Throughout most of the twentieth century the Copenhagen interpretation of Bohr and Heisenberg has endured as the orthodox interpretation, replete with contradictions and paradoxes such as duality, the necessity for an observer before a quantum system can attain physical meaning, and the reduction of the wave function upon observation. The *reductio ad absurdum* of such paradoxes was the example of Schrödinger's cat [Schrödinger 1936; Gribben 1984,1995], in which a cat inside a closed chamber remained in limbo as a linear superposition of $|dead\ cat\rangle + |live\ cat\rangle$ until an observer determined whether or not a radioactive nucleus had decayed, releasing a deadly poison.

During the last several decades, nonlinear dynamics and chaos theory have become well-enough developed that they can be used to intercede in some of these seeming paradoxes of quantum mechanics. Since chaotic systems are fundamentally deterministic, yet have to be treated statistically, it is worth investigating as to whether chaos can form a bridge between the determinism of classical mechanics and the probabilistic aspects of quantum mechanics. Perhaps both Einstein and Bohr could have been correct in their interpretations: At heart chaos theory provides the determinism so dear to Einstein; yet for most practical purposes it reduces to the probabilities of the Copenhagen interpretation. Interestingly enough, although authors of the earlier (not altogether successful) attempts to impose determinism on

quantum mechanics did not have access to modern chaos theory, in many ways they toyed with ideas that we now can see as arising naturally in chaotic systems.

More recently, nonlinear extensions to quantum mechanics have been promulgated by a number of authors [Weinberg 1989; Gisin 1989, 1990; Mielnik 2001; Czachor and Doebner 2002]. Again, their efforts have been but partially successful, sometimes introducing superluminal (nonphysical) signals into multi-particle correlations. Mielnik sums up their thinking, "...perhaps, it resists embedding into too narrow a scheme...the nonlinear theory would be in a peculiar situation of an Orwellian 'thoughtcrime' confined to a language in which it cannot even be expressed...A way out, perhaps, could be a careful revision of all traditional concepts..." Their efforts centered around corrections and perturbations applied to traditional, *linear* quantum mechanics — and in such weakly nonlinear systems chaotic behavior cannot develop!

From a different perspective, viz., a consideration of the possibility that nonlinearities can arise at the Planck length ($\leq 10^{-33}$ m), has come the recent work of t'Hooft [2003] and Krasnoholovets [2003]. However, this is more concerned with reconciling quantum mechanics with relativity than in dealing with the (more simplistic?) imponderables encountered with the Copenhagen interpretation.

Perhaps the time is ripe to inquire into the possibility that chaos and nonlinear dynamics could be an inherent component of quantum mechanics — only heretofore not recognized as such. In a series of papers [McHarris 2001, 2003, 2004] I have cautiously put forth the idea that certain imponderables — or paradoxes — encountered with the Copenhagen interpretation of quantum mechanics might have parallel explanations in terms of nonlinear dynamics. This is not to be construed as any sort of proof of the existence of chaos underlying quantum mechanics — indeed, just as quantum mechanics itself cannot be derived, but only postulated, such a proof cannot be forthcoming. And these ideas are still at the "from the bottom up," even "quasi-experimental" stage: Examples must be collected and analyzed before any broad formulations can even be considered. Nevertheless, the very existence of such parallel examples makes raising the question(s) worthwhile.

Even if eventually it becomes accepted that quantum mechanics can contain deterministic, if nonlinear components, for the most part this will have relatively little effect on the day-to-day use of quantum mechanics. This results from the fact that most scientists use it simply as the superb procedure — or computer formulation — that it is and care little about the quandaries associated with its foundations. And they would be trading one set of difficult mathematics for an equally messy set of nonlinear numerologies. The primary exception to this that I foresee lies in the field of quantum information and computing, the very field that has helped so much to reinstate interest in reexamining the foundations of quantum mechanics. For the possibility of massively parallel quantum computing rests firmly on the principle of linear superposition of states, which can be manipulated simultaneously but independently. In a quantum mechanics containing nonlinear elements, this basis might have to be reexamined.

X.2 Quantum Mechanical Imponderables with Nonlinear Parallels

At least seven so-called imponderables or paradoxes associated with the Copenhagen interpretation of quantum mechanics have analogous nonlinear interpretations that logically are quite compelling. Some of these have been investigated much more thoroughly than others. They are summarized here in decreasing order of effort spent in trying to fathom them.

X.2.1 The Exponential Decay Law and the Escape Group from Unimodal Maps

Radioactive decay and atomic and molecular transitions — indeed, all first-order processes, including first-order chemical reactions — follow exponential decay laws, exhibiting time-independent half-lives. These are often justified by analogy with actuarial tables, such as those used by the life insurance industry. Although it is difficult, if not impossible, to determine when an individual will die, given a sufficiently large sample, the statistical predictions become quite precise, allowing insurance companies assured profits. By analogy, it is impossible to predict when, say, a given radioactive nucleus will disintegrate; however, given a large enough sample of nuclei, a statistical exponential decay law is followed very precisely.

Upon further consideration, such an analogy should not hold up. Actuarial tables are based on complexity: There are large numbers of *different* people having *widely diverse* causes of mortality. On the other hand, one of the fundamental premises of quantum mechanics is that *identical* particles are truly *identical* and *interchangeable*; thus, completely different statistics should apply.

A nonlinear parallel can be found in the iteration of unimodal maps in their chaotic regimes, where extreme sensitivity to initial conditions applies. Consistent with (but not dependent on) the Uncertainty Principle, an initial, say, radioactive nuclear state, having a finite width, can be likened to a tiny interval in initial input values. Different individual nuclei in this state can then be represented by random initial values selected within this interval. The final nuclear state can similarly be represented by a second interval, corresponding to possible final values. And the decay dynamics — a transition probability is at least quadratic in nature — can be considered analogous to iterating the map. One keeps a record of the number of initial states remaining, i.e., the number that have not escaped into the final state, after each iteration. A plot of this remaining number against the number of iterations yields an exponential decay curve.

This analog is treated in considerable detail in [McHarris 2003], where both the quadratic and sine maps are considered. Tens of thousands of randomly-generated initial states within intervals typically having widths of 10^{-11} were followed, and this procedure consistently generated exponential decay curves. The process of iteration can be justified physically if one makes a correspondence with a physical process such as the number of oscillations of, say, a nuclear dipole or the number of attempts of an α particle at barrier penetration. Unfortunately, because of the “universality” of chaos, it is difficult to make further mechanistic predictions, and any sort of time series analysis is unlikely to retain significant correlations because of the enormous difference between the laboratory and nuclear times scales. (Nevertheless, because of the relative ease with which time-delay experiments could be performed with radioactive species, such experiments should be performed on the off chance that some faint remnant of an attractor could be perceived.)

X.2.2. Bell's Theorem and Nonextensive Entropy

The EPR paradox [Einstein, Podolsky, and Rosen 1935] was designed to demonstrate that quantum mechanics was incomplete ; it involved correlations between separated particles (Einstein's "spooky action at a distance"), but it was cast in the form of an abstract *Gedankenexperiment*. Bohm [Bohm 1951] made the EPR more specific and less abstract by considering a pair of spin-1/2 fermions, but it was Bell [Bell 1964] who reanalyzed it into something that touched upon physical reality. There have been various refinements and variants on Bell's inequality, but perhaps the simplest — *designed to be experimentally friendly* — is the CHSH inequality [Clauser, Horne, Shimony, and Holt 1969], which is used as the illustration here. (Also, cf. [McHarris 2004]).

Consider the following correlation experiments on pairs of particles, using the standard information theory cartoon characters, Alice and Bob, who are stationed at an effectively infinite (incommunicado) distance apart. Pairs of particles having binary properties, e.g., spin up vs spin down or perhaps horizontal vs vertical polarization, are prepared, then one particle from each pair is sent to Alice and the other to Bob. Examples of such pairs could be two electrons or two photons.

Alice can make measurements Q or R on each of her particles, each measurement having a possible outcome of $+1$ or -1 . For example, Q could be a measurement of spin with respect to a vertical axis, while R would be with respect to an oblique axis. Similarly, Bob can make measurement S or T on each of his particles. Alice and Bob each choose which measurement to make at random, often waiting until the particles are already on their way in flight, thus assuring no communication between them or with the originator of the particles. After making many pairs of measurements in order to attain statistical significance, the two get together to compare notes. The quantity of interest based on their measurements is

$$QS + RS + RT - QT = (Q + R)S + (R - Q)T. \quad (1)$$

Note the single minus sign — because Q and R independently can have the values $+1$ or -1 , one of the terms on the right side of the equation must be 0. Either way,

$$QS + RS + RT - QT = \pm 2, \quad (2)$$

or in terms of probabilities, where $E(QS)$, for example, is the mean value of the measurements for the combination QS , we come up with the CHSH inequality,

$$E(QS) + E(RS) + E(RT) - E(QT) \leq 2. \quad (3)$$

This so-called "classical" derivation of a specific variant of Bell's inequality places an upper limit on the statistical correlations for a specific combination of products obtained by presumably independent (and randomly chosen) measurements.

The quantum mechanical version is obtained by starting off with the pairs of particles in the *entangled* Bell singlet state,

$$|\Psi\rangle = (|01\rangle - |10\rangle)/\sqrt{2}. \quad (4)$$

The first qubit from each ket is sent to Alice, the second from each ket to Bob. Measurements are carried out as before, but on the following combinations of observables:

$$Q = Z_1, \quad R = X_1, \quad S = \frac{(-Z_2 - X_2)}{\sqrt{2}}, \quad T = \frac{(Z_2 - X_2)}{\sqrt{2}} \quad (5)$$

Here X and Z are the “bit flip” and “phase flip” quantum information matrices, corresponding to the Pauli σ_1 and σ_3 spin matrices. It can be shown that the expectation values of the pairs QS , RS , and RT are all $+1/\sqrt{2}$, while that of QT is $-1/\sqrt{2}$. This leads to the quantum mechanical analogy to the CHSH inequality,

$$\langle QS \rangle + \langle RS \rangle + \langle RT \rangle - \langle QT \rangle = 2\sqrt{2}. \quad (6)$$

Thus, quantum mechanics, within the framework of entangled states, predicts a possibly larger statistical correlation than was allowed by the so-called classical inequality. Bell’s theorem predicts that classical systems will obey such inequalities, while quantum systems might violate them under the right circumstances.

During the last several decades, several dozen “Bell-type” experiments have been performed [Bertlmann and Zeilinger 2003], and they have consistently violated the inequalities. Quantum mechanics wins, classical mechanics loses! As with most ideas connected with quantum mechanics, interpretations vary — but most interpretations involve the elimination of “local reality.” Two isolated, far-apart but entangled particles have some sort of influence on each other. A down-to-earth experimental example of this might be the following: Two electrons are emitted in a spin-singlet state. Their individual spin directions are unknown (undefined according to the Copenhagen interpretation), but they must be opposite. When Alice arbitrarily measures the direction of her electron, say, with respect to a z axis and gets $\uparrow$, this information is instantaneously conveyed to Bob’s electron, whose wave function reduces to $\downarrow$ with respect to this same axis. Einstein’s “spooky” — and superluminal — action at a distance is real!

But wait a minute. Is this really a contest between quantum vs. classical mechanics, or is it between correlated vs. uncorrelated statistics. In the so-called classical derivation, the particles were presumably prepared in correlated pairs, but these correlations were then tacitly ignored, while the quantum mechanical entangled pairs necessarily retained the highest correlations. And correlated statistics are known to exist in nonlinear systems:

The codification of correlated statistics was introduced by Tsallis and his co-workers [Tsallis 1988, Curado and Tsallis 1991], when they formulated so-called “nonextensive” (meaning nonadditive) thermodynamics. Correlations in classical systems result in a generalized entropy,

$$S_q = (1 - \sum_{i=1}^W p_i^q) / (q - 1). \quad (7)$$

Here the phase space has been divided into W cells of equal measure, with p_i the probability of being in cell i . For the exponent q (termed the “entropic index”) having a value of 1, the generalized entropy reduces to the standard Boltzmann entropy,

$$S_1 = - \sum_{i=1}^W p_i \ln p_i. \quad (8)$$

As q varies from 1, the deviation from standard distributions becomes greater, with “long-range” correlations becoming greater. When such correlations are present, the entropy becomes nonextensive, and the entropy of the total system becomes

$$\frac{S_q(A+B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1-q) \frac{S_q(A)S_q(B)}{k^2}. \quad (9)$$

When $q < 1$, the entropy of the combined system is greater (superextensive) than the sum of its parts, and when $q > 1$, it is less (subextensive) than the sum of its parts. This concept has found widespread applications in classical systems, ranging from winds velocity distributions in tornadoes to the energy distributions of cosmic rays [i.a., Gell-Mann and Tsallis 2004].

What is pertinent is that systems “at the edge of quantum chaos” have recently been studied [Weinstein, Tsallis, and Lloyd 2004], and both for the quantum kicked top and for the logistic map [Baldovin and Robledo 2002; Borges et al. 2002] values of $q > 1$ could be applied. [One has to be careful here with quantitative interpretations because these values were derived within the context of standard (linear) quantum mechanics with “quantum chaos”; however, the crossover into classical chaos is similar, and it seems that both systems exhibit long-range correlations.] For the logistic equation these groups found that a value of $q \approx 2$ seemed reasonable.

From the above it seems rather clear that nonlinear classical systems can indeed exhibit correlations in which “long-range” correlations play an important role. (This does not necessarily mean long-range forces or “action at a distance,” as has been known for a long time from the behavior of cellular automata and self-evolving systems.) Thus, the “classical” derivation of the CHSH inequality — and most if not all of the other guises that Bell’s inequality takes on — is suspect. Classical systems can easily involve correlated statistics, which raises the apparent upper limit of inequalities such as Eqn. (3). With a value of q in the vicinity of 2, one could easily obtain something closer to an exponential rather than a Gaussian distribution. In

other words, Bell's inequality is moot in ruling out the existence of local reality in quantum mechanics.

X.2.3 Other Possible Nonlinear Parallels with Quantum Mechanics

Other parallels between nonlinear dynamics and quantum mechanics should also be considered. These have been less extensively investigated, so are only listed here as a prod to one's imagination.

• **Attractors and innate quantization.** Nonlinear systems have preferred modes of oscillation, *independent of boundary conditions or external influence*. Many deterministic but nonlinear classical systems obey eigenvalue equations, i.e., they are quantized innately without having to invoke such artifices as wave interference.

• **Spontaneous symmetry breaking — parity nonconservation.** Nonlinear systems can spontaneously break both temporal and spatial symmetry. Odd iterators, for example, exhibit this property. And practical applications include chemical reactions and the separation of powders in nonlinear tumblers [cf. McHarris 2004]. Might this have some bearing on the nonconservation of parity in weak interactions?

• **Decoherence and the destruction of KAM tori.** Decoherence and the reduction of wave functions are among the more intriguing paradoxes associated with the Copenhagen interpretation. The nonlinear alternative would be for an observer to perturb, ever so slightly, a knife-edge equilibrium in a Hamiltonian system, perhaps resulting in its orderly breakdown of KAM tori. This would remove the observer from having to be an integral part of the system. Weinberg [Weinberg 1989] touches on ideas similar to this.

• **Diffraction — the existence of order in chaos.** A possible mode of attack on problems such as the double-slit experiment would be to examine the intricate mixing of windows of order with regions of chaos in many chaotic regimes. Windows of order would correspond to "constructive interference," whereas chaos would correspond to "destructive interference." It is well known that two first-order differential equations can be combined to produce a single second-order equation. Thus, two identical slits could possibly lead to chaotic behavior, but closing one slit (or doing anything else to remove one of the equations) would do away with the possibility of chaos.

• **Barrier penetration.** Again, many nonlinear systems exhibit a type of barrier penetration, e.g., water waves crossing a barrier. Chap. 7 of [Hey & Walters 2003] gives an intriguing overview of this field, which might have deeper implications for quantum mechanics than they realized.

X.3. Conclusion

This paper is intended more to be thought provoking than to proclaim definite conclusions. Nevertheless, I hope to have raised serious questions about our current, orthodox thinking about quantum mechanics. Two of the paradoxes of quantum mechanics have been shown to have reasonably quantitative alternative explanations in nonlinear, possibly chaotic dynamics, while five others simply raise reasonable speculations. Chaos applies to almost every other discipline in nature, so why is quantum mechanics exempt from nature's preferred feedback and nonlinearities? Perhaps, as Mielnik suggested, we have unconsciously been using a scientific linear

“newspeak,” which has prevented us from expressing any nonlinear “thoughtcrimes.” The consequences of nonlinearities and determinism underlying quantum mechanics should shock us, but then it should make us think again — and investigate the situation without wearing (linear) blinders. After all, perhaps Einstein and Bohr were both right — but couldn’t realize it at the time.

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Chapter 29

The use of fractal dimension calculation algorithm to determine the nature of autobiographical memories distribution across the life span

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In the given research we offer the technique for the calculation of the density of events which people retrieve from autobiographical memory. We wanted to prove a non-uniformity nature of memories distribution in the course of time and were interested with the law of distribution of these events during life course.

The hypothesis that “The important events are grouped with more density around the critical events in non-uniform way” was confirmed in the study. For testifying and specification of this hypothesis we chose a formal model, proceeding from which the important events were represented by fractal sets in one-dimensional intervals, centered around the critical events of the personal past.

Fractal dimensions for centered one- and two-sided neighborhood intervals of different radius were calculated.

On the material of the reports of 40 subjects it has been statistically proved, that fractal dimension grows while approaching the center of the neighborhood from the right side faster than the cubic function. The results let us make a conclusion that critical events as a rule are connected in personal consciousness with directly following important events. However there is a question here for the further research: what is a real direction of this correlation.

For a long time it has been supposed that «the forgetting curve» in autobiographical memory has the form similar to classical Ebbinghaus law, i.e. represents monotonously decreasing function: old events should be forgotten gradually, giving a up the place to recent ones. This assumption found substantial evidence in a number of studies.

C.P.Thompson et. al. [1996] built a forgetting curve for real events in individual life, applying for these purposes a diary method. Their results have shown, that on

short intervals (no more than an year) autobiographical memory functions similar to other kinds of long-term memory, but on more extended intervals of time the given forgetting law is not kept.

The research carried out by D.Rubin and M.Conway, unequivocally testify that the function describing subjective existence of our past during the life as a whole has completely different character. The periods of subjective "emptiness" about which we have no clear memories, and the periods of subjective "completeness", which remain in our memory for a long period, replace each other. Reminiscence bump effect that people recollect disproportionate high amount of autobiographical events which happened between 16 and 26 years old was described by D.Rubin with his colleagues in the middle of 80th [Rubin et al. 1986]. The found bump effect appeared to be the steadiest. Recurrence of research in six various cultures (Japan, Bangladesh, UK, China, Spain, US) has led to comparable results [Conway, Hague,1999]. Rubin and colleagues postulated that the obtained curve is a composition of three independent factors: childhood amnesia; recency factor and bump effect, which means that the graph of percent of memories depending on age at time of event looks like general cubic curve with maximum in age between 20 and 30 and minimum about 50 [Rubin, Schulking, 1997].

At present there are several explanations of the bump effect in autobiographical memories' concerning late youth and early maturity. First, the bump effect is interpreted as evolutionary phenomenon. The second approach explains the bump effect from the standpoint of the general laws of memorization – the best conditions for memorization are created in the beginning of the period of stable stimulation. As the youth is characterized by a maximum number of changes at biological, social and personal levels, the following years are remembered in the best way. Some researchers explain "peak" by needs of personal history creation and characterized mentioned age period as the most emotional and novelty. One more approach comprehends the bump effect as a result of assimilation of cultural life scenarios, which mostly fall into the age of 16-30 years. [Conway, Pleydell-Pearce, 2000; Nourkova, Mitina, Yanckenko 2005].

As we see, all above mentioned explanations insist on universal character of the bump effect in autobiographical memoirs. However, in our opinion, there are reasons to believe that behind the universal causes of bump effect there are also individual causes. Proceeding from functional understanding of autobiographical memory, it is possible to assume that preservation of high "density" of memoirs from the period of the past happens in case when a person gets into a situation which can be named conditionally «diachronic disunity» [Lampinen et al., 2003].

The given situations are marked in autobiographical memory as memoirs about critical events [Nourkova, 2000; Nourkova, Mitina, Yanckenko 2005]. Critical event as a special type of unit of the organization of autobiographical memory structure has critical importance and causes reorientation of the subject from the assimilation of the events from an external world to the accommodation to these new events, breaking the continuity of usual existence (from «I change the world» to «the World changes me»). The main difference of critical event from simply important one is that in the second case we interpret the life situation, and in the first – the person himself (herself). While the important events exist in autobiographical memory in the context of life history, critical event determines the history of personal changes. Critical events qualitatively and sharply modify the self-estimation in various fields of activity, the representation of the psychological qualities, the self-image. The

structure of autobiographical memoirs about critical event is based upon substantial comparison of two systems of self-descriptions, occurring at different times, in their relation to the point of discontinuity. The subject should answer the question "What is me?", "Who am I" again and again, being based on the reference to memoirs about the events of cardinal personal changes that happened in this period.

As it comes from general speculation about memory, the period following the critical event is the beginning period of subjective stability. It seems to be reasonable to predict that the period following qualitative shift in personal development will be the most available for both voluntary and involuntary recollections. It means that each person has his/her own unique configuration of recollective "bumps", which reflect the time followings critical experiences.

Therefore, it is possible to assume, that the individual sequence of "bumps" of a saturation of autobiographical memory repeats in itself the configuration of critical events of personal life.

Thus, the primary goal of our empirical research is an attempt to answer the question whether the bump effect has individual character connected with the individual configuration of critical events. The hypothesis to be tested is formulated as follows: The important events are grouped around the critical events in non-uniform way. Critical events are condensed points in this geometric structure.

3. Method

3.1 Participants and procedure

For carrying out the experimental research the «Line of a life» technique based on the reference to the events of the already lived part of the life, revealing a schematic image of the past as a way of personal movement along the axis of time has been used. The subject is offered to draw an arrow, symbolizing life as a vector of time directed from the past in the future, and the particular events of the past.

In the instruction the respondent was offered first of all to draw «a vector of destiny», *«only those events without which your life would not be yours, without which it could not come true»*, and then one more form was given with the request *«to specify the events which changed your personality, made you different»*. Thus among the set of events some are allocated as important (specified in the beginning), and critical (specified in the second stage).

As a rule the number of important events was about 20 and the number of very important, critical ones was no more than 7.

40 examinees took part in the research. Among them were 29 women (mean age was 24.4; in the range of 18-47 years) and 11 men (mean age was 29.7; in an interval of 19-62 years). Education: high school graduates – 3; some college degree – 27; MA (or equivalent) – 10.

3.2 Technique

For testifying and specification of this hypothesis we chose a formal model, proceeding from which the important events were represented by fractal geometrical structures in one-dimensional intervals, centered around the critical events. Testifying and specification of the main hypothesis about non-uniform distribution of important autobiography events, how they are presented in personal memory and what is their thickness around critical events can be made by calculation of Fractal dimensions of different parts of this geometrical structure (Sprott, 1993) (for all subjects) and

further statistical confirmation of difference between empirical indices and theoretical values which could be expected in the case of uniform distribution.

With this goal we offered the following way of calculation. For each subject all his or her course of life was marked by critical events. In the neighborhood of each critical event the system of centered intervals which lengths correspond among themselves as $\frac{1}{2} : \frac{1}{3} : \frac{1}{4}$ was constructed. (See fig.1)

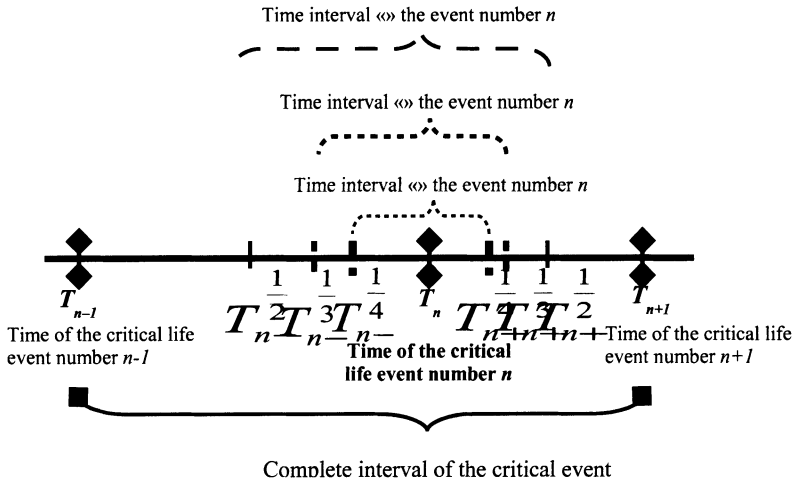


Fig 1. The diagram of the partitioning of the interval of life course around critical event number n

Table of symbols:

$$T_{n-}^{\frac{1}{2}} = T_n - \frac{(T_n - T_{n-1})}{2};$$

$$T_{n-}^{\frac{1}{3}} = T_n - \frac{(T_n - T_{n-1})}{3};$$

$$T_{n-}^{\frac{1}{4}} = T_n - \frac{(T_n - T_{n-1})}{4};$$

Analogically

$$T_{n+}^{\frac{1}{2}} = T_n + \frac{(T_{n+1} - T_n)}{2};$$

$$T_{n+}^{\frac{1}{3}} = T_n + \frac{(T_{n+1} - T_n)}{3};$$

$$T_{n+}^{\frac{1}{4}} = T_n + \frac{(T_{n+1} - T_n)}{4}$$

In the Figure 1 intervals $\left[T_{n-}^{\frac{1}{2}}; T_{n+}^{\frac{1}{2}} \right] \supset \left[T_{n-}^{\frac{1}{3}}; T_{n+}^{\frac{1}{3}} \right] \supset \left[T_{n-}^{\frac{1}{4}}; T_{n+}^{\frac{1}{4}} \right]$ can be

considered as convergent centered system of intervals.

Complete interval for the event T_n is $[T_{n-1}, T_{n+1}]$.

Complete interval for the event T_1 is $[T_0, T_2]$. $T_0=0$ (the moment of personal birth).

If the subject during experiment session mentioned N critical events, then complete interval for the event T_N is $[T_{N-1}, T_{N+1}]$. T_{N+1} – actual subject's age.

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It should be noticed that distances (measured in years) between different critical events are not equal, so the limits of centered intervals are not symmetrical around the center – the corresponding critical event.

Let designate the number of important event which happened during the time period

(time interval) $\left[T_{n-}^{\frac{1}{2}}; T_{n+}^{\frac{1}{2}}\right]$ as S_n^v , the number of important event which

happened during the time interval $\left[T_{n-}^{\frac{1}{3}}; T_{n+}^{\frac{1}{3}}\right]$ as S_n^3 , and the number of

important event which happened during the time interval $\left[T_{n-}^{\frac{1}{4}}; T_{n+}^{\frac{1}{4}}\right]$ as S_n^4 . If

important events happened uniformly during the life course not depending upon (approaching/moving away from the points of) critical events, then the number of events which belong to each centered interval and happened there were in the same ratio as the intervals' lengths.

$$\frac{S_n^4}{S_n^v} = \frac{1}{3} = 0.33, \quad \frac{S_n^3}{S_n^v} = \frac{2}{3} = 0.667, \quad \frac{S_n^4}{S_n^3} = \frac{3}{4} = 0.75 \quad (*)$$

If we accept the hypothesis that the frequency of important events is higher near critical event, the ratio between the numbers of events from each time interval should be different.

If we admit that the density of important events increases linearly during approaching to the critical event (that means that while approaching to a critical event people more often memorize important events which happened in their life during that time), then the ratio will be the following:

$$\frac{S_n^4}{S_n^2} = \frac{7}{12} = 0.583, \quad \frac{S_n^3}{S_n^2} = \frac{20}{27} = 0.741, \quad \frac{S_n^4}{S_n^3} = \frac{63}{80} = 0.788 \quad (S_n^k = 2 \int_{1-\frac{1}{k}}^1 Cx dx) \quad (**)$$

If we admit theoretically that the density of important events increases in concordance with the quadratic law while approaching to critical event, then the ratio will transform:

$$\frac{S_n^4}{S_n^2} = 0.661, \quad \frac{S_n^3}{S_n^2} = 0.804, \quad \frac{S_n^4}{S_n^3} = 0.822 \quad (S_n^k = 2 \int_{1-\frac{1}{k}}^1 Cx^2 dx) \quad (***)$$

For cubic model it will be:

$$\frac{S_n^4}{S_n^2} = 0.729, \quad \frac{S_n^3}{S_n^2} = 0.856, \quad \frac{S_n^4}{S_n^3} = 0.851 \quad (S_n^k = 2 \int_{1-\frac{1}{k}}^1 Cx^3 dx) \quad (****)$$

Thus in any model different from uniform (which we will call basic) the ratios between indices $\frac{S_n^k}{S_n^1}$ are always higher than corresponding basic ratios.

So to test our hypothesis that subjective representation of important events in personal memory is not uniform and has points of thickness in the neighborhood of a critical event we should test the fact that the set of indices computed for all subjects and their corresponding means are higher than the basic ones.

So for each subject i we compute the sets of empirical indices

$$\left\{ \frac{S_n^4}{S_n^2} \right\}_i, \left\{ \frac{S_n^r}{S_n^v} \right\}_i, \left\{ \frac{S_n^i}{S_n^v} \right\}_i \quad \text{for all } N_i \text{ critical events during life course of this}$$

subject, that's mean that n belongs to the range from 1 to N_i and then we get average values

$$\frac{S^{i4}}{S^{i2}} = \frac{\sum_{n=1}^{N_i} \frac{S_n^4}{S_n^2}}{N_i}, \quad \frac{S^{ir}}{S^{iv}} = \frac{\sum_{n=1}^{N_i} \frac{S_n^r}{S_n^v}}{N_i}, \quad \frac{S^{i4}}{S^{i3}} = \frac{\sum_{n=1}^{N_i} \frac{S_n^4}{S_n^3}}{N_i}$$

And then we compute means for data sets $\left\{ \frac{S^{i4}}{S^{iv}} \right\}$, $\left\{ \frac{S^{ir}}{S^{iv}} \right\}$, $\left\{ \frac{S^{i4}}{S^{ir}} \right\}$ and using

statistical T-test test the hypothesis that empirical means are significantly higher than the predicted theoretical means of the uniform model (*).

Besides, we were interested to investigate not only for two-side intervals, when the critical events were situated in the centers of the analyzed intervals, but also for so called right- and left- one-side intervals. In the case of left-side intervals we compared the frequencies of important events which had happened only before the corresponding critical event and in the case of right-side intervals we compared the frequencies of important events which happened only after. The procedure of indices computation was the same as for tow-side intervals, but from the logical point of view the interpretation of results should be changed. In the case of two-side intervals the proof of non-uniformity can testify just the correlation of facts: a person regards an event as critical and high-density important events in the same time period are connected with each other. In the right-side case the increasing density of important events near the critical one, but after it, testifies that after the critical event happened (in some way we can say that the personality has changed) all around it is considered more sharply, from the new standpoint. The person memorizes more events and regards events which follow the critical one as important.

Here we should remember the statement mentioned above that the beginning of stability is memorized best of all.

In the left-side case we can assume that the increase in the frequency of important events in the life course happens not accidentally and a person him or herself (consciously or unconsciously) builds this sequence, and realizing or not realizing prepares for a critical event which should happen according common life scenarios.

Let designate corresponding indices as $L \frac{S_n^4}{S_n^2}$, $L \frac{S_n^r}{S_n^v}$, $L \frac{S_n^4}{S_n^3}$ for left-side case and as $R \frac{S_n^4}{S_n^2}$, $R \frac{S_n^3}{S_n^2}$, $R \frac{S_n^4}{S_n^3}$ for right-side case. The Table 1 presents results of analysis of empirical data using the suggested method.

As shown in the table in all three cases – two-side, left- and right- one-side intervals - the hypothesis about the uniform and linear distribution of the frequencies of important events happening in the course of life can be rejected with the probability to make error less than 0.0005. Testing the hypothesis about the quadratically increasing frequency of important events while approaching to a critical event the probability to make error having rejected H_0 hypothesis for two-side intervals increases a little, but no more than 0.05. So rejection H_0 still is possible for all intervals' types.

Testing the hypothesis about cubically increasing frequency it is possible to say that for two-side intervals H_0 hypothesis is confirmed, for left-side intervals the increasing numbers of important events as approaching to a critical event is a little higher and for right-side intervals the statement that the decreasing frequency of important events is going more faster than the cubic function is possible with the probability of error less than 0.0005.

In general it should be noted that the above mentioned trends demonstrate more contrast in case of right-side intervals, that's why we can make conclusion that critical events as a rule are connected in personal consciousness with directly following important events. However there is a question here for the further research: what is a real direction of this connection. Is each critical event the reason for the whole sequence of the important events, or for an explanation of the whole cascade of the important events, so that the person tries to find in his or her life some «trigger», consciously or unconsciously, in a retrospective way and then call it the critical event.

Table 1. Results of the statistical analysis for the ratios of frequencies of important events

	Means	St.Dev	Test for rejection H_0 -hypothesis about			
			uniform distribution	linear distribution	quadratic distribution	cubic distribution
			Testable	Testable	Testable	Testable
			value= 0.5	value=0.583	value=0.661	value= 0.792
Two-side S_n^4	.7454	.16245	9.553***	6.308***	3.296**	.631
intervals $\frac{S_n}{S_n^2}$	.8883	.12121	20.262***	15.914***	11.877***	8.305***
Right-side S_n^2	.7804	.17728	10.002***	7.029***	4.268***	1.826*
intervals						
Left-side						
intervals			Testable	Testable	Testable	Testable
			value=0.667	value= 0.741	value= 0.804	value=0.856

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Two-side	S_n^3	.8475	.14224	8.039***	4.747***	1.924*	-.376
intervals	$\frac{n}{n}$	.9177	.10925	14.528***	10.242***	6.566***	3.571***
Right-side	S_n^2	.8680	.12741	9.995***	6.319***	3.167**	.599
intervals							
Left-side							
intervals							
				Testable	Testable	Testable	Testable
				value=0.75	value= 0.786	value= 0.822	value= 0.852
Two-side	S_n^4	.8822	.13144	6.360***	4.556***	2.917**	1.459
intervals	$\frac{n}{n}$	.9564	.08558	15.253***	12.482***	9.966***	7.725***
Right-side	S_n^3	.9022	.12666	7.599***	5.727***	4.027***	2.513**
intervals							
Left-side							
intervals							

Level of significance of rejection H_0 hypothesis by T-test *** – $p < 0.0005$,

** – $p < 0.01$, * – $p < 0.05$

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Chapter 30

An formally exact solution for a time-dependent quantum system

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1. Introduction

Since the beginning of quantum mechanics, different methods have been developed to solve the Schrödinger equation; however there are a few systems whose solution is exact. These exactly solvable systems are used to construct an approximated solution for the non-exactly solvable systems. For example, a lot of systems whose solution is not exact, are commonly solved through the use of the harmonic oscillator in the modeling of the system. Whatever, in general when the Hamiltonian is an explicit function of time, the solution is frequently either an analytical approximated solution or a numerical solution.

The use of invariants theory to solve quantum systems, whose Hamiltonian is an explicit function of time, has the advantage to offer an exact solution for problems solved by the traditional time-dependent perturbation theory [Landau 1975]. There is a class of exact invariants for time-dependent harmonic oscillators, both classical and quantum, that has been reported in [Lewis 1968].

The invariants method is very simple due to the relationship between the eigenstates of the invariant operator and the solutions to the Schrödinger equation by means of the phases; in this case the problem is reduced to find the explicit form of the invariant operator and the phases.

In this work, we try to show how the invariants theory method works to solve a time-dependent oscillator. In the second section we present what an invariant operator means and what is the condition to be filled by its eigenstates and the solutions to the time-dependent Schrödinger equation. In the third section we show how to get the invariant operator by means of an adequate canonical transformation. In the fourth section we apply the proposed method to get an exact solution for a time-dependent quantum oscillator.

2. Time-dependent Invariants operators

Suppose the existence of a Hermitian, explicitly time-dependent, non trivial and invariant operator $\hat{I}(t)$; that means, $\hat{I}(t)$ satisfies

$$\hat{I}(t) = \hat{I}^\dagger(t) \quad (2.1)$$

$$\frac{d\hat{I}}{dt} \equiv \frac{\partial \hat{I}}{\partial t} + \frac{i}{\hbar} [\hat{H}, \hat{I}] = 0 \quad (2.2)$$

where the Hamiltonian operator $\hat{H}(t)$ is an explicit function of time and satisfies the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} | \rangle = \hat{H} | \rangle \quad (2.3)$$

It is easy to see that the action of the invariant operator in a Schrödinger state vector produces another solution of the Schrödinger equation, that is

$$i\hbar \frac{\partial}{\partial t} (\hat{I} | \rangle) = \hat{H} (\hat{I} | \rangle)$$

which is a valid result for any invariant operator.

We can choose some invariant operators, which are some of a complete set of observables, in order to assure the existence of a complete set of eigenstates of $\hat{I}(t)$, in this case

$$\hat{I} |\lambda, \kappa; t\rangle = \lambda |\lambda, \kappa; t\rangle \quad (2.4)$$

and

$$\langle \lambda', \kappa'; t | \lambda, \kappa; t \rangle = \delta_{\lambda, \lambda'} \delta_{\kappa, \kappa'} \quad (2.5)$$

The eigenvalues λ are real because $\hat{I}(t)$ is an hermitic operator and it is easy to show that λ are time-independent so the eigenstates are time-dependent.

Lewis [Lewis 1969] has showed there exists a simple and explicit rule for choosing the phases of the eigenstates of $\hat{I}(t)$ such that these states satisfy themselves the Schrödinger equation with the only requirement the invariant does not involve time differentiation. The new eigenstates $|\lambda, \kappa; t\rangle_\alpha$ of $\hat{I}(t)$ are

$$|\lambda, \kappa; t\rangle_\alpha = e^{i\alpha_{\lambda, \kappa}(t)} |\lambda, \kappa; t\rangle \quad (2.6)$$

and the phases $\alpha_{\lambda, \kappa}(t)$ must satisfy the first-order differential equation

$$\hbar \frac{d\alpha_{\lambda, \kappa}}{dt} = \langle \lambda, \kappa; t | \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) | \lambda, \kappa; t \rangle \quad (2.7)$$

In this way, every new eigenstate $|\lambda, \kappa; t\rangle_\alpha$ of $\hat{I}(t)$ satisfies the Schrödinger equation, and we can write the general solution to Schrödinger equation as

$$|t\rangle = \sum_{\lambda, \kappa} C_{\lambda, \kappa} e^{i\alpha_{\lambda, \kappa}(t)} |\lambda, \kappa; t\rangle \quad (2.8)$$

where $C_{\lambda, \kappa}$ are time-independent coefficients.

3. Invariant operator obtained by means of a Canonical Transformation

Suppose a system whose associated Hamiltonian operator is $\hat{H}(p, q; t)$ and for which there exists an invariant operator $\hat{I}(p, q; t)$ defined as in the previous section. Now consider the following transformation

$$\begin{aligned}\hat{q} &\rightarrow \hat{Q} \\ \hat{p} &\rightarrow \hat{P}\end{aligned}$$

defined by means of

$$\begin{aligned}\hat{p} &= \frac{\hat{P}}{a} + b\hat{Q} \\ \hat{q} &= a\hat{Q}\end{aligned}\tag{3.1}$$

and inverse

$$\begin{aligned}\hat{Q} &= \frac{\hat{q}}{a} \\ \hat{P} &= a\hat{p} + b\hat{q}\end{aligned}\tag{3.2}$$

where the parameters $a = a(t)$ and $b = b(t)$ are time-dependent. The new operators $\hat{Q}$ and $\hat{P}$ satisfy the canonical commutation relation $[\hat{Q}, \hat{P}] = [\hat{p}, \hat{q}] = i\hbar$, i.e. the above transformation is a canonical transformation.

Under this transformation the invariant operator is

$$\hat{I}(\hat{p}, \hat{q}; t) = \hat{I}\left(\frac{\hat{P}}{a} + b\hat{Q}, a\hat{Q}; t\right) = \hat{J}(\hat{P}, \hat{Q}; t)$$

and the Hamiltonian

$$\hat{H}(\hat{p}, \hat{q}; t) = \hat{H}\left(\frac{\hat{P}}{a} + b\hat{Q}, a\hat{Q}; t\right)$$

In this case, we must write the condition (2.2) for the new invariant operator as

$$\frac{\partial}{\partial t} \hat{J}(\hat{P}, \hat{Q}; t) + \frac{i}{\hbar} \left[\hat{H}\left(\frac{\hat{P}}{a} + b\hat{Q}, a\hat{Q}; t\right) - \frac{\dot{a}}{2a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) - \frac{1}{2} (\dot{a}b - \dot{b}a) \hat{Q}^2, \hat{J}(\hat{P}, \hat{Q}; t) \right] = 0 \tag{3.3}$$

where the point over the parameters means time derivation. Then, to have an invariant operator for the Hamiltonian depending on the new variables, we need to solve equation (3.3). Even if the new operator $\hat{J}$ had not shown dependence on time, the old invariant $\hat{I}$ would be still dependent on time because the transformation includes

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the parameters a and b that do; in such case the partial derivative will vanish and the equation to solve would be

$$\left[\hat{H} \left(\frac{\hat{P}}{a} + b\hat{Q}, a\hat{Q}; t \right) - \frac{\dot{a}}{2a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) - \frac{1}{2} (\dot{a}b - \dot{b}a) \hat{Q}^2, \hat{J}(\hat{P}, \hat{Q}) \right] = 0 \quad (3.4)$$

A particular solution for this equation is

$$\hat{J}(\hat{P}, \hat{Q}) = \lambda(t) \left\{ \hat{H} \left(\frac{\hat{P}}{a} + b\hat{Q}, a\hat{Q}; t \right) - \frac{\dot{a}}{2a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) - \frac{1}{2} (\dot{a}b - \dot{b}a) \hat{Q}^2 \right\} \quad (3.5)$$

where $\lambda(t)$ is chosen in such a way that $\hat{J} = \hat{J}(\hat{P}, \hat{Q})$, and that depends on the explicit form of Hamiltonian.

IV. Application to the Time-dependent Forced Oscillator.

To take advantage of the previous sections, we will consider a time-dependent forced oscillator, in which case the Hamiltonian is

$$\hat{H}(\hat{p}, \hat{q}; t) = \frac{1}{2} \left[e^{-F(t)} \hat{p}^2 + e^{F(t)} \omega^2(t) \hat{q}^2 \right] \quad (4.1)$$

with

$$F(t) = \int_{t_0}^t f(t') dt'$$

any time-dependent function. The Schrödinger equation to solve is

$$i\hbar \frac{\partial}{\partial t} |t\rangle = \frac{1}{2} \left[e^{-F(t)} \hat{p}^2 + e^{F(t)} \omega^2(t) \hat{q}^2 \right] |t\rangle \quad (4.2)$$

Following the previous ideas, the problem is reduced to find an invariant operator and the suitable phases of its eigenfunctions to take them as the solution for the Schrödinger equation.

Considering the canonical transformation (3.1) our Hamiltonian is transformed into

$$\hat{H} \left(\frac{\hat{P}}{a} + b\hat{Q}, a\hat{Q}; t \right) = \frac{1}{2} \left[e^{-F(t)} \left(\frac{\hat{P}}{a} + b\hat{Q} \right)^2 + e^{F(t)} \omega^2(t) a^2 \hat{Q}^2 \right]$$

and, in accordance with (3.4) the invariant operator is obtained if we solve the equation

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$$\left[\frac{1}{2} \left[e^{-F} \left(\frac{\hat{P}}{a} + b\hat{Q} \right)^2 + e^F \omega^2 a^2 \hat{Q}^2 \right] - \frac{\dot{a}}{2a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) - \frac{1}{2} (\dot{a}b - \dot{b}a) \hat{Q}^2, \hat{J} \right] = 0$$

or

$$\left[\frac{1}{2} \left[e^{-F} \left(\frac{\hat{P}^2}{a^2} + b^2 \hat{Q}^2 + \frac{b}{a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) \right) + e^F \omega^2 a^2 \hat{Q}^2 \right] - \frac{\dot{a}}{2a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) - \frac{1}{2} (\dot{a}b - \dot{b}a) \hat{Q}^2, \hat{J} \right] = 0$$

whose solution is

$$\hat{J} = \lambda(t) \left\{ \frac{1}{2} \left[e^{-F} \left(\frac{\hat{P}^2}{a^2} + b^2 \hat{Q}^2 + \frac{b}{a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) \right) + e^F \omega^2 a^2 \hat{Q}^2 \right] - \frac{\dot{a}}{2a} (\hat{P}\hat{Q} + \hat{Q}\hat{P}) - \frac{1}{2} (\dot{a}b - \dot{b}a) \hat{Q}^2 \right\}$$

Now we choose $\lambda(t) = a^2 e^{F(t)}$ and the invariant becomes

$$\hat{J} = \frac{1}{2} \left\{ \hat{P}^2 + \left[a^2 b^2 + e^{2F} \omega^2 a^4 - a^2 e^F (\dot{a}b - \dot{b}a) \right] \hat{Q}^2 + (ab - \dot{a}a e^F) (\hat{P}\hat{Q} + \hat{Q}\hat{P}) \right\}$$

Since we want $\hat{J}$ had not shown dependence on time, we should take

$$a^2 b^2 + e^{2F} \omega^2 a^4 - a^2 e^F (\dot{a}b - \dot{b}a) = k_0 \quad (4.3)$$

and

$$ab - \dot{a}a e^F = k_1 \quad (4.4)$$

where k_0 and k_1 are constants. In this case our invariant is

$$\hat{J} = \frac{1}{2} \left\{ \hat{P}^2 + k_0 \hat{Q}^2 + k_1 (\hat{P}\hat{Q} + \hat{Q}\hat{P}) \right\}$$

Doing the inverse transformation from the invariant $\hat{J}$ to the invariant $\hat{I}$, considering the equations (2.10), (4.3) and (4.4), and after some algebra we have

$$\hat{I}(\hat{p}, \hat{q}; t) = \frac{1}{2} \left\{ (a\hat{p} - \dot{a}e^{F(t)}\hat{q})^2 + k^2 \frac{\hat{q}^2}{a^2} \right\} \quad (4.5)$$

where we have recalled $k_0 - k_1^2 = k^2$. Now, inserting (4.4) into (4.3) we can find the auxiliary equation for this invariant

$$\ddot{a} + \dot{F}\dot{a} + \omega^2 a = \frac{k^2}{a^3} e^{-2F} \quad (4.6)$$

The operator (4.5) is an invariant for the Hamiltonian (4.1) under the condition a satisfying (4.6). Now the task is to find the eigenstates for the invariant operator and to solve the equation (2.7) in order to obtain the appropriate phases for the general

solution. This is very easy if we consider the new transformation for the variables in (4.5)

$$\begin{aligned}\hat{Q}' &= \frac{\hat{q}}{a} \\ \hat{P}' &= a\hat{p} + \dot{a}e^{F(t)}\hat{q}\end{aligned}$$

Notice that the new variables satisfy the canonical commutation relation $[\hat{Q}', \hat{P}'] = i\hbar$, so the invariant can be written as

$$\hat{J}' = \frac{1}{2} \left\{ \hat{P}'^2 + k^2 \hat{Q}'^2 \right\} \quad (4.7)$$

which have the Hamiltonian form for a harmonic oscillator whose solutions are well known [DeLange 1991, Borowitz 1967]. Factorizing (4.7) by means of

$$\hat{J}' = \frac{\hbar\kappa}{2} (\hat{A}\hat{A}^\dagger - 1) \quad \text{or} \quad \hat{J}' = \frac{\hbar\kappa}{2} (\hat{A}^\dagger\hat{A} + 1)$$

where the operators

$$\hat{A} = \frac{1}{\sqrt{\hbar k}} (\hat{P}' - ik\hat{Q}') \quad \text{and} \quad \hat{A}^\dagger = \frac{1}{\sqrt{\hbar k}} (\hat{P}' + ik\hat{Q}')$$

are the annihilation and creation operators, respectively, for the states of the invariant operator, we can rewrite the Hamiltonian as

$$\begin{aligned}\hat{H} &= \frac{1}{2} \left\{ \frac{\hbar k e^F}{4a^2} (\hat{A}^2 + \hat{A}^{\dagger 2} + \hat{A}\hat{A}^\dagger + \hat{A}^\dagger\hat{A}) + \frac{\hbar e^F}{4k} (\dot{a} + \omega^2 a^2) (\hat{A}^\dagger\hat{A} + \hat{A}\hat{A}^\dagger - \hat{A}^2 - \hat{A}^{\dagger 2}) \right. \\ &\quad \left. + \frac{i\hbar\dot{a}}{2a} (\hat{A}^2 - \hat{A}^{\dagger 2}) \right\}\end{aligned}$$

Then, taking into account the properties of the annihilation and creation operators, and denoting with $|n\rangle$ the eigenstates of $\hat{J}'$, we are able to get the phases beginning with the right side of (2.7)

$$\langle n | \left(i \frac{\partial}{\partial t} - \frac{1}{\hbar} \hat{H} \right) | n \rangle = \left[\frac{e^F}{4k} (a\ddot{a} + a\dot{a}\dot{F} + a^2\omega^2) + \frac{e^{-F}k}{4a^2} \right] (2n+1)$$

Using the auxiliary equation (4.6) for the invariant, we have

$$\langle n | \left(i \frac{\partial}{\partial t} - \frac{1}{\hbar} \hat{H} \right) | n \rangle = -\frac{e^{-F} k}{2a^2} (2n+1)$$

substituting it in equation (2.7) for the phases

$$\frac{d\alpha_n}{dt} = -\frac{e^{-F} k}{2a^2} (2n+1)$$

where we can immediately get the solution for the phases

$$\alpha_n = -\frac{k}{2} (2n+1) \int \frac{e^{-F}}{a^2} dt$$

As mentioned in the second section, the general solution of the Schrödinger equation for our oscillator is

$$|t\rangle = \sum_n C_n e^{i\alpha_n(t)} |n\rangle$$

which is, formally, an exact solution.

V. Conclusion

Using the invariant operators method to solve a time-dependent quantum oscillator, we have observed the advantages it offers to found a formally exact analytical solution without solving the complicated equations that appear when another methods are used. It has been demonstrated that canonical transformations help obtaining the invariant operator and its auxiliary equation, depending on the specific problem. In general, the invariant operators has a great advantage over the other methods since we can obtain the Schrödinger equation's solution for systems whose Hamiltonian has a dependence on time, and this solution is formally exact.

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Chapter 31

Human-technology Integration

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Human-technology integration is the replacement of human parts and extension of human capabilities with engineered devices and substrates. Its result is hybrid biological-artificial systems. We discuss here four categories of products furthering human-technology integration: wearable computers, pervasive computing environments, engineered tissues and organs, and prosthetics, and introduce examples of currently realized systems in each category. We then note that realization of a completely artificial system via the path of human-technology integration presents the prospect of empirical confirmation of an aware artificially embodied system.

1.1 Introduction

At least since Turing [1], the *intelligence* of machines has been benchmarked in terms of performance compared to a human's on some set of tasks. One way to realize an artificial system intelligent in this sense is to build a system *de novo* to approximate some aspect of human behavior. In this paper we discuss an alternative means toward engineered systems with human-like performance: *human-technology integration*. The human-technology integration approach begins with existing humans and proceeds by augmenting or replacing “natural” parts with engineered devices and substrates, to result in hybrid biological-artificial systems.

Human-technology integration proceeds via the development of engineered systems that allow the extension of human senses and capacity to act into the environment. Such systems include (wearable) computing devices and pervasive

computing environments, as well as products that substitute or modify aspects of human's existing organic structure, e.g., prosthetics and engineered tissues and organs. Such means will be discussed in brief.

Continued progress in human-technology integration will conceivably allow the creation of entirely artificial systems by its means. The possible observational consequences of replacement of each and every human part with an artificial substitute are the subject of the last section of this paper. We formulate a *replacement experiment* in which a human observer transfers their embodiment completely to engineered devices or substrates, and present two possible outcomes of such an experiment. Interestingly, the replacement experiment presents an empirical means to confirm the possibility of an aware artificial system.

1.2 Wearable computers

Advances in computer technology have brought the human user closer to computational power, where *closer* means having the ability to access computational power in a less conditional sense. The advent of the personal computer and portable computers removed barriers separating the user from access to computer power, and the wearable computer, or wearable, works to further diminish barriers that remain.

Wearables package computing power in a form that goes wherever the user does, embedded in clothing or carried on the head or body. Wearable developer Steve Mann prompts

Let's imagine a new approach to computing in which the apparatus is always ready for use because it is worn like clothing. The computer screen, which also serves as a viewfinder, is visible at all times and performs multimodal computing (text and images). [2]

Wearables effectively allow the user to extend their ability to compute into their environment regardless of their primary task, allowing access to computational power in settings in which the use of a traditional portable computer is cumbersome or impossible. For example, wearables may assist soldiers in combat situations in which the use of traditional portable computing devices is not feasible. The 'Objective Force Warrior' (OFW) project of the United States Army currently explores the "synergistic result" of combining soldiers with wearables. The "overall warrior system" in development includes a helmet with 180 degree integrated display with voice control command software, video/data links to networked sensors, multi-spectral vision, thermal management and temperature control, biometric sensors, hemorrhage control, virtual reality/3D visualization software, tactics, techniques and procedures (TTP) recall, and integrated mission rehearsal capability [3].

The *always ready* mode of wearables allows their users to assimilate information processing tasks more seamlessly into their activities. For example, the Mobile Assistant wearable computer from Xybernaut Corp. has been used by

the service personnel of the telecommunications carrier Bell Canada International Inc. since 2000 to speed data processing tasks in the field, allowing an estimated time savings of 50 minutes per day per worker. The pilot version of the Mobile Assistant used by Bell was a head-mounted display (HMD), which was soon replaced with flat-panel 8-in. display that allows pen input on the screen or with an electronic keyboard attached to a processor embedded in a vest, belt or knapsack [4]. Because such devices ease human-computer interaction in such a way as to allow businesses to operate more efficiently, their use is rapidly spreading.

1.3 Pervasive computing environments

Pervasive computing environments seek to provide a seamless continuum between the computing environment and the physical environment, and may be compared to a nervous system for the environment being sensed [5]. Human-technology integration is facilitated by allowing human users an unprecedented opportunity to collect information from (sense) and act on their environments.

Sensors and sensor networks are a component of pervasive computing environments that allow their users an extended ability to monitor their surroundings. A common and relatively mature such technology is the closed-circuit television (CCTV) camera, which is used by individuals and institutions worldwide to extend a “watchful eye” into the environment. The British government, for instance, has installed 1.5 million CCTV cameras in public and semi-public places. Cameras currently line nearly every road and public square in the country, manned by human operators that decide whom to survey in detail and for how long, allowing for increasingly ubiquitous presence of governmental agents.

Another pervasive computing technology in wide use to increase user’s capacity to survey the physical environment are radio frequency identification (RFID) sensors, which turn the objects they are affixed to into network nodes that up-link IDs and data to databases. The tags are dormant until activated by a RFID reader, which stimulates the RDID to broadcast information. They are currently used by businesses (e.g. Procter and Gamble, Gillette and Wal-mart) to manage inventory, several U.S. state governments to track cars in order to levy tolls (via the EZPass system), and a wide range of institutions to track the activity of employees via tags embedded in ID badges. Applications for personal use are in development.

1.4 Engineered tissues and organs

Engineered tissues and artificial organs act to restore function to human patients in the case of tissue or organ damage due to injury, age or disease. Unlike the technologies of human-technology integration discussed thus far, engineered

tissues and organs may actually replace (as opposed to merely augment) existing human parts.

A strong impetus for the development of artificial organs exists because of the donor shortage—in excess of 70,000 individuals in the U.S. alone wait for organ transplantation each year, but fewer than 11,000 donors (cadaveric and living) are available [6]. Some of this donor shortage is currently remedied via use of artificial organs. The artificial heart is the oldest example of a functional artificial organ. In 1957 Willem Kolff and his associates successfully implanted the first artificial heart in an animal. In 1969 Denton A. Cooley, founder and became the first heart surgeon to implant an artificial heart in a human patient. The first fully self-contained artificial heart was successfully implanted in 2001. The device, manufactured by the AbioCor Corporation, is currently in U.S. Food and Drug Administration (FDA)-approved clinical trials. Other artificial organs, such as livers and kidneys, have also been in long development, and are meeting increasing success in clinical applications.

Artificial tissues differ from artificial organs in that they are typically comprised of biologically-derived materials. Tissue engineering itself is defined as the application of principles and methods of engineering and life sciences toward the development of biological substitutes to restore, maintain or improve tissue function [7]. The engineered tissue most common use today is skin. Creation of replacement skin typically involves *in vitro* seeding and attachment of human cells to a biodegradable polymer or collagen scaffold, which is then bathed with growth factors, causing proliferation, migration and differentiation of the seed cells. Upon implantation, the scaffold is gradually reabsorbed into the body. Skin created in this way is presently used as a replacement for the damaged skin of burn victims and the sufferers of diabetic ulcers, among others. Research in progress in the creation of other artificial tissues, including blood vessels, connective tissues, and blood itself promises to help meet the health needs of many more.

1.5 Prosthetics

A prosthetic is generally defined to be a corrective consisting of a replacement for a part of the body. In general, prosthetics can “restore lost mobility to individuals if (i) they can express cognitive control over relevant motor functions somewhere in their residual anatomy and (ii) a device can pick up and decipher that cognition [8].”

Myoelectric limbs, for instance, operate by sensing electric signals generated by the muscles of the remnant limb. Sensors embedded in tight-fitting rubber prosthetics pressed against the remnant limb pick up electric electromyographic (EMG) signals, which are then amplified and sent to microprocessors that operate motors in the joints of the artificial limb. The devices help amputees worldwide toward functional replacement of their upper-limbs.

Even patients with complete paralysis, or locked-in syndrome, may use prosthetics to direct activity. In locked-in patients, the series of electrical impulses

that pass from brain cells along nerves to trigger the release of chemical messages that result in movement of the muscles is blocked, leaving the brain fully conscious but unable to control the body. Brain computer interfaces (BCIs) allow such patients to direct external devices such as computer mice or robotic arms by voluntarily and reliably changing in their electroencephalographic (EEG) activity. Since 1997 BCIs have been implanted in locked-in patients who learn to use their brain waves to “will” a cursor to move and then stop on a specific point on a computer screen. The screen is typically made to contain a list of options or characters from which the patient may choose in order to construct messages. The technology has been extended to allow control of robotic limbs [9, 10].

Since the successful development of proof-of-concept devices, interest in the development of BCIs has grown. In the U.S., The National Institutes of Health awarded \$3.3 million in late 2002 to a partnership headed by the Wadsworth group to help match BCI software to patients, and DARPA awarded a Duke University research team \$26 million in 2003 to improve its implanted BCI technique. A DARPA spokesperson reports that the agency is interested applications such as enabling “soldiers to push buttons with their brains, giving them speedier control of submarines and aircraft and enabling them to more adeptly manipulate robotic arms that move munitions [11].”

Artificial eyes, or visual prosthesis, are another promising prosthetic device that seek to provide functional visual perception to a individuals blinded by disease or trauma. The devices are based on neuronal electrical stimulation at different locations along the visual pathway (i.e., cortical, optic nerve, epiretinal, subretinal) [12]. Several researchers have reported successful restoration of some part of lost vision via implantation of artificial retinas, e.g., [13, 14]. The ongoing Artificial Retina Project will standardize and extend the current state-of-the-art in artificial stimulation of the retinal nerves with three rounds of clinical trials of progressively more sophisticated devices. Five U.S. national laboratories, three universities, and the private sector are collaborating on the project, which will receive \$9 million in funding from the U.S. Department of Energy’s Office of Science over three years [15].

1.6 The future of human-technology integration

The categories of technologies described in previous sections, among others, allow for the creation of hybrid biological-artificial intelligent systems. These hybrid systems offer their human components either i) an extension of the capability to collect, interpret and act on environment information, or ii) the maintenance of “normal” or healthy functionality of damaged, diseased or aging parts. Since there is considerable demand for both i) and ii), there exists a strong impetus to further the means of human-technology integration.

As this impetus enables humans to replace or extend more and more of their components with artificial devices and substrates, it will become possible for the resulting intelligent biological-artificial systems to become increasingly artificial. At some future point it is conceivable that a human will be able to replace *all*

“natural” parts with engineered components, to result in a completely artificial system with human-like performance on some set of tasks.

Whereas there is general consensus that human parts and even the human whole may be replaced in principle by a *functionally* isomorphic artificial system, there remains debate regarding whether artificial systems can be made to be aware (i.e., conscious, feeling, with qualia, etc.). This debate is philosophic since observable qualities by which to distinguish matter that merely *acts* as though it has awareness from matter that actually *has* awareness are not known to exist. On the debate regarding whether it is possible for an artificial (i.e., non-biological) system to be aware, Marvin Minsky comments

Many thinkers firmly maintain that machines will never have thoughts like ours, because no matter how we build them, they'll always lack some vital ingredient. They call this essence by various names—like sentience, consciousness, spirit, or soul. Philosophers write entire books to prove that, because of this deficiency, machines can never feel or understand the sorts of things that people do. [16]

From the intrinsic privacy of experience, it seems that detectable properties to ascertain the awareness of other systems (i.e., other humans, animals, robots) will remain elusive. However, human-technology integration nevertheless presents a path toward observational confirmation of the possibility of an aware artificially embodied system. Given the means to replace each and every natural human part with an engineered device or substrate the following *replacement experiment* may be made:

The experimenter begins replacing their parts with engineered substitutes, continuing until they are completely comprised of engineered parts, realizing one of two possibilities:

- 1) Ability to observe remains as before. In this case the experimenter obtains empirical evidence of the possibility of an aware artificial system.
- 2) No ability to observe remains. In this case the original observer has been destroyed.

The above described experiment offers a means to end the debate regarding the possibility of aware artificial systems simply in that a human observer who is able to transfer their embodiment to artificial devices and substrates cannot argue against the possibility of aware artificial systems. Currently, skeptics of the possibility of aware artificial systems may argue that when one carries out the replacement experiment sufficiently far, the following scenario necessarily results

You find, to your total amazement, that you are indeed losing control of your external behavior. You find, for example, that when doctors test your vision, you hear them say “We are holding up a red object in front of you; please tell us what you see.” You want to cry out “I can’t see anything. I’m going totally blind.” But you hear your voice saying in a way that is completely out of your control, “I see a red object in front of me” . . . Your conscious experience slowly shrinks to nothing, while your externally observable behavior remains the same. [17]

Performing the replacement experiment will offer the skeptic a means of testing their prediction that 2) necessarily results. The following scenario, or some variant of it, would put to rest the skeptic's reservations regarding the possibility of aware artificial systems

You've just been wheeled into the operating room. A robot brain surgeon is in attendance, a computer waits nearby. Your skull, but not your brain, is anesthetized. You are fully conscious. The robot surgeon opens your brain case and places a hand on the brain's surface. This unusual hand bristles with microscopic machinery, and a cable connects it to the computer at your side. Instruments in the hand scan the first few millimeters of brain surface. These measurements, and a comprehensive understanding of human neural architecture, allow the surgeon to write a program that models the behavior of the uppermost layer of the scanned brain tissue... The process is repeated for the next layer, and soon a second simulation resides in the computer, communicating with the first and with the remaining brain tissue. Layer after layer the brain is simulated, then excavated. Eventually your skull is empty, and the surgeon's hand rests deep in your brainstem. Though you have not lost consciousness, or even your train of thought, your mind has been removed from the brain and transferred to a machine. [18]

Via realization of such a scenario, human-technology integration offers the only known experimental means of ending the debate regarding the possibility of aware artificial systems.

1.7 Conclusions

The human-technology integration approach toward artificial systems with human-like performance has been introduced and discussed in terms of example products by which it currently proceeds. Future progress in human-technology integration will allow biological systems to become increasingly, and even entirely, artificial. By transfer of embodiment to a completely engineered substrate, skeptics will have the possibility of testing their convictions regarding the impossibility of aware artificial systems.

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Chapter 32

Crafting a Social Context for Medical Informatics Networks

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Abstract

Effective healthcare delivery is increasingly predicated upon the availability, accuracy, and integrity of personal health information. Tracking and analysis of medical information throughout its lifecycle may be viewed through the lenses of both physical network architecture and the broader social context in which such information is gathered and applied. As information technology and evidence-based practice models evolve in tandem, the development of interlinked multimodal and multidimensional databases has shown great promise for improving public health. To this end, providers, regulators, payers, and individual

patients each share rights and responsibilities in creating a milieu which both fosters and protects the practice and promise of medical information.

1. Introduction

Medicine has transitioned over the past century from a healing art, characterized by artisinal apprenticeship and empirical knowledgesets, to an increasingly algorithmic, scientific endeavor, buttressed by measures of individual and population health parameters, clinically-validated and peer-reviewed treatments, and consistent, longitudinal, evidence-based assessment. The latest era of developments in this realm have been enabled to a large degree through compounding rates of information collection, manipulation, and distribution.

In practice settings ranging from primary care clinics to tertiary-level academic hospitals, and in development settings including device and drug research, databases are growing in scope, size, and interoperative capabilities. A transparent, comprehensive system for storage and manipulation of medical histories, imaging data, cytologic, and genetic profiles, and treatment outcomes is universal objective of healthcare providers, payers, and entrepreneurs, and researchers. Such integration must not proceed, however, devoid of the broader contextual framework of economics, ethics, and civil rights. The study of complex systems and social dynamics offer important clues to help direct this process.

2. Economic Impact

Networked information systems represent significant contributors to, and modulators of, the economic environment of health provision. Much of the economic benefit of databases emerges from cost savings in the provider space, and from identifying novel targets in the research and development space. Maximum effort should be focused not only upon the provision of services, but upon how to maximally exploit the linkages between these datasets. The magnitude and scope of this charge will necessitate the training of librarians and data custodians to assist in data mining methods. Emergent behaviors of groups of individuals in health pools, including specific consumption patterns and demographic trends, may be particularly valuable. Additionally, treatment cost trends over

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loco-regional, disease-centered, and culturally-based strata will be targets of keen interest to healthcare financing organizations.

Inconsistencies and errors in administration may be reduced through standardized in billing and data transfer practices. Such savings have already been demonstrated in the New England Healthcare Electronic Data Interchange Network due to reduced administrative overhead, forecasted to lead to annual savings greater than 65 million dollars [1].

Furthermore, complex health data systems hold the promise of reducing costs associated with medico-legal liability. Post-hoc analysis of medical errors often begins with an inquiry into provider activity, and blame is usually assigned at an individual practitioner level. This is not always a useful approach, particularly when a case is handled by multiple teams interacting at various points in the treatment process. While the majority of malpractice lawsuits allege wrongdoing of willful neglect of selected parties, it is likely that a significant number of poor patient outcomes are the result of a breakdown in the system of diagnosis, treatment, and follow-up. The aviation transport, package shipping, and automobile design industries have successfully implemented parallel quality assessment protocols over the prior two decades.

Witness the enactment of an 80 hour work-week limitations for residents in accredited training programs at U.S. hospitals, a response to claims that fatigued residents are more likely to commit errors. One consequence of these regulations is that the care of a patient may be passed among several separate care teams within an initial span of 24-48 hours; the demands of multiple transfers of recent patient information may lead to altered content, granularity, and quality of these findings. By examining each node in the web of healthcare delivery, potential sources of systematic and random error may be identified and reduced, overall decreasing the cost of effective care.

Telecommunication-enabled services, initially involving remote diagnosis and supervision, and later in the fields of remote surgical intervention, may facilitate cost savings by increasing access and decreasing utilization of conventional inpatient care [2]. Paradoxically, the aggregate demand for costly services such as radiologic imaging, angiography, and other procedural exams, aided by this ease of information interchange, may actually increase costs in the short term, as care providers reach new equilibria in balancing payer cost, health outcomes, personal liability, and diagnostic accuracy.

3. Advancing Public Health

In the domain of ensuring population health, an electronic system of healthcare providers offers a novel and potentially powerful tool for indentifying emergent trends in acute and chronic healthcare settings, helping identify patterns of both endemic and epidemic pathology. For instance, IBM [3] and SAS [4] research groups have proposed a methodology of Unstructured Data Mining that may be particularly well-suited to the task of sifting through arrays of disparate patient datasets. Implementation of methods in biostatistics and predictive analytics will all be necessary in order to fully exploit a large and accessible database of health measures and outcomes. The challenges of integrating large datasets into the American public health infrastructure are daunting, however. The variable granularity and format of information fields is a limiting characteristic of current electronic medical systems, making cross-datatype and cross-database comparisons difficult. Further downstream, large networks of interlinked providers will enable the agile creation and modification of best-practice guidelines over abbreviated timescales. At the Johns Hopkins School of Medicine, an email broadcast system was created in response to the anthrax attacks of 2001; after 12 months, an estimated 18,000 subscribers received regular updates from the service.

4. Public, Institutional, and Personal Rights

The struggle between the public interest and individual autonomy is rooted in a body of prior case-law. The US Supreme Court, in *Jacobson v. Massachusetts* (1905), ruled that mandatory vaccination is justified to protect public welfare, notes that “the Constitution of the United States...does not import an absolute right in each person to be, at all times and in all circumstances, wholly freed from restraint. There are manifold restraints to which every person is necessarily subject for the common good.” Despite this overarching principle, multiple questions of ownership, fair and appropriate use, and intellectual property loom large as the consolidation of data networks transforms the healthcare landscape. For instance, in the majority of US local jurisdictions, the record creator, not the patient, has primacy over the use of database, and only in selected instances do individual privacy rights trump authorship rights [5]. When databases span states and even countries, whose laws reign supreme? Can individual data records be de-identified and yet remain complete and transparent? To what extent may a

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governmental agency exercise powers of “*eminent domain*” over health data?

Additionally pressing is the conundrum of the rights of corporate entities conflicting with those of individuals in the marketplace of ideas, goods, and services. These issues are becoming increasingly relevant with the rise of “*computational medicine*,” which correlates drug reactions and efficacy with specific patient populations. In cancer treatment, personalized drug selection based upon histologic exam of patient pathologic tissue and genetic markers is already in clinical trials.

Another vexing question, yet to be fully answered: is personal health data a discoverable item under legal proceedings? That is, can plaintiffs in lawsuits obtain access to defendant party data? Finally, how may individuals audit and ensure the accuracy of their records? This is a pressing problem due to the lack of current regulation explicitly prohibiting “*genetic discrimination*” by insurance companies.

These issues, clearly beyond the scope of the federal Health Insurance Portability and Accountability Act of 1996 (HIPAA), will soon demand legislative attention and the establishment of common standards for privacy.

It may be helpful to approach public debate and legislation using the precautionary principle of the David Kreibel. This model proposes that preventative action is indicated in uncertain times, that the proponents of an activity bear the burden of proof, that alternative actions must be explored, and that public participation is key in the decision-making process [6].

5. Information Security

For collections of individual records assembled in databases, which themselves are linked in various ways, the topology of the network formed at each level attains particular importance. Yook, et al. have modeled the structure of Internet connections, and proposed that such a network may be classified as “*scale-free*” [7] such that a relatively small number of central nodes are responsible for a disproportionate level of the connectivity within the system [8]. The implications of identifying such a structure are important for several reasons: first, they offer an insight into the underlying communications load that various elements of the system must bear. Second, the central nodes are those which generally subserve critical functions (*i.e.*, house data which is of particular utility). The random failure of such a node may be a rare event, but a coordinated attack upon several nodes may be catastrophic for the system [9].

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A given health-care network, much like the Internet, is a system with connectivity directed by human parsing, that relies heavily upon centralized data-centers for specific information such as patient identification numbers, allergies, and prior history. This implies that, to ensure robustness of a health care network, the most important nodes should be identified and the majority of available resources should be directed towards protecting these centers against failure.

The potential for theft and abuse by legitimate providers will only rise as perceived value of personal medical records increases. Through rigorous auditing processes [10], and security hardening against software and hardware exploits, both the private and public sector may be able to cooperate in developing a secure and reliable data services infrastructure for medical practice, education, and research.

In summary, the potential for dramatic shifts in public health and the public welfare secondary to medical data accumulation and analysis is indeed promising, but only in the context active and continuous engagement by government entities, health-care providers, industry leaders, scientists, and the citizenry at large.

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Chapter 33

Modeling Safety Outcomes on Patient Care Units

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1.1 Introduction

In its groundbreaking report, “To Err is Human,” the Institute of Medicine reported that as many as 98,000 hospitalized patients die each year due to medical errors (IOM, 2001). Although not all errors are attributable to nurses, nursing staff (registered nurses, licensed practical nurses, and technicians) comprise 54% of the caregivers. Therefore, it is not surprising, that AHRQ commissioned the Institute of Medicine to do a follow-up study on nursing, particularly focusing on the context in which care is provided. The intent was to identify characteristics of the workplace, such as staff per patient ratios, hours on duty, education, and other environmental characteristics. That report,

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“Keeping Patients Safe: Transforming the Work Environment of Nurses” was published this spring (IOM, 2004).

In the last five years, AHRQ also funded a number of research studies directed at patient safety issues. The Impact Study described in this paper is one of those efforts. In the Impact Study, we chose to focus on studying workplace characteristics (organization and patient care unit) that can affect patient safety and quality outcomes. To do so, we collected data from 37 patient care units in 12 Arizona hospitals. Hospitals that participated in the research included teaching and non-teaching hospitals, as well as public and privately funded hospitals ranging in size from 60 to over 400 beds. To ensure a more comparable analysis across units, only adult medical or surgical units were included in the sample. Data were collected in two “waves;” patient care units from half the hospitals were assigned to each wave. Each wave of data collection required six months to complete. Data related to each of the model components were collected through surveys of patients, staff, managers, quality improvement (QI) departments, and information services (IS). In all, 1179 patients and 867 staff were surveyed.

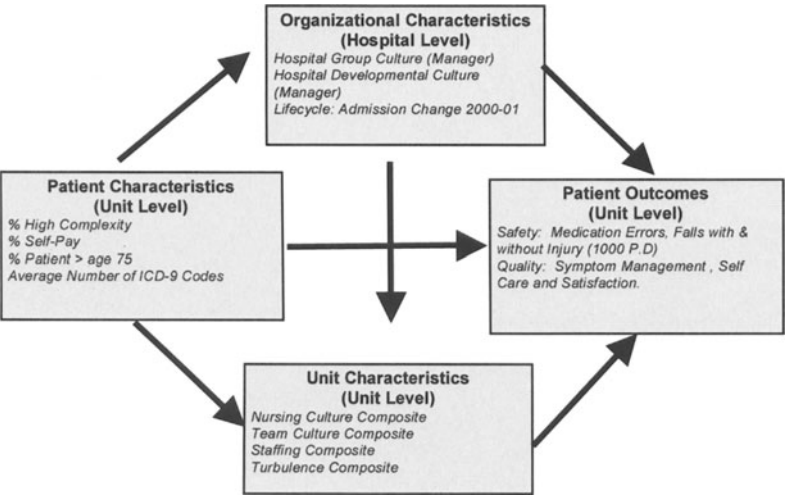


Figure 1. The Conceptual Model Used to Guide the Impact Study showing only the variables used for computational modeling

The framework for the research was based on the 1996 American Academy of Nursing Health Outcomes Model (Fig. 1) (Mitchell, Ferketich & Jennings, 1998). Patient safety outcomes studied included medication errors and patient falls, with and without injury. Quality outcomes investigated included symptom management, simple and complex self care, and perception of being well cared

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for. In this paper, we will focus only on the safety outcomes. The data were subjected to descriptive analysis, as well as causal modeling prior to their being used to develop the computational model. Our emphasis was on identifying changes that nurse managers could make at the patient unit level, because organizational changes are not under their control. Similarly, nurse managers cannot change the characteristics of the patients they see on their units; instead patient characteristics were treated as risk adjusters in the analysis.

1.2 Using OrgAhead to Create Virtual Patient Care Units

1.2.1 Orgahead

We used *OrgAhead*, a computational modeling program, to create virtual units that functionally matched our actual units and then evaluated the patient safety outcomes for the virtual units under various conditions. *OrgAhead* is a theoretically based computational modeling program developed by Dr. Kathleen Carley and her team at Carnegie Mellon University. The theoretical perspectives grounding *OrgAhead* derive from social network, complexity, and organizational theories (Carley & Hill, 2001) and are consistent with the theoretical basis of the conceptual model used for the Impact Study. *OrgAhead* had been used in a number of military and business settings, but this provided its first application in healthcare.

1.2.2 The modeling process

The computational modeling process (Fig. 2) included four distinct steps: First, variables in our research model were matched to the variables in *OrgAhead*. Variables that were found to be significant in our model that were not initially in *OrgAhead* were created for *OrgAhead* in collaboration with Dr. Carley and her team at Carnegie Mellon University. Next, we determined the range for each independent variable in *OrgAhead*. In the third step, values were set for all other variables used in *OrgAhead*. Finally, experiments were run to validate the virtual model with actual data and then to generate hypotheses about the kinds of changes that might be made to improve patient outcomes (Effken et al., 2003, Effken et al., in preparation) using a static version of the model.

One of the strengths of computational modeling is its ability move beyond static, snap-shot analyses to examine organizational performance over time. To explore how patient safety outcomes might change under various changes in structure and unit characteristics, we utilized the annealing characteristics of the model. In Orgahead, individual learning occurs through a standard stochastic learning model for boundedly rational agents (Carley, 1996). Organizational adaptation or learning occurs as a simulated annealing process. The annealing model was developed originally to solve complex combinatorial optimization

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problems (Kirkpatrick, 1983; Rutenbar,1989). Simulated annealing is a heuristic for optimization and a computational analog of the physical process of annealing (heating and cooling) a solid, in which the goal of the process is to find the atomic configuration that minimizes energy costs. In organizations, this is analogous to a design problem in which the organization is trying to optimize organizational performance under various constraints (Carley, 1997). For our purposes, we assume that the patient care unit endeavors to optimize performance (e.g., achieving desired quality and patient safety outcomes) while reducing or maintaining costs.

Organizational adaptation, for our modeling purposes, has two components: executive decisions about particular restructuring goals and strategies and individual employees' experiential learning (Carley, 1996). Executive decisions are commonly assumed to be "satisficing," rather than optimizing. That is, the manager doesn't consider all possible strategies are compared; instead the first one that seems likely to move the organization toward the goal is selected (March, 1958; Simon, 1954). Similarly, nurse managers do not consider every possible intervention, but select the first one that seems likely to work, given their current constraints.

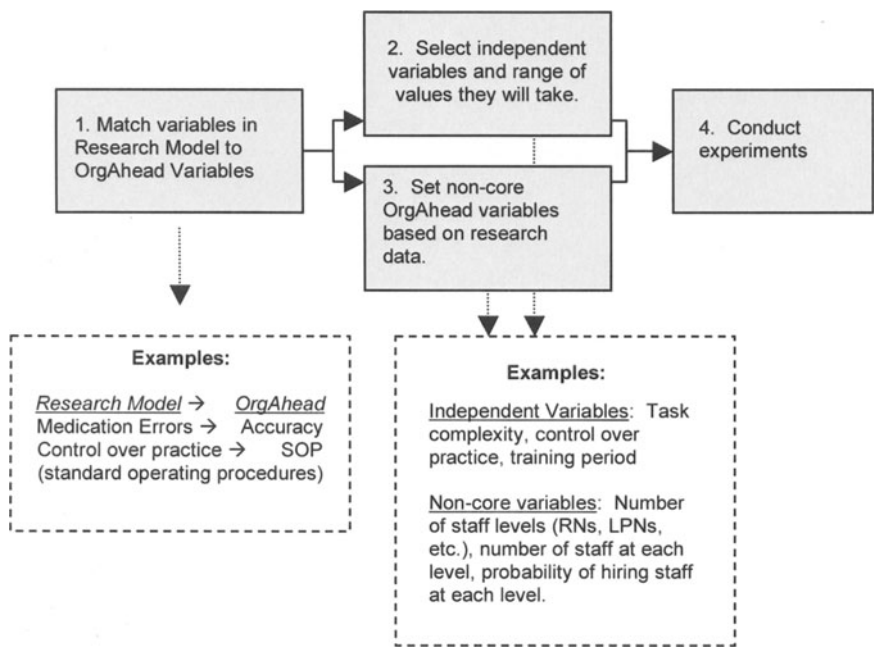


Figure 2. The Computational Modeling Process

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1.2.3 Modeling the patient care unit

The patient care unit is modeled as two interlocking networks: an authority structure (who reports to whom?) and a resource management structure (who has access to which resources?). We assume a 3-layered structure with RNs at the top level, LPNs and patient care technicians (PCTs) at the second level, and unit clerks at the bottom level. Individuals may have one or more subordinates and report to one or more managers. This allows us to model teams, hierarchies, matrix structures, etc.

Both the organization and individual employees operate in a “task” environment where a “task” equals a patient. In Orgahead, patients are modeled as 9-bit binary choice tasks. For each “patient,” which is modeled as a 9-bit series of a’s and b’s, the organization (patient care unit, in our research) has to determine whether there are more a’s or b’s in the string. Different levels of staff see different numbers of bits. RNs see 4 bits, LPNs and PCTs see 2 and Unit Clerks see 3. No individual can make a patient unit decision alone (assuming bounded rationality and distributed decision making); instead the unit decision is created as a majority vote of the individual decisions. For more details, see Carley, 1998.

1.3 Results and Discussion

For the static experiments with the 32 virtual units, the correlation coefficient (r) of the rank order for accuracy (virtual units) and total errors (actual units) was found to be 0.83. This exceeded our target of acceptable level of correspondence of 0.80 (Effken et al, 2003). The correlation co-efficient for the actual values for accuracy and total errors was found to be -0.55, which is acceptable at the value level.

The results of our static experiments to improve performance by varying the initial values of various independent variables (task complexity, workload, turbulence, standard operating procedures (SOP), training and memory) are summarized in Table 1 for 6 pilot units. These 6 pilot units are different in their key characteristics, as well as in their safety outcomes. Improvement in accuracy was obtained by varying the independent variables in the static experiments is given. A 5% improvement in accuracy in the virtual world corresponds to a decrease in 5 errors in the real world. Managers could potentially select a number of strategies to decrease task complexity or increase training, for example, to achieve this level of improvement in their real units.

Dynamic simulations involved setting up annealing parameters and allowing the virtual units to adapt over time. Figure 3 shows a snapshot of how the 6 pilot units adapt over time by changing the authority and resource management structures resulting in the performance varying over time.

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Unit	A	B	C	D	E	F
Task Complexity	15 (17)	12 (14)	8 (11)	9 (12)	8 (9)	11 (13)
Training	834 (234)	1000 (365)	903 (303)	943 (343)	404 (404)	903 (403)
Memory	500 (100)	1000 (100)	900 (100)	800 (100)	100 (100)	800 (100)
SOP						
(a) RN	0.4 (0.0)	0.3 (0.28)	0.1 (0.30)	0.3 (0.33)	0.1 (0.24)	0.3 (0.51)
(b) LPN/PCT	0.8 (0.6)	0.6 (0.33)	0.5 (0.29)	0.8 (0.23)	0.5 (0.35)	0.6 (0.71)
(c) Unit Clerk	0.9 (0.62)	0.99 (0.46)	0.9 (0.39)	0.9 (0.42)	0.9 (0.18)	0.8 (0.67)
% Accuracy	80.16 (77.72)	83.78 (82.22)	86.07 (78.16)	85.16 (76.55)	86.39 (79.98)	78.19 (74.95)
%Improvement	2.44	1.56	7.91	8.61	6.41	3.24

Table 1. Percentage Improvement in Accuracy (based on static modeling) achieved for 6 Pilot Units modeled. The numbers shown in parentheses are the values for the corresponding actual unit; all other numbers are those values used in *OrgAhead*.

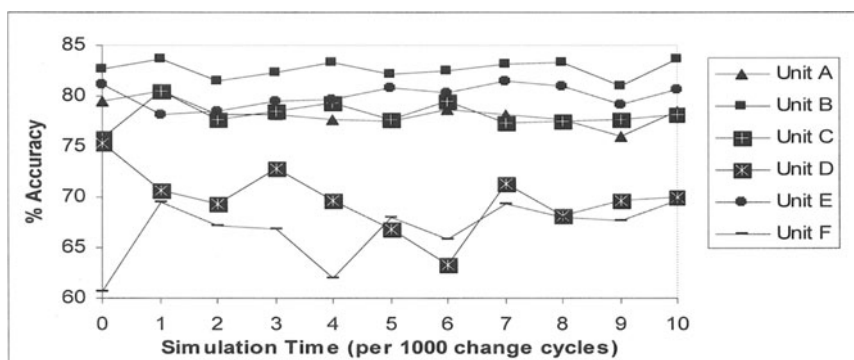


Figure 3. Accuracy (safety outcomes) by Time for 6 pilot units

The average accuracy over time for the dynamic run for each unit was consistent with the total errors reported on the actual units. For example, Figure 3 shows that Units C and D initially had similar levels of accuracy, but over time

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performed differently, reflecting their actual performance values. The actual Unit C produced 4.73 errors, but its corresponding virtual unit showed better performance (avg. accuracy = 79.99%) as compared to Unit D, for which the actual unit reported total errors of 26.18, and the virtual unit showed an average accuracy of 70.04%.

After validating that the dynamic average accuracy values for the 6 modeled units reflected their actual outcomes, we selected some of the best and the worst accuracy values during the adaptation process and studied the respective authority and resource management matrices to see how they influenced the outcomes. This gave us some insight into the structures that lead to both successful and unsuccessful performance. Of these values, we picked only those structures that are most likely to occur in the real scenario. The result of one such successful structure for Unit E along with its initial structure is as shown in Figure 4.

Interestingly, the better performing structures were flatter. This generally resulted in eliminating the unit clerk position, which is probably not realistic because of their pivotal roles on the unit. This may represent a limitation of the modeling, which assumes that all members of the team are working on the same problem. In fact, the unit clerk has a rather different role. These results suggest that, in the future, we may need to omit the clerks from the models and perhaps include the nurse manager instead. Further modeling will be needed to inform that decision.

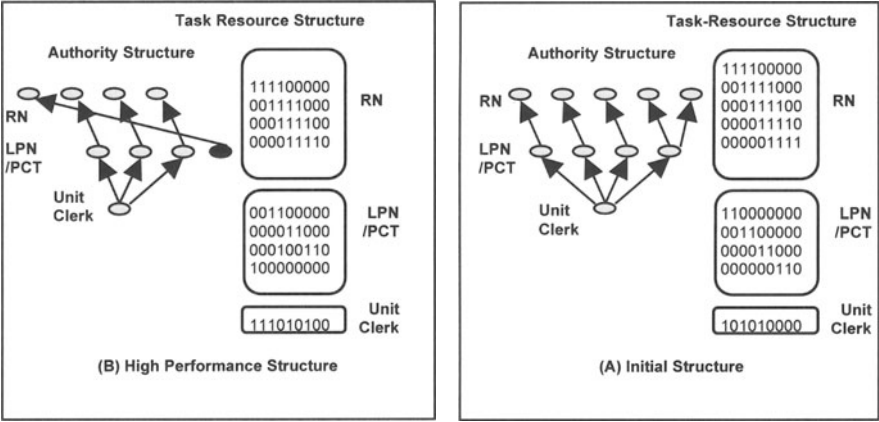


Figure 4. The initial and high performance structures for Unit E.

1.4 Conclusion

Using OrgAhead, we created 32 virtual patient care units that were functionally similar to the actual units in their key characteristics and safety outcomes with

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the outcomes (accuracy with total errors) having an acceptable level of correspondence. Using these virtual units, for the static model we varied the various independent variables for 6 pilot units, and studied how each would improve the safety outcomes. We then used OrgAhead dynamically, and verified that the average dynamic accuracy is consistent with the safety outcomes. Using the dynamic runs, we were able to pick the authority and resource management structures that produced the best and worst safety outcomes. Our computational model could be a very effective tool for nurse managers to visualize various structures and strategies that they could use to improve patient safety outcomes on their units, before extending them to the real world.

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Chapter 34

Defining Emergent Descriptions by Information Preservation

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We propose a formalized approach for the characterization of the phenomenon of *emergence*, based on information-theoretic criteria. The proposed mechanism of description fits in well with existing approaches for the characterization of complex systems and also has ramifications towards existing algebraic models for coordinatizations of complex systems.

1.1 Introduction

Among the most fascinating phenomena in the field of complex systems and Artificial Life is the phenomenon of *emergence*. Informally, one speaks of emergence if some phenomenon occurs in a complex system that is not “obviously” deducible from the microdynamics of the system. Here, we must emphasize, the crucial notion is the word “obviously”. Generally, given a specific scenario, human observers will, on an intuitive level, usually agree whether emergence is present or absent in that system. It would be desirable to achieve a more objectifiable access to these phenomena and to move away from the implicit and subjective identification of emergence by human observers to a mathematically

accessible and operationally relevant characterization. However, the intuitive “emergence detection” capability of humans seems to be grounded in a “gestalt”-like perception of the phenomena in question, and the phenomenon itself turns out to offer a surprising degree of resistance to formalization.

Consequently, not a unique, formal and operational notion of emergence has “emerged”. Some approaches characterize emergence informally as “surprising” effects [19] which gain their existence only in “the eye of the beholder” [12], thus making the human observer mentioned above an indispensable ingredient in the characterization of the phenomenon.

On the other end of the spectrum, one finds highly formalized approaches, using the powerful language of category theory. Among these are [16], and, in particular, the approach developed in [18]. One of the problems remaining with definitions based on meta-models like category theory is that, while precise, in practice they are often computationally inaccessible and they make it difficult to allow for a “natural” concept of emergence to arise from the intrinsic structure of a system.

What one would like to have is a formalized concept of emergence which would be able to capture essential aspects of the “gestalt”-like detection of emergence phenomena by humans, which would be operational and thus computationally relevant and useable and which, ideally, would be forged out of the dynamics of the given system without having to resort to additional assumptions not present in the original system under consideration.

In the present paper, we propose to characterize emergence via the formal concept of *emergent description* as a decomposition of a stochastic dynamic system into approximately independent subsystems which, individually, preserve information (in sense of Shannon’s information theory) as much as possible. The following chapters will develop the rationale for this approach, introduce the formalism and give a discussion.

1.2 Motivation and Related Work

1.2.1 An Instructive Example: Collective Modes in Crystal Lattices

One of the motivations of our approach is the natural decomposition of the collective dynamics in crystal lattices into individual oscillatory modes, *phonons* [5]. This phenomenon is particularly instructive because it demonstrates, on the one hand, how “holistic”, “gestalt”-like phenomena can arise (“emerge”) in a well-understood way as collective modes from the natural dynamics of a dynamical system. Furthermore, if symmetries are present, they even pre-induce an a priori dynamics decomposition structure in a universal fashion via a generalized Fourier decomposition [3, 20]. This shows how additional aspects of structure can be seamlessly worked into a definition of a canonical partition into subsystems. This case is, however, limited by the fact that it requires the systems to be linear.

1.2.2 Dynamics Decomposition in Nonlinear Systems

The field of synergetics develops an approach to decompose also nonlinear systems in a natural fashion [10]. Here, the natural decomposition of dynamical systems near fixed points into stable, central and unstable manifolds is reinterpreted in a heuristic way, separating *fast foliations* and *slow manifolds* in the system [14]. Slow degrees of freedom (*master modes*) of the system dynamics are said to “enslave” the fast degrees of freedom (*slave modes*), because they essentially dominate the dynamics of the system. The *master modes* can be construed as “emerging” from the system dynamics. This decomposition into individual subsystems arises naturally from the system dynamics and is therefore not due to a subjective observer as in [12]. The synergetics decomposition typically requires the systems to exhibit a splitting into different time scales. However, it turns out that under certain conditions it is even possible to decompose nonlinear (even chaotic) dynamical systems canonically into weakly coupled subsystems if they have no separate time scales [23].

It is well-known that dynamical systems can be well described using information theory using the Chaitin-Kolmogorov Entropy (e.g. [8]) measuring the information flow from microstates towards macrostates. Here, the dynamics of the system is translated into the information-theoretical language via an a priori choice of the space partition. However, it would be desirable to have an approach where the decomposition “emerges” naturally from the structure of the dynamical system and is not imposed upon it¹.

Information-theoretic principles have been used for the characterization of complex systems [7, 24, 4]. In [1, 2], a notion of complexity is introduced as the *persistent* information captured in an individuals’ genome during an evolution process. This shows significant parallels to the synergetics view that persistence of certain aspects of a system description over time can be important; however, it is felt that the information-theoretic formulation of synergetics has not exploited the persistence paradigm to its full potential [11].

In the crystal-lattice example or the synergetics model, the “persistence” idea is incarnated as the decomposition of the system into modes. Defining such a decomposition of the system dynamics for a general nonlinear system is non-trivial. Heuristic approaches can be used for this purpose, stemming either from nonlinear dynamics analysis [17], or clustering methods [25]. The constructive creation of a stable subdynamics (as opposed to a decomposition of an existing system) has been addressed in the context of the “homeokinesis” [9].

1.3 Emergent Descriptions

These developments formed the motivation for our present approach to introduce a formal characterization of emergence. It is based on information theory, is fully formal and operational in the sense that it can – in principle – be calculated

¹In this context, studying the relation between the notion developed in Sec. 1.3.2 and the concept of generating partitions from nonlinear dynamics would be of particular interest.

for any given stochastic dynamical system. The present section introduces the concept. In Sec. 1.4 we will indicate how the stringency of our approach can be relaxed to become relevant for the study of practically relevant cases.

1.3.1 Concept Overview

We will define emergent descriptions as a *complete* decomposition of the system into *independent* subsystems which are *individually predictable*.

1.3.2 Strong Emergent Descriptions: Formal Definition

From above considerations, we see that several aspects have to be incorporated to attain a notion of emergence: an aspect of temporal persistence, a notion of partition of the system states into roughly independent subsystem states (this partition may be “holistic” in the sense that the states of each subsystem needs to encompass a state description of all constituents of the total system and thus may be “oblique” with respect of possible system constituents). Also, the notion should be capable to deal naturally with inherently nonlinear systems.

The approach we use is to mimic information-theoretically the decomposition of linear dynamical systems into independent subsystems, *eigenmodes*, whose individual dynamics, while induced by the global dynamics, can be considered separately and independently of each other. We interpret these subsystems as “emerging” from the global system dynamics.

First, we introduce some notation. Given a random variable X (uppercase), the set of its possible values will be denoted by (calligraphic) $\mathcal{X}$ and a concrete value for X by (lowercase) $x \in \mathcal{X}$. Write $P(X = x)$ for the probability that X assumes a value x or, if no confusion is possible, $p(x)$ by abuse of notation. Similarly, write $p(y|x)$ for the conditional probability $P(Y = y \mid X = x)$ when no confusion is expected.

We introduce probabilistic maps as a generalization of deterministic maps. Let event sets $\mathcal{X}, \mathcal{Y}$, and a conditional probability $p_M(y|x)$ be given. The probabilistic map M from the event set $\mathcal{X}$ to an event set $\mathcal{Y}$ maps any random variable $X \in \mathcal{X}$ to a random variable $M(X) \in \mathcal{Y}$, such that $P(MX = y \mid X = x) = p_M(y|x)$ and, conditioned on X , the variable $M(X)$ is independent of any other random variables in the model, i.e. $M(X)$ has a Markovian dependence on X .

For two random variables X and Y , let $H(X) = -\sum_{x \in \mathcal{X}} p(x) \log p(x)$ denote the entropy of X and $I(X; Y) = H(X) + H(Y) - H(X, Y)$ denote the mutual information between X and Y . For details of the properties of these notions, see e.g. [6]. We proceed now to define strong emergent descriptions.

Definition 1.3.1 (Strong Emergent Description) *Let $\mathcal{S}$ be a (for sake of technical simplicity) finite set of states. Further let on $\mathcal{S}$ a stochastic dynamics be recursively defined via a transition probability $p(s(t+1)|s(t)) \equiv P(S(t+1) = s(t+1) \mid S(t) = s(t))$ (t may be limited to a finite range $\{0 \dots T\}$) and an initial probability distribution $p(s(0))$, thus defining a Markovian process with initial conditions. $\mathcal{S}$ together with the dynamics defined by the Markov process forms*

a stochastic dynamic system which can be characterized by a (possibly finite) sequence $S(0), \dots, S(t), \dots$ of random variables with values in $\mathcal{S}$.

A strong emergent description is then defined as a sequence of probabilistic maps (projections) $Q_t : \mathcal{S} \rightarrow \hat{\mathcal{S}}^{(0)} \times \hat{\mathcal{S}}^{(1)} \times \dots \times \hat{\mathcal{S}}^{(k)}$, inducing subsystems such that for all $t \in \{0 \dots T\}$

1. the totality of $Q_t = \hat{Q}_t^{(1)} \times \dots \times \hat{Q}_t^{(k)}$ is information conserving with respect to the total state, i.e.

$$H(S(t)) = I(S(t); Q_t(S(t))) ; \quad (1.1)$$

2. the dynamics of the individual subsystems are independent from each other:

$$\forall i \neq j : I(\hat{Q}_t^{(i)}(S(t)); \hat{Q}_t^{(j)}(S(t))) = 0 ; \quad (1.2)$$

3. and with exception of subsystem 0, the subsystem dynamics is information conserving:

$$\forall i \in \{1 \dots k\} : H(\hat{Q}_{t+1}^{(i)}(S(t+1))) = I(Q_t^{(i)}(S(t)); \hat{Q}_{t+1}^{(i)}(S(t+1))) \quad (1.3)$$

(note that $\hat{Q}_t^{(i)}(S(t))$ is the subsystem state description). Here, subsystem $\hat{\mathcal{S}}^{(0)}$ is the perfectly random subsystem, i.e. $I(\hat{Q}_t^{(0)}(S(t)); \hat{Q}_{t+1}^{(0)}(S(t+1))) = 0$. Subsystem 0 takes into account the nonpredictable part of the dynamics.

A subsystem is called trivial, if for all t :

$$H(\hat{Q}_t^{(i)}(S(t))) = 0 . \quad (1.4)$$

Note that in a strong emergent description, the random subsystem may be trivial. Apart from it, without loss of generality, one can exclude emergent descriptions with trivial subdynamics. Note also that Criterium (1.2) can be strengthened requiring the subsystems to be independent with respect to multi-information, i.e. $\sum_i H(\hat{Q}_t^{(i)}(S(t))) - H(Q_t(S(t))) = 0$

1.4 Discussion and Future Work

The strong emergent description is a notion that provides a criterium to decide whether a collection of (projection) maps decomposes a stochastic dynamical system into independent subdynamics. For systems continuous in both state S and time t , it is possible to give a definition that is similar in spirit to that from Sec. 1.3.2, but technically more involved.

As example for the notion, consider the dynamics of the crystal lattice from Sec. 1.2.1. It is a deterministic dynamical system and thus a special case of a stochastic dynamical system, allowing to apply the notion from Sec. 1.3.2. Its decomposition into independent eigenmodes (for any initial state distribution) is a strong emergent description for that system, since the complete set

of eigenmodes covers the whole space, the individual modes are independent of each other and each of them individually fully predicts the future states of its subsystem.

The present concept is related, but goes significantly beyond Independent Component Analysis and deterministic annealing by introducing additional structure in form of a temporal dimension. Due to the subdynamics of the individual projection spaces, they can be interpreted as closed subsystems.

The strong emergent description is a criterium that can be applied to a very general class of systems, going beyond systems that can be studied with linear (as in the crystal lattice) or nonlinear localized analysis (as is done e.g. in synergetics). Although in this paper the space is too limited to discuss the entire spectrum of ramifications of the concept, it should be mentioned that it captures many central aspects and phenomena commonly associated with emergent phenomena. Apart from addressing the issues from Sec. 1.2, the concept of the strong emergent description opens the path towards “soft” probabilistic generalization of algebraic coordinatization models [15] which provide powerful possibilities to decompose systems in a natural fashion; it also opens new perspectives in the study of the emergence of structured information processing in agents from first principles [22, 13].

At this point, neither necessary nor sufficient conditions for the existence or uniqueness of nontrivial strong emergent descriptions in a given system are known. There are indications that, if existing, minimal descriptions might be unique under certain circumstances, but in general, this will not be the case and may not even be desirable: different strong emergent descriptions may lead to alternative valid “views” of a system.

On the practical side, it is possible to construct approximations to strong emergent descriptions, namely *weak emergent descriptions*, by optimizing (maximizing or minimizing, respectively) the terms from the three conditions in Sec. 1.3.2 using either Lagrange multipliers (similar to the multivariate bottleneck models, which also might be modified to provide possible algorithms to compute such a decomposition [21]) or multiobjective optimization. The results of such an optimization may or may not be proper strong emergent descriptions. In systems with a certain amount of mixing, one will not expect to achieve anything beyond a weak description, but for practical purposes weak emergent descriptions can be sufficiently powerful. It should also be mentioned that the limited time range incorporated in the definition in Sec. 1.3.2 allows the possibility to have different emergent descriptions at different times, allowing “paradigm” shifts in the descriptions that may be induced by the dynamics or by the observer.

Future work will refine the computation of the notion, apply it to a larger range of systems, study its utility and investigate the connections of the presented concept to other notions used in the analysis of complex systems.

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Chapter 35

Universality classes of complexity

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We give several criteria of complexity and define different universality classes. According to our classification, at the lowest class of complexity are random graph, Markov Models and Hidden Markov Models. At the next level is Sherrington-Kirkpatrick spin glass, connected with neuron-network models. On a higher level are critical theories, spin glass phase of Random Energy Model, percolation, self organized criticality (SOC). The top level class involves HOT design, error threshold in optimal coding, language, and, maybe, financial market. Alive systems are also related with the last class.

1.1 Introduction

The definition of statistical complexity is an entirely open problem in statistical mechanics (see [1,2] for the introduction of the problem and [3] for the recent discussion). There are a lot of different definitions having sometimes common context. A certain success was the discovery of an idea of "schema", a highly compressed information, introduced by Gell-Mann for complex adaptive (we assume, for all complex) systems. Some attempts, based mainly on entropy concepts, have been undertaken to define the concept of complexity. The approach [4-6], relevant for our investigation, is of special interest. A very interesting aspect of complex phenomenon is related to the edge of chaos (the border between chaotic and deterministic motion), the phase of complex adaptive systems

(CAS) [2],[7]. The concept of edge of chaos, independently suggested by P. Bak, S.A. Kauffman and C.Langton , is not well defined quantitatively. However, it is widely accepted this concept to be connected with the sandpile [8]. This concept is of special importance due to its possible relation to the birth of life and evolution [7]. This paper is devoted to relations between this phenomenon and some aspects of information theory and optimal coding [9]. We assume that the definition of a single (or best) complexity measure is a subjective one, even with a reasonable constraint that complexity should vanish for totally ordered or disordered motion). More strict is the definition of different universality classes of complexity, which is presented in the paper. We suggest several numerical criteria for complex adaptive property. In practice we suggest to identify the universality class of complexity from the experimental data and to choose a model from the same class to describe the phenomenon.

We assume the following picture of complex phenomenon. The following hierarchy is presented: instead of microscopic motion of molecules or spins we deal with the macroscopic thermodynamic variables. Besides those, some new structures arose, sometimes proportional to fractional degree of particles number. One can understand qualitatively the complexity as a measure of new structures. We are not going to scrutinize into the concrete feature of those structures. We will just evaluate total measure of structures on the basis of free energy expression, including finite size corrections. For interesting cases of complex adaptive system, a hierarchy in the definition of a model, either a disorder ensemble (as in spin glasses), or scale of the system (spatial or temporal) should be represented. The structures themselves are derived from microscopic motions of spins via order parameters. When those order parameter fluctuates, they can be handled like the microscopic spins or molecules. Therefore, in such cases, including the optimal coding of the article, we can identify complex phenomenon as a situation with changing reality or birth of new reality (the thermodynamic reality is a mapping of molecular motions into few thermodynamic variables).

We suggest to apply subdominant free energy as a measure of complexity for any system, as one of complexity criteria. For the situation, when there is no explicit free energy one should try to find some equivalent statistical mechanical formulation of the theory and investigate free energy. In this work we give the first list of universality classes.

1.2 Definition of complex adaptive property

Let us consider ferromagnetic version of Random Energy Model (REM), the border between spin-glass and ferromagnetic phases. There is a Hamiltonian

$$H = - \sum_{1 \leq i_1 \dots \leq i_p \leq N} [j_{i_1 \dots i_p}^0 + j_{i_1 \dots i_p}] s_{i_1} \dots s_{i_p}. \quad (1.1)$$

for N spins $s_i = \pm 1$. Here $j_{i_1 \dots i_p}^0$ are ferromagnetic couplings

$$j_{i_1 \dots i_p}^0 = \frac{J_0 N + j_0 \sqrt{N}}{\binom{p}{N}} \quad (1.2)$$

For quenched disorder $j_{i_1 \dots i_p}$ we have a distribution

$$\rho_0(j_{i_1 \dots i_p}) = \frac{1}{\sqrt{\pi}} \sqrt{\frac{\binom{p}{N}}{N}} \exp\left\{-j_{i_1 \dots i_p}^2 \frac{\binom{p}{N}}{N}\right\}.$$

In this model there are three phases: ferromagnetic (FM), paramagnetic (PM) and spin glass (SG). The choice $j_0 = 0$ corresponds to the exact border FM-SG phases. Using the methods of articles [11,12], we derive for the free energy finite size corrections (bulk free energy is $(\sqrt{\ln 2} + \frac{j_0}{\sqrt{N}})N$)

$$\langle \ln Z \rangle - (\sqrt{\ln 2} + \frac{j_0}{\sqrt{N}})N \sim \beta \sqrt{N} \exp[-j_0^2]. \quad (1.3)$$

We calculated the magnetization m , and derived for its derivative:

$$\frac{dm}{dj_0} = \frac{1}{\sqrt{\pi}} \exp[-j_0^2]. \quad (1.4)$$

We derive an edge of chaos parameter as

$$C = \langle P_1^2 \rangle - \sum_{\alpha > 1} \langle P_\alpha^2 \rangle. \quad (1.5)$$

where $P_1 = \exp[-\beta E_1]$ is a Boltzmann weight of the ferromagnetic configuration (probability of ordered motion), and P_α are Boltzmann weights of other configuration (connected with chaotic motion). C takes the maximal value at the critical point $j_0 = 0$. At $T = 0$ we have

$$C = \frac{1}{2} \exp[-j_0^2]. \quad (1.6)$$

At $j_0 = 0$ probabilities of ordered and disordered motions are equal, then C damps exponentially, when j_0 deviates from the fine tuned value $j_0 = 0$.

Let us define the complex adaptive property. Free energy is the fundamental object in statistical mechanics. The bulk free energy is proportional to the number of particles (spins). It is well known that in case of some defects on geometrical manifolds (lines, surfaces), besides the bulk term in the asymptote expression of free energy, there are subdominant terms proportional to some roots of N . Thus, the subdominant term in free energy could be identified with existence of some structures (much more involved than simple geometrical defects) in the system. In our case of REM, the formulation of the model was homogeneous in the space, but we got a square root subdominant term. In complex system we assume the following hierarchy: bulk motion and some structures above it. The subdominant free energy is related to the structures. If we are interested just in structure, we can ignore bulk free energy. Therefore:

A. We define the complexity as subdominant free energy.

We have seen that in case of error threshold via REM it scales as a square root of number of spins. We assume that it is the most important class of complex phenomena, connected with alive systems. In complexity phase intermediate scale free energy (or entropy, or Kolmogorov complexity) becomes strong, and the subdominant term scales as a square root with the number of degrees.

What do we mean by intermediate scale? There is a minimal scale (ultraviolet cutoff) and maximal scale (infrared one). The intermediate scale is just their geometric average. The complexity in our definition is free energy on a higher hierarchy level (connected with the structures). One should remember that free energy itself is a second level on hierarchy. The energy is on the ground level of hierarchy. Due to thermodynamic motion, only its smaller part is manageable on macroscopic level (only free energy could be extracted as a mechanical work while changing the global parameters). Therefore, complexity is a level on a hierarchy of the following modalities: energy, free energy and subdominant free energy ones. Every higher level is more universal. It is explicit in quantum field theory approach to critical phenomenon [13]. Different renormalization schemes can give different bulk free energies, but the same logarithmic subdominant one. Thus we observe a hierarchy of modalities (non-categorical statement about reality, see [14]). In principle, the hierarchy could be continued, and at some level the life could appear. Our view (rather statistical mechanical, than mathematical) is close to the one by M. Gell-Mann and S. Lloyd in [2], defining system complexity as "length of highly compressed description of its regularities".

Due to above mentioned hierarchy, the identification of complexity with a subdominant free energy is more universal, than the entropy approach of [4,5]. Sometimes the existence of structure could be identified in entropy or Kolmogorov complexity subdominant terms as well. In our case the free energy (sic!) reveals a huge subdominant term, but not the entropy.

We assume that other features of our toy model are characteristic for complex adaptive systems:

B. There is an emergent property, maximally unstable under the change of ordered external parameters, Eq.(1.4). Sometimes it can be characterized as a second derivative of free energy via ordered parameter.

C. The probability of ordered and disordered motions should be at the same level.

D. The complex adaptive properties could be exponentially damped in case of even small deviation of ordered parameter (6).

1.3 Universality classes

Analyzing error threshold phenomena in REM, we have found several criteria of complexity: (3),(4),(39) and (5) which could be applied for complex adaptive systems. In [4-5] has already been suggested to consider the subdominant part of the entropy as a measure of complexity. We have enlarged their idea, suggesting to use a subdominant part of free energy as a measure of complexity. It is more

universal, than the bulk free energy, and could be considered as the next step in the hierarchy energy-free energy-subdominant term in free energy. This hierarchy could be continued. Complexity appears on the third level, at some higher levels the life could appear. We admit that our approach catches the qualitative idea about edge of chaos: in the complex phase, the probabilities of ordered and disordered motions are equal, and complexity properties damp exponentially outside the error threshold point, Eqs (3),(4) and (6). There are few classes of subdominant term behavior: zero, or exponentially decreasing subdominant terms for Markov, and Hidden Markov models [6]; logarithmic corrections for critical theories [13]; cubic root corrections for Sherrington-Kirkpatrick model; square root corrections for error threshold, long-range SG model [5] and, maybe, language. HOT design belongs to error threshold universality class of complexity. First a complexity class should be identified from the empirical data, to model complex phenomenon. As percolation or SOC models belong to the universality class [13], it is improbable that they can describe financial markets. Originally only SOC criticality has been identified with a qualitative idea of "edge of chaos". But we see that error threshold class is higher, than the SOC, and this complexity class is likely connected with alive-like systems [7]. We have suggested to investigate, at first, the main features of complexity to identify the large universality classes. What other characteristics could be used for the further characterization of complex phenomenon? Perhaps the language of the system with its grammar, or, in physical systems, the existence of local gauge invariance. The spin-glass phase and error threshold border in REM reveal the advantage of subdominant free energy approach to complexity compared with the subdominant entropy one. The latter, if be used as a complexity measure, produces lower classes ($\sim O(1)$ instead of $\ln N$ or $\sqrt{N}$). We have used free energy to define the complexity. In general, when direct statistical mechanics formulation of the problem is impossible, one can use a variable, describing a manageable amount of motion on macroscopic level. The context of the problem can contribute greatly make a proper choice.

We assume that it is an important feature of complex system: the real state of the system is in abstract hidden space, and can be observed in reality only in a probabilistic way. In case of spin glasses, the real state of the system is defined in the replica space, with some probability followed by the projection to the zero replicas (in Parisi's theory). In case of Hidden Markov Models the state is not directly observable again, as we get an information via probabilistic process. In quantitative linguistics, an abstract linear space has been applied to catch the meaning of the words [16]. Perhaps, the first example is quantum mechanics: there is a unitary evolution of the state in Hilbert space, and during the measurement we have some probabilistic results. In all those examples the state of complex system is not formulated directly via observable, but instead in some hidden abstract space, where the interpretation of the system (its motion) is rather simple one (the formulation of spin-glass statistical physics in replica space is much easier, than the zero replica limit, and formulation of Schrodinger equation is easier than quantum theory of measurement). Therefore we suggest

a "principle of expanded pre-reality": to solve complex problem one should reformulate the problem in some internal,hidden, wider space ("pre-reality"), then return back to the observable space ("reality") in a probabilistic way.

It is very important to investigate the language models [16], and latent semantic analysis in our approach. The investigation of the semantic is much deeper than the word entropy analysis. The singular value decomposition in [16] qualitatively resembles the fracturing of couplings into ferromagnetic and noisy ones.

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Chapter 36

Networks of genetic loci and the scientific literature

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This work considers biological information graphs, networks in which nodes correspond to genetic loci (or “genes”) and an (undirected) edge signifies that two genes are discussed in the same article(s) in the scientific literature (“documents”). Operations that utilize the topology of these graphs can assist researchers in the scientific discovery process. For example, a shortest path between two nodes defines an ordered series of genes and documents that can be used to explore the relationship(s) between genes of interest. This work (i) describes how topologies in which edges are likely to reflect genuine relationship(s) can be constructed from human-curated corpora of genes annotated with documents (or *vice versa*), and (ii) illustrates the potential of biological information graphs in synthesizing knowledge in order to formulate new hypotheses and generate novel predictions for subsequent experimental study. In particular, the well-known LocusLink corpus is used to construct a biological information graph consisting of 10,297 nodes and 21,910 edges. The large-scale statistical properties of this gene-document network suggest that it is a new example of a power-law network. The segregation of genes on the basis of species and encoded protein molecular function indicate the presence of assortativity, the preference for nodes with similar attributes to be neighbors in a network. The practical utility of a gene-document network is illustrated by using measures such as shortest paths and centrality to analyze a subset of nodes corresponding to genes implicated in aging. Each release of a curated biomedical corpus defines a particular static graph. The topology of a gene-document network changes over time as curators add and/or remove nodes and/or edges. Such a dynamic, evolving corpus provides both the foundation for analyzing the growth and behavior of large complex networks and a substrate for examining trends in biological research.

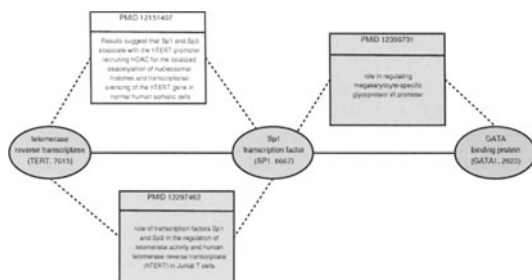


Figure 1.1: A visual depiction of three PubMed citations (squares) that link the three genes TERT, SP1 and GATA (circles). The free-text statement in a box is a synopsis of the article with the stated standard PubMed identifier (PMID).

Introduction

Graphs with large numbers of nodes and edges have been employed to represent and investigate social, information, biological and technological networks [4]. Since such graphs may contain $\sim 10^3 - 10^9$ nodes, statistical methods are required to quantify and characterize their large-scale properties. In biology, most efforts have focused on metabolic, gene regulatory, and protein interaction networks where nodes are molecules and edges are genetic or biophysical associations. Biological information graphs have received less attention despite, for example, their unique capacity to connect nodes representing genes from different species. As shown here, networks capturing the relationships between “genes” and “documents” have to potential to become important research topics in both graph theory and molecular biology.

A study such as a high-throughput molecular profiling study usually uncovers genes unfamiliar to the investigator. For example, a cancer-related mRNA microarray study may highlight the importance of the genes telomerase reverse transcriptase (TERT) and GATA binding protein (GATA1). How can the investigator efficiently learn about these genes and hypothesize new relationships between them? The prevailing approach is a simple keyword search of PubMed¹. However, a PubMed query using the text string “TERT GATA1” is uninformative. Thus, the problem becomes one of discovering indirect links between genes, *i.e.*, that two specific PubMed citations relate TERT to the transcription factor Sp1 (SP1) and another relates SP1 to GATA (Figure 1.1). Given a biological information graph, this information retrieval problem can be recast as a standard convex optimization problem: find the shortest paths between the nodes corresponding to TERT and GATA1. The nodes and edges linking these genes define an ordered sequence of genes and published studies that can assist in discovering the relationship(s) between TERT, GATA1, and cancer.

Previously, text analysis techniques such as natural language processing have

¹URLs discussed: PubMed, <http://www.ncbi.nlm.nih.gov/pubmed>; LocusLink, <http://www.ncbi.nlm.nih.gov/LocusLink>; WormBase, <http://www.wormbase.org>; SGD, <http://www.yeastgenome.org>; FlyBase, <http://www.flybase.org>; Gene Ontology (GO), <http://www.geneontology.org>; SAGEKE, <http://sageke.sciencemag.org>; HuGE, <http://www.cdc.gov/genomics/hugenet>; R, <http://www.r-project.org>; Graphviz, <http://www.research.att.com/sw/tools/graphviz>.

been used to determine associations between given genes/proteins and specific MEDLINE abstracts [2, 8]. However, a problem inherent to these “automated” approaches is entity recognition, the task of ascertaining whether the abstract contains a reference to a specific gene. The complexity of biological terminology means that the frequency of erroneous edges (false positives) and missed edges (false negatives) is likely to be non-negligible. In contrast, this work shows that by viewing widely-available biomedical resources such as LocusLink, WormBase, SGD, and FlyBase as human-curated corpora of annotated data (genes with documents or *vice versa*), gene-document networks can be produced that emphasize quality rather than quantity. Specifically, a biological information network is derived from LocusLink, examined in terms of its large-scale statistical properties, and used to enhance understanding of genes implicated in aging.

Materials and Methods

LocusLink gene-document (GeneRIF) network

LocusLink is a database of genetic loci created by the NCBI in 1999. LocusLink entries (“loci”) are maintained via a process that includes both automated computational methods and manual data curation. A locus may be associated with any number of references into the primary literature, termed “Gene References Into Function” (GeneRIFs). GeneRIFs are assigned by professional NCBI indexers and the scientific community. A GeneRIF consists of the PMID for a relevant article and a free-text synopsis of the pertinent article, written by the GeneRIF submitter. Since every locus is associated with zero or more GeneRIFs, LocusLink can be viewed as a corpus of “genes” annotated with “documents”. A GeneRIF network is defined as a graph in which nodes represent loci and an edge denotes that each of the two connected loci includes a GeneRIF referencing the same PMID. The absence of an edge between loci can indicate either the known absence of a direct relationship between the loci or a lack of knowledge about a relationship.

The GeneRIF network described here was derived from the April 2004 release of LocusLink, containing 181,380 loci from 14 model organisms. The most represented organisms were *M. musculus*, *H. sapiens*, *D. melanogaster*, *R. norvegicus*, *C. elegans*, and *D. rerio*. Genes with no GeneRIFs or whose GeneRIF PMIDs were not shared by any other gene were excluded, resulting in a final network with no isolated nodes. All research was performed using LocusLink LL_tmp1 and GO flat files housed in a custom relational database, the R statistics package, the C++ Boost Graph Library, and GraphViz.

Species and molecular function assortativity

Assortativity refers to the preference of nodes with similar attributes to be neighbors in a network. The notion of preferential association can be quantified via an assortativity coefficient, $0 \leq r \leq 1$, computed using a normalized symmetric

mixing matrix (Eq (17) in [4]). Investigated here were two types of assortativity of loci: by species origin and by function.

For species assortativity, an element of the mixing matrix specifies the fraction of edges that connect genes from two given species. Assessing functional assortativity is more challenging because proteins can have multiple functions, distinct functions are not necessarily independent, and functional annotation is incomplete. The approach used here exploits ongoing efforts to characterize gene products via the assignment of terms from an extensive controlled vocabulary known as the Gene Ontology (GO). Each GO term belongs to one of three orthogonal aspects, and the ontology itself is organized as a directed acyclic graph. Given this source of node-specific attributes in LocusLink, the task of calculating functional assortativity becomes one of computing the similarity between the associated GO terms of all connected loci. A simple similarity score was estimated using an approach developed to take into consideration the GO graph structure and the frequency of GO terms assigned to genes [3, 7]. For the GeneRIF network, functional assortativity was assessed by computing pairwise GO molecular function semantic similarity scores using only GO **Molecular Function** terms accompanied by a **Traceable Author Statement Evidence Code**, i.e., GO assignments of high-confidence since they reflect knowledge present in the primary literature.

Gene-document network-based analysis of aging-related genes

The SAGEKE database of known aging-related genes was analyzed using the following heuristic. The shortest path (SP) between two nodes in a network can be computed using standard algorithms such as breadth-first search [1]. An SP for a pair of genes in a collection defines a sequence of genes in which neighbors are related via knowledge found in the scientific literature. The union of shortest paths (USP) subgraph is the set of nodes and edges defined by the SPs for all distinct node pairs in a collection. Centrality refers to the influence a node has over the spread of information in a network. A simple measure of this notion is stress centrality, the number of SPs between node pairs that pass through a node of interest. Given nodes in the USP subgraph ranked by their stress centrality score, good candidates for genes for additional study are nodes with high scores but that are not present in the original collection. Stress centrality was computed for SAGEKE USP genes in the GeneRIF giant component.

Unweighted and weighted networks

A weighted GeneRIF network was estimated using an approach proposed for scientific collaboration networks in which nodes correspond to scientists and an edge indicates that two scientists are co-authors [5]. The weight of an edge is the sum, over all common documents, of $1/(n-1)$, where n is the number of genes associated with a document.

GeneRIF component(s)		
	All 1229	Giant
n	10,297	7,167
m	21,910	19,372
z	4.26	5.41
l	5.54	5.54
$C^{(1)}$	0.153	0.146
$C^{(2)}$	0.365	0.401
r	0.141	0.108

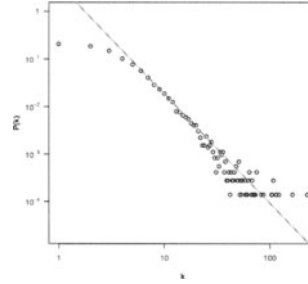


Figure 1.2: Left: Large-scale statistical properties of the unweighted GeneRIF network. n , number of nodes; m , number of edges; z , mean degree (number of edges per node, k); l , SP distance between node pairs (Eq (2) in [4]); $C^{(1)}$, clustering coefficient (mean probability that two nodes that are network neighbors of the same third node are themselves neighbors; Eq (3) in [4]); $C^{(2)}$, alternative clustering coefficient (weights the contribution of nodes with few edges more heavily; Eq (6) in [4]); r , degree correlation coefficient. Right: Log-log plot of the degree, k , and degree probability (fraction of nodes with degree k), $P(k)$, for the giant component. The tail follows an approximate power law, $P(k) = ck^{-\alpha}$ ($\alpha \approx 2.3$, $c \approx 2.7$ for the line shown).

Results

Large-scale statistical properties, including assortativity

The GeneRIF network contains 10,297 nodes and 21,910 edges organized into 1229 distinct components (two or more nodes connected transitively to each other but not to other nodes in the graph). The basic statistics of this gene-document network are similar to those of networks studied previously (Table 1 in [4]; Figure 1.2). Since the degree distribution follows an approximate power law, most genes are related to each other by a small cabal of highly-connected genes. These are human TP53, tumor protein p53 (annotated with 510 documents/number of edges or degree $k = 226$); human TNF, tumor necrosis factor (319/164); human VEGF, vascular endothelial factor (236/122); human MAPK1, mitogen-activated protein kinase 1 (124/115); human TGF β 1, transforming growth factor, beta 1 (176/114); human NF κ B1, nuclear factor of kappa light polypeptide gene enhancer in B-cells 1 (113/108); mouse Trp53, transformation related protein 53 (148/108); mouse Tnf, tumor necrosis factor (150/105); and human SP1, Sp1 transcription factor (72/104).

The biological properties of signaling and kinase activity distinguish well-connected genes (105 genes having the top 1% of degrees, $k \geq 33$) from all genes (7,167 genes in the giant component). For GO terms assigned to $\geq 10\%$ of genes in both sets, the ratio of the relative frequency of a GO term in well-connected genes to its relative frequency in all genes was computed. GO terms with a ratio greater than 2.0 are MAP kinase activity, cell proliferation, cell-cell signaling, kinase activity, apoptosis, signal transduction, regulation of cell cycle, protein amino acid phosphorylation, immune

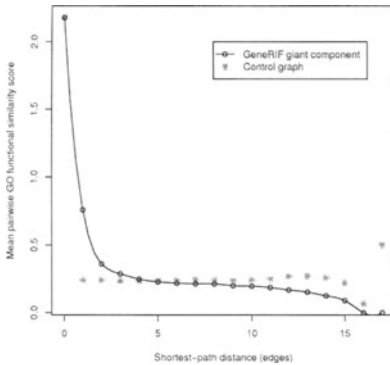


Figure 1.3: Functional assortativity of nodes in the GeneRIF network giant component and a topologically identical network generated by randomly shuffling the identities of nodes in the giant component. At distances of 1 to 4, genes in the real network are more similar to each other than might be expected (the distance of a gene to itself is defined as zero). The fluctuation at large distances is due to small sample sizes.

response, protein serine/threonine kinase activity, protein kinase activity, transferase activity, ATP binding, extracellular, cytoplasm, and transcription factor activity.

Nodes in the giant component of the GeneRIF network exhibit extensive segregation on the basis of both species and molecular function. The species assortativity coefficient of $r = 0.73$ suggests that this gene-document network is closer to a perfectly assortative network (if $r = 1$, every edge connects nodes of the same type) than a randomly mixed network ($r = 0$). The functional similarity between pairs of nodes (pairwise GO molecular function semantic similarity score) decreases as the SP distance between them increases (Figure 1.3).

GeneRIF network: known and novel aging-related genes

In order to investigate previously identified aging-related genes and suggest new genes with potential roles in this phenomenon, a weighted GeneRIF network was used to analyze a collection of genes implicated in aging (Figure 1.4). The presence of mouse (Trp53, Igf1, Tnfsf11, Tnfrsf11b, Akt1) and fly (W) genes amongst human genes highlights a unique property of biological information graphs. Because edges can link nodes from different organisms, gene-document networks provide an ability to navigate both intra- and inter-species relationships, a facet absent in protein interaction and other biological networks.

Nodes in the SAGEKE USP subgraph that have high stress centrality scores include some genes that are highly-connected in the giant component of the GeneRIF network (large degree k): human TP53, mouse Trp53, and human VEGF. The higher score and degree of TP53 compared to its mouse homolog (Trp53) reflect the greater scrutiny to which this gene has been subjected (to date, SAGEKE has only linked the mouse gene explicitly with aging). Other highly-connected GeneRIF genes are human VEGF, human TNF and mouse TNF. One heuristic for identifying new genes with possible roles in aging is to equate them with nodes that have high centrality scores in the SAGEKE USP subgraph but are less well-connected in GeneRIF network. Using these criteria, additional studies of IGF1/Igf1, PTEN, Tnfsf11, Tnfrsf11b/TNFRSF6,

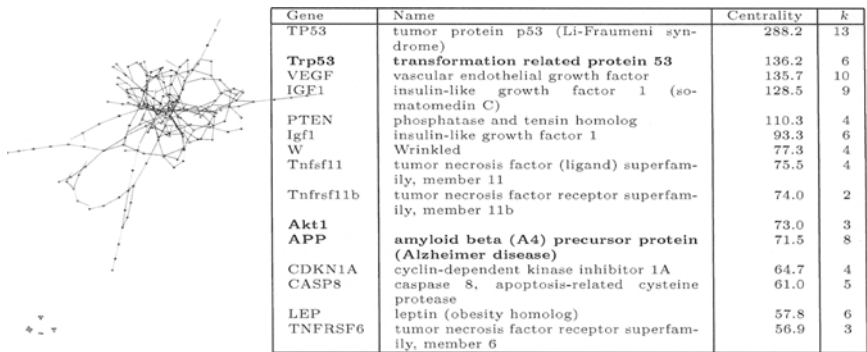


Figure 1.4: Left: The 185 nodes and 268 edges of the weighted GeneRIF network that constitute the union of shortest-paths (USP) subgraph for 51 known aging-related (SAGEKE) genes (note that some SAGEKE genes correspond to nodes that are not in the giant component, small clusters of nodes in the bottom left). Right: Genes in the SAGEKE USP subgraph with the 15 highest stress centrality scores. Genes in bold are SAGEKE genes.

CDKN1A, CASP8, and LEP could prove informative.

Discussion

The biological information graph investigated here is similar to the literature citation network first studied four decades ago [6] in that semantic links between nodes come exclusively from published research. Gene-document networks have a variety of strengths and applications. As suggested by the analysis of aging-related genes using a LocusLink-derived GeneRIF network, they have potential as tools in the scientific discovery process. Such networks provide an individual with little expertise in given domain ready and simple access to an extensive body of prior work allowing them to formulate hypotheses and generate predictions for subsequent investigation. Especially noteworthy, although rare, are edges between genes from different species because the associated documents provide a useful bridge for comparative genomics and biology studies of similar processes such as aging. By ascertaining isolated components in the GeneRIF network, NCBI indexers can be alerted to genes that might benefit from systematic efforts to identify publications that link them to other and larger components.

Gene-document networks are limited by a number of factors, not the least of which is the corpus of annotated data used to construct the network. The very origin and nature of LocusLink means that the GeneRIF network is neither comprehensive nor complete. The focus of GeneRIF is papers pertinent to basic gene structure and function rather than, for example, evolution. Because GeneRIF was initiated in 2001 as a manual curation effort by a small group of experts, only those relationships between genes in recent publications are present in the LocusLink. Some of these deficiencies may be overcome by building gene-document

networks using multiple manually curated gene-centered corpora, for example, the HuGE database of published epidemiology articles on human genes.

Since the nodes in gene-document, protein interaction and related networks correspond to genetic loci, such sources of heterogeneous data could be fused to yield biological information graphs of greater scope and enhanced utility. Such an operation would provide a simple method for synthesizing disparate information. Since most biomedical resources are ongoing efforts, the size and coverage of such corpora is increasing over time. Building biological information graphs using each release would yield new real-world examples of large, complex, dynamic, networks. In addition to theoretical studies of their properties and behavior, these networks would be useful not only for researchers and clinicians, but also policy makers, historians, and sociologists interested in the evolution of different disciplines in biology.

Acknowledgements

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Chapter 37

A Multi-Modeling Approach to the Study of Animal Behavior

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1.1. Introduction

Animals are paradigms of complex systems. Therefore, models must be used to fully understand their emergent individual, group, and social behavior. Models can be physical, symbolic, mathematical, or computational, but they are always simpler than the animal systems they represent. Thus, models always have limitations. Viewed as tools for understanding, some models are better fit for investigating particular systems than others. Indeed, using models in science is much like using tools to build things. The use of tools is typically coordinated for the best success. For example, to drill a precise hole in a sheet of metal, several tools are needed: a ruler, pencil, punch, hammer, and drill. Holes can be made without some or all of these tools, but there will be a cost in precision and accuracy. To use models effectively in science, we need to understand their specific functions and limitations. Understanding these properties of models as tools is essential for their coordinated and effective use.

In this chapter, we discuss and illustrate several dimensions of modeling with our research program. We believe this research provides a nice example because it is not so complicated that it cannot be outlined in a single chapter, but it is also sufficiently complex to illustrate the need for multi-modeling approaches and the consideration of the properties of different models.

1.2. Models and their Dimensions

We have found it useful (Schank & Koehnle, 2007; Koehnle & Schank, 2003) to characterize models in terms of several dimensions of modeling. We (Schank & Koehnle, 2007) have extended previous frameworks (e.g. Webb's (2001), which extended Levins (1966) framework to discuss the role of robotics in behavioral research) for discussing the properties and functions of models to 9 dimensions. Each of these dimensions we believe is important, but none are completely independent or dependent on the others: (1) *Realism* concerns the degree to which the properties of a model accurately represent an intended system. (2) *Detail* concerns the number of variables and parameters in a model. (3) *Generality* of a model concerns the applicability of a model to a broad domain of systems, but what makes a model general has been confused with detail (Schank, 2001). (4) *Match* concerns the relationship between data and the model but matching failures can also guide us in building better models (Wimsatt, 1987). (5) *Precision* concerns how quantitatively precise a model is in its predictions, explanations and even its degree of match. (6) *Tractability* concerns how analyzable or manipulable a model is. (7) *Integration* concerns how well the model can be coordinated with the use of other models, to facilitate their use, and thereby add synergy to the modeling process. (8) *Level* concerns either levels of analysis or organization. Some models are appropriate for populations of organisms, types of behavior (e.g., game theoretic models), or physiological process in an organism. Finally, (9) *Medium* concerns the nature of a model itself. Is it mathematical, computational, or physical? This taxonomy of model properties allows us to specify the dimensions along which models imperfectly represent their targets. Different models will score well on some, and poorly on others. Understanding the diverse behavior of animals will likely require models spanning all nine dimensions.

1.3. Locomotor Behavior in Developing Rats: An Example

To illustrate these dimensions and the use of multiple models in research, we will outline our research program, which is still in its early stages. Though we illustrate dimensions of modeling with a specific example, we believe that many aspects of our use of models apply to other areas research. In addition, the issue of integrating and comparing multiple models is not well understood and we hope that this chapter will stimulate further discussion of the use of multiple models in research.

1.3.1. Discrete Agent-Based Models

Agent-based modeling (ABM) is a strategy (though not a specific technique), which focuses on modeling the interacting components of a system rather than its macro-level behavior (Bonabeau, 2002). Agents interact according to sets of rules that modulate individual behavior and interactions with other agents. Even simple sets of rules can give rise to interesting and emergent patterns of behavior at both individual and group levels. ABM can be an especially promising modeling strategy when little is understood about the dynamics of individual or group patterns of behavior. This

can be accomplished by exploring plausible sets of individual rules or even using genetic algorithms to evolve rules that generate observed individual and group patterns of behavior. For example, we have used discrete ABMs to model the patterns of individual locomotion and group aggregation in infant Norway rats (see Fig. 1; Schank & Alberts, 1997; Schank & Alberts, 2000; & Schank, 2008).

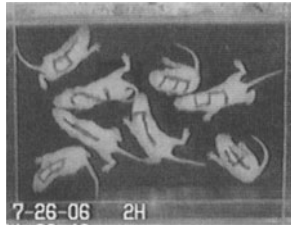


Figure 1. Ten-day-old infant rats (pups) in a 20.32 cm × 30.48 arena (Schank, 2008).

The first version of these ABMs modeled pups as moving discretely between cells of a grid representing an arena (Schank & Alberts, 1997). Movement was probabilistic and movement probabilities were determined by simple rules for assigning thigmotaxis weights to the three cells in front of a pup depending on the content of the cells—thigmotaxis is an orienting response to contact with objects (Frankel & Gunn, 1961). Whether an agent was active or inactive was determined by transition probabilities from active to inactive and inactive to active. The model did a reasonably good job of matching the behavioral data for 7-day-old pups (Schank & Alberts, 1997), but did not work well for 10-day-old pups (Schank & Alberts, 2000).

The second generation ABM extended the modeling of transition probabilities from constants to functions of time and the activity states of other pups contacted (Schank & Alberts, 2000). The new model better explained aggregation in 10-day-old pups and revealed that by day 10, pups exhibit coupled activity (i.e., the locomotor activity of pups dependent on the activity states of other pups, which does not occur at day 7; Schank & Alberts, 2000). The coupling of activity in 10-day-old pups often led to synchronized quiescent activity towards the end of an experimental session, when pups aggregated into one or two groups (Schank & Alberts, 2000).

The third generation ABM added a new feature to the second generation ABM to model kinematics of whole-body directional movement and its development in infant rats (Schank, 2008). This new feature was a kinematic matrix $\mathbf{K}$ of probabilities of moving to any of eight adjacent cells surrounding an agent when there are no objects or stimuli influencing the direction of movement. In this extension, $\mathbf{K}$ is assumed to have lateral symmetry of directional movement probabilities

$$\mathbf{K} = \begin{bmatrix} fl & f & fl \\ l & 0 & l \\ bl & b & bl \end{bmatrix} \quad (1)$$

where, f (forward), b (turn around), l (lateral), fl (forward lateral), and bl (lateral and to the back) are probabilities of moving to adjacent cells. Genetic algorithms were

used to fit the model to data on 7- and 10-day-old pups, which were placed in an arena either as individuals or in groups of eight. For 7-day-old pups, $\mathbf{K}$ in both individual and group context was characterized by a relatively high proportion of $b/$ and b movements. This produced punting-like behavior (turning around an axis of rotation) and reduced aggregation. For 10-day-old pups, the story was more complex. In the context of groups, forward movement occurred over 40% of the time, but in individual contexts, forward movement was converted into over 60% lateral movement. The group $\mathbf{K}$ facilitated aggregation and the individual $\mathbf{K}$ fit the zigzag movement observed in day 10 individuals. These different $\mathbf{K}$ matrices at day 10, can be mapped onto the developing corticospinal tract (Clarac et al., 2004; Schank, 2008).

Dimensions of Modeling. Discrete ABMs are realistic in representing the dynamics of individuals moving on the surface of an arena and responding to stimuli. They are unrealistic in representing space and time as discrete units and ignoring physical properties of the body morphology and the environment. The models taken together incorporate increasing detail and their abstraction from physical properties allows them to generalize to other animal systems. With each generation of ABM, the match between model and data improved as well as the quantitative precision in explaining behavior. The tractability of ABMs depends largely on the computational power available, which is exponentially improving and likely to for a long time (Lloyd, 2000). We will hold off discussion of integration of this model with the other models we have developed until the end. The level modeled was the individual, but the analysis of these models was at both individual and group levels. Finally, the medium was computational, which means there are concerns that do not arise in mathematical models such as numerical precision and pseudo-random number generation.

1.3.2. Robotic Models

Concerns about physical realism of models of animal behavior suggest that physical models may be well-worth pursuing (Webb, 2001). Robotic models typically do not share the same physical properties as the system modeled, but they can be scaled to share key formal properties in common. Shape and motion are key variables of pups we aimed to represent in our robots (**Figs. 1 & 2**).

The first generation robot (Joshi et al., 2004) was designed to have roughly the shape and tactile sensory capabilities of pups. It exhibited wall following and corner “burrowing” behavior typical of pups. After establishing that a robot could generate some behaviors that were similar to rat pups, we designed a second generation of robots with a higher fidelity morphology, better control of movement, and more realistic tactile sensory system (**Fig. 2**). The shape of a pup (**Fig. 1**) is long with a somewhat pointed head, rounding out at the nose. Because we hypothesized that shape strongly influences arena behavior, robots were custom-constructed to have the same shape. They have the same length: width ratio as rat pups, approximately 3:1, where the head constitutes 1/3 of the length. An aluminum skirt was outfitted with 14 micro/limit (touch) switches. Brass strips connecting these binary switches allowed for a 360° sensory range. Sensor cluster density is substantially higher at the nose, mimicking a rat’s sensory montage. Since rat pups’ front legs are underdeveloped

and aid only in steering, they primarily use their back legs for locomotion. Accordingly, the robots were equipped with rear-driven wheels (differential drive) on a single chassis.

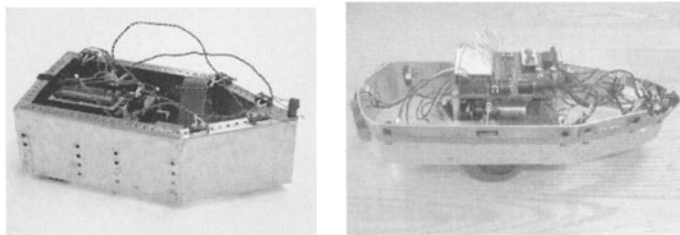


Figure 2. First (left) and second (right) generations of robotic rat pups (cf. **Fig. 2**).

Robots were tested both individually and in groups, yielding interesting results (Schank et al., 2004; May, et al., 2006). First, the implementation of a simple thigmotaxic control architecture (i.e., orientation and movement towards objects contacted; Frankel & Gunn, 1961) generated stereotypical behavior in which a robot repeatedly circled the arena. Pup behavior, however, is much more variable (Schank, 2008). This suggested that the behavior of pups was not likely explained solely by sensorimotor control. Second, robots that processed no tactile sensory input and moved randomly in the arena behaved more realistically. They could aggregate (**Fig. 3**) into groups, and behaved intermediate between 7- and 10-day-old pups (May et al., 2006).

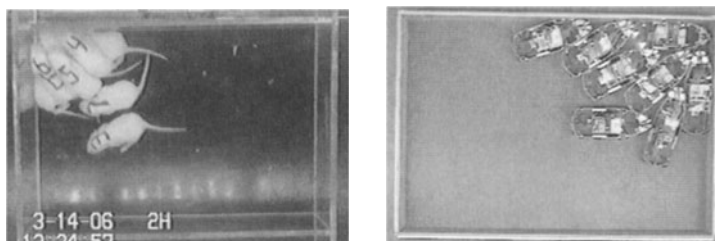


Figure 3. An example of aggregation of pups (left) and random robots (right).

Dimensions of Modeling. The development of robotic models represented a change in medium, which implied that these models were more realistic in the sense of having physical properties, representing the physical environment, and body morphology. Physical robots, however, created problems of tractability. First, they have to be analyzed experimentally, which requires considerable time and only allows small-sample size statistical comparisons with data. Second, the physical parameters of these robots are not easily modified. One concern about realism made tractability especially salient: our robot have rigid bodies, but pups have flexible bodies (cf. **Figs. 1, 2, 3**). There are many ways to implement flexible bodies, but the development of alternative physical robots takes time.

1.3.3. Dynamic Systems Models

The standard engineering strategy in robotics is to develop system dynamic models of robots. If we were to explore aspects of body morphology and body flexibility, the first thing we had to establish is that we could develop adequate models of our robots. Dynamic system models of behavior attempt to represent individuals interacting with a physical environment. Physical and geometrical properties are represented, but the difficult problems concern which physical properties are relevant, how are they adequately represented, and how to measure the relevant physical properties in the system modeled.

In Bish et al., (2007), we developed a detailed dynamic system model of our second-generation robot with a Newtonian dynamics-based simulation (**Fig. 4**), which included mathematical formulation and computer implementation. The computer simulation had three parts: (1) dynamics of the robot including sensors and actuators; (2) environmental coupling dynamics of the arena and robot; and (3) implementation of robot control algorithms. We showed that the mathematical model and corresponding virtual robot behaved very similarly to our physical robots.

Dimensions of Modeling. The dynamic system model verified that we could adequately simulate our physical robots and therefore model different morphologies virtually. The detailed realism of this model, however, came at the cost of computational tractability. Our MATLABTM implementation of the mathematical model was computationally extremely intensive, prohibiting the investigation of group behavior.

1.3.4. Heuristic Physics and Agent-Based Models

To achieve a more computationally tractable model, we implemented our virtual robots in the breve open-source simulation platform (Klein, 2002). Breve is a three-dimensional simulation environment designed for modeling multi-agent systems with heuristic physics. Our first aim was to determine whether an agent implementing heuristic physics could replicate the behavior of our robots and our dynamic system model, which it did (May, 2006; May & Schank, submitted). Rigid-bodied agents were then modified to create 3-segmented agents. To do this, passive revolute joints were added to create a head and a body that could flex body up to $\pm 72.5^\circ$. Thus, if an agent hit a wall at an angle, one of more body segments would flex (**Fig. 4**).

Two notable results were that both flexibility and the kinematics of turning dramatically altered behavior (May et al., 2006, May & Schank, submitted). Whereas individual rigid-bodied agents behaved like our physical robots and were intermediate between 7- and 10-day old pups in locomotor behavior, the flexible agents behaved more like 10-day-old pups. Second, flexible agents that only moved forward (or had a high probability of moving forward) behaved like our robotic thigmotaxic agents (Schank et al., 2004): they typically repeatedly circled the arena.

Dimensions of Modeling. Breve-implemented virtual agents allowed us to overcome the computational tractability issues of the dynamic systems agent implemented in MATLABTM. The implementation of flexible-bodied agents illustrates an important issue in modeling that is little discussed, namely, that radically

1.4. Discussion

In our research, one type of model drives the development of a different type to overcome particular limitations. For example, discrete ABMs led to the creation of robotic models with increased physical realism. This realism caused an appreciation of the role of body morphology in constraining and generating patterns of behavior. In turn, this led to the development of dynamic system models to explore the effects of different morphological designs. These simulations enabled an exploration of different kinematic implementations (an increase in detail), which dovetailed with the third generation ABMs described above (which have higher generality).

The use of multiple models has revealed that modeling locomotor behavior in even relatively simple animals such as infant rats involves multiple levels of organization and analysis. Understanding behavior does not reduce to understanding stimulus-response relationships or even the computational processes that mediate stimuli and responses. In addition, we must understand body morphology and how it passively and actively constrains and generates behavior. This kind understanding requires the use of multiple models to explore the effects of diverse variables at multiple levels of organization on emergent behavior.

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Chapter 38

Patterns of Negotiation

A new way of looking at marketplace B2B Negotiations

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1.1. Introduction

Traditionally, face-to-face negotiations in the real world have not been looked at as a complex systems interaction of actors resulting in a dynamic and potentially emergent system. If indeed negotiations are an outcome of a dynamic interaction of simpler behavior just as with a complex system, we should be able to see the patterns contributing to the complexities of a negotiation under study. This paper and the supporting research sets out to show B2B (business-to-business) negotiations as complex systems of interacting actors exhibiting dynamic and emergent behavior. This paper discusses the exploratory research based on negotiation simulations in which a large number of business students participate as buyers and sellers. The student interactions are captured on video and a purpose built research method attempts to look for patterns of interactions between actors using visualization techniques traditionally reserved to observe the algorithmic complexity of complex systems. Students are videoed negotiating with partners. Each video is tagged according to a recognized classification and coding scheme for negotiations. The classification relates to the phases through which any particular negotiation might pass, such as laughter, aggression, compromise, and so forth – through some 30 possible categories. Were negotiations more or less successful if they progressed through the categories in different ways? Furthermore, does the data depict emergent pathway segments considered to be more or less successful? This focus on emergence within the data provides further strong support for face-to-face (F2F) negotiations to be construed as complex systems.

1.2. Research Challenges and Literature Review

The central proposition relates to exploring the concept of F2F (or marketplace) negotiation research in business from the perspective of complex systems and emergence. The authors believe that negotiations exhibit emergent characteristics whether over the short or even long term with respect to military acquisitions or large ticket value corporate tenders or purchases. Traditionally, negotiation research is heavily process based following a conventional negotiation cycle of opening, middle and closing. This can be seen no more clearly than in the definition "Business negotiation is the process of bargaining over a set of issues for the purpose of reaching an agreement" [Holmes 1991]. Furthermore, the author's literature review classifies this research into:

Accounting and auditing, education, social interaction and communication, marketing, behavior, accountability and time pressure, culture, conflict management, law as well as "e-" and automated negotiation.

More specifically, the area of complexity science and marketplace negotiation exhibits paucity of published work and at this stage, there appears to be only one publication [Wheeler, 2002] covering this area of interest.

A clear challenge of the research from the onset is to determine how the complex system of marketplace negotiations is represented. We wished to avoid what we saw as a failing of the traditional negotiation research and overcome capturing a single dimension (e.g. process map). The more we pondered B2B negotiations we recognize:

- a.) Buyer and seller especially in multi-body (more than two players) negotiations do not comprehend how the negotiation operates even if they have a process map to guide actions.
- b.) An outside observer will never have a perfect view of information since we cannot under normal circumstances look inside the minds of participants and understand the multiple mental processes [Woodside, 2005].

In light of this, the only representation of the negotiation is the negotiation itself or a comprehensive multi-dimensional simulation capturing the entire system. This is consistent with Kolmogorov-Chaitin complexity. Therefore, the negotiation is explored as a complex system by looking both inside and outside the negotiation through video ethnography and self reports from buyer and seller.

1.3. Research Methodology

1.3.1 Complex Systems Representation

From the onset, the desire is to utilize the ethnographic observation represented by the video footage to understand “what is actually going on in the negotiation?” The research is exploratory or investigative in nature rather than hypothesis driven. In effect, our desire is to see what the complex systems representations would tell us rather than imposing traditional beliefs.

An important aspect of the work is to break with the traditional process based approach that aims to answer questions of the nature “how many steps did it take to achieve the end result?” Rather, the researchers see potential in capturing video footage in lieu of a traditional paper based ethnographic observation to help analyze and consider the negotiation process as being built atop at times an unstructured interaction between buyers and sellers.

The source of negotiations is course 24723 Business-to-Business Electronic Marketing [Young and Sood, 2002]. Furthermore, this course has a negotiation simulation in which students are asked to participate as buyers and sellers. Using these negotiations, an initial digital video footage of five negotiation sessions from this teaching is captured as an initial research set against which to refine the research method. This content constitutes an actual ethnographic record of the student negotiations. The footage covered negotiations of two as well as three actors. Supporting information includes self-reports from participants.

The video taping of the sessions attempt to capture a negotiation in entirety. This content is isolated and recorded onto CD ROM media for ease of further editing and analysis. Subsequent steps created a complex systems representation of the negotiation.

1.3.2 Method

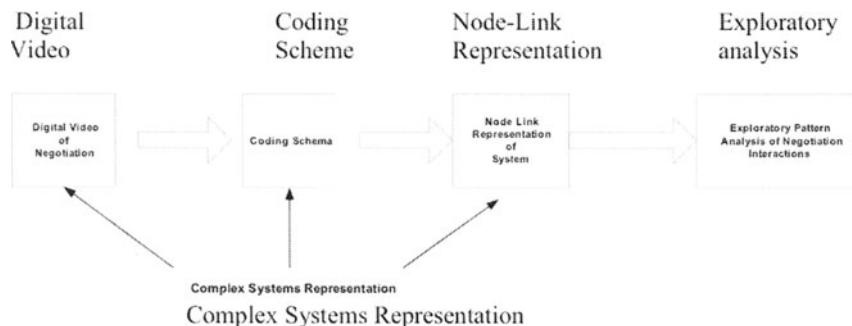


Figure. 1. End to end method to represent negotiation as a complex system

The Interpersonal Negotiation Coding Scheme [Campbell 1997] is ideally suited for the video coding strategy. This scheme operates at the lowest possible level of communications (micro events) between actors suiting the motivations of the researchers to explore system interactions via linkages. The coding schema is not process based but focuses on the personal interaction between actors at a fundamental level. If indeed negotiations are an outcome of a dynamic interaction of simpler behavior just as with a complex system we should be able to see the patterns contributing to the complexities of the negotiation under study.

A time code is inserted by a video editing software application at the beginning and end (if applicable) or just at the beginning of the observed behavior in accordance with the coding scheme.

The video segments need to be viewed over a number of times to pick up “what is actually going on” and therefore code the micro level activities. At the highest level it is expected that the negotiation follows a communication process between normally 2 parties

Each player of the game does not automatically accept what the other party offers. At some stage during the negotiation one may indeed witness conflict resolution, joint collaboration and a decision on a final outcome. Price may not be the only deciding factor. These macro events are recorded in terms of time code start & end.



Figure. 2. Video segment coding – micro events

1.3.3 Related Video & Visualization Software

Researchware HyperRESEARCH software is selected because of the ready ability to cope with video as well as other data types. This software is a code-and-retrieve data

analysis program with a hypothesis tester. HyperRESEARCH is used to conduct the pre-processing and coding before analyzing the occurrence of any patterns to fingerprint the complex system.

Netmap Analytics software is used for visualization and exploratory pattern analysis. The Netmap software helps provide the most direct representation of a complex system as nodes and links. An Australian scientist, Dr John Galloway developed Node and Link Analysis (NALA) in the 1980's.

Netmap has numerous features not seen in other packages including the ability to view emergent data sets. These emergent data sets exhibit more relationships between themselves than outside.

The bottom up representation of the negotiation as nodes and links considers the nodes as participating actors with links denoting the observed behavior as represented by the coding scheme at an associated time.

1.4. Findings - Patterns of Negotiation



Figure 3. Sequential pathway patterns for all negotiation groups (left hand side), showing the categories (vertical) traversed to complete the negotiation (right hand).

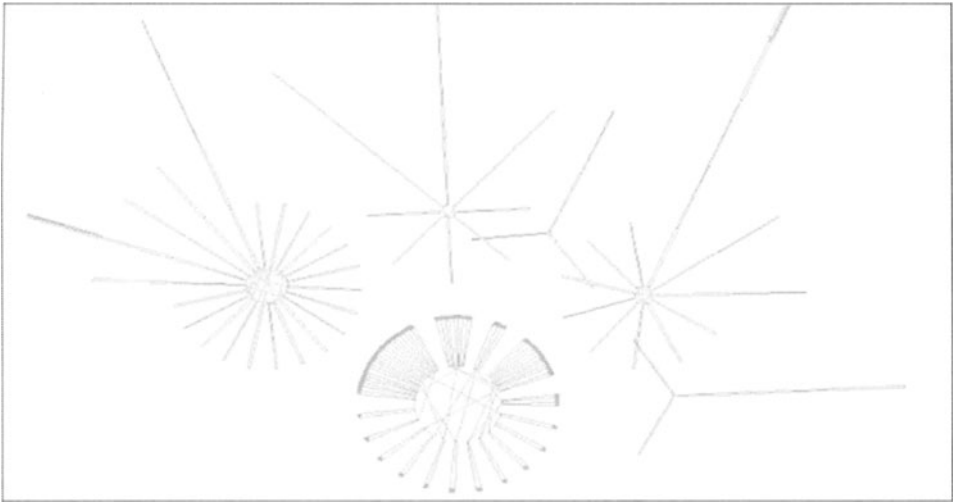


Figure. 4. Emergent pathways discovered by the Netmap software and each group is comprised of negotiations following through the coded categories sequentially in a very similar manner. Each group of groups has distinctive pathways. The pathway is very similar to each other if they belong to the same emergent group and different to each other if they belong in different emergent groups. This is essentially what the data visualization depicts from the bottom up.

1.5. Discussion and Future Research

The research to date has served to bring together a laboratory “demonstrator” which is capable of taking video based negotiations, creating a complex systems representations and attempts to look for patterns of interactions between actors. The research needs to be extended to a much larger data set to demonstrate any practical value.

The demonstrator if developed further can be of significant value in for instance, very large trade negotiations or the purchase of extremely complex industrial goods [Koop, 2004] in which a multitude of working groups come together to conclude an overall negotiation. The scenario of looking at trade talks such as Cancun [Bailey, 2003] starts to look more like a true complex system with a significant number of actors, groups and behavior envisaged to be emergent. The unexpected outcome of the talk points to what we would expect of a complex system resultant counterintuitive behavior. Such a tool as described could be used for diagnostic purposes during the course of a negotiation alongside any traditional process based intervention techniques.

Other areas for further research consideration include the integration of self reports and capture of physiological factors that can be collected automatically alongside the video capture to move towards a more complete representation of the negotiation as a complex system. Additionally, future research intends to explore synchronizing the real time negotiation activities with cognitive scripts based on a corpus of successful pathways generated using the techniques outlined in this paper. Can indeed such a complexity-based approach guide negotiations to achieve successful outcomes?

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Chapter 39

Organized All the Way Down: The Local Complexity of “Thick” Social Systems

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1. Introduction

At least since Adam Smith’s *The Wealth of Nations*, it has been understood that social systems can be considered as having emergent properties not reducible to the actions of individuals. The appeal of this idea is obvious, no different now than in Smith’s time: that aggregates of persons can be ordered without such order being intended or enforced by any particular person or persons. A search for such an “invisible hand” is what brings many of us to the study of complexity and the construction of various types of computational models aimed at capturing it. However, in proceeding along these lines, we have tended to focus on particular types of social systems – what I will in this paper call “thin” systems, such as markets and populations – and ignored other types, such as groups, whose base interactions are “thick,” i.e., constructed as one of many possibilities, by the participants, at the moment in which they take place. These latter systems are not only ubiquitous but pose particular modeling problems for students of complexity: the local interactions are themselves complex and the systems display no strongly emergent features.

2. Emergence in thin social systems

2.1. Typical thin systems

It is convenient to start by considering the type of social systems commonly modeled in the agent-based literature. A classic example is Sugarscape [Epstein and Axtell 1996]; although the characterizations which follow also apply to many other studies, including those with which I was involved [e.g., Cederman 1997; Ormerod 1998; Majeski et al. 1999; Bhavnani and Backer 2000; Lustick 2000; Macy and Willer 2002; Sylvan and Majeski 2003; Watts 2003]. The social system in Sugarscape can

best be characterized as a population whose members are defined by dint of their ability to interact with others locally. This population, in itself, has no particular significance for the agents themselves; it is simply a set of agents able (because of geographical propinquity and agent characteristics) to interact. (Even when there is positive feedback from the percentage of the system in a given state to the probability of agents “opting” for that state the next time around, this does not mean that the agents perforce perceive, much less consider as relevant, the system as a whole.) In this sense, the boundary separating the system from other systems is a purely quantitative measure of interaction likelihood and the system cannot, except in a purely operationist sense, be said to display any “entitativity” [Campbell 1958].

To say that a social system, whether in Sugarscape or in other agent-based studies, is a population is to treat that system as having several characteristics. First, the system is incapable of acting, wishing, or displaying any type of agent-like qualities. That is, the system is not in any sense analogous to an organism or some other higher-level entity. This is not to deny either the reality or the patterned quality of the system; but it is to deny that the system has some sort of behavior proper to it. For example, an economic market does not act. It may well display price convergence (and, indeed, have that convergence operate slowly or quickly) and, through those prices, may affect the behavior of buyers and sellers; we may therefore speak of the market as operating smoothly or poorly, with some among us going so far as to look for information on market-wide prices or to pursue policies aimed at affecting market operations; but the market cannot in itself do anything.

(One might argue that certain Sugarscape-like social systems, if not themselves agents, at least display certain pseudo-agent qualities. Such claims are often made for crowds or mobs, or even of “publics,” mass or otherwise. However, to use this sort of language is somewhat misleading, since to say, for example, that a mob stormed the palace is not to say anything other than that a large number of persons stormed the palace, with each being encouraged in his/her behavior by the fact that many others were acting in the same way. Even cooperation among persons in the mob – say, pulling together on a rope – is not action by the mob but by small and momentary clusters of individuals.)

Second, instead of having agentive qualities, a population-like social system has what might be termed statistical emergent qualities. That is, one can talk about averages and variation in certain agent properties; one can depict clumping and clustering at any given moment or over a certain period of time. Obviously, these qualities are genuinely emergent: they apply only to the system and not to individual members. Such characteristics may well have qualitative import, as when certain types of agents either disappear or crowd out other types. Nonetheless, the complexity often attributed to social systems of the Sugarscape sort by dint of their emergent properties is statistical in nature, meaning, among other things, that its significance may well pass unperceived by the systems’ agents.

The implication of the first two points is the third and perhaps most important characteristic of these systems: the semantically limited quality of their agents’ interactions. It is well known that Sugarscape-style social systems are built up from highly stylized, sharply limited repertoires of local interactions. Agents can either

move or not move; trade or not trade; cooperate or defect; befriend each other or not; kill, not kill, or flee; and so forth. There is of course no logical necessity for agents to be confronted with such binary or threefold choices, but in order for systems to have statistical emergent qualities, all interactions must enter into the calculation of the latter, which means that the significance of the formal alternatives open to agents must be the same across every interaction. Put differently, in Sugarscape-type social systems, the semantics of agent interactions must be “thin.”

A good example of this thinness and its link to statistical emergence can be seen in Epstein and Axtell’s well-known “tag-flipping” model of cultural transmission. When the number of 0s in an agent’s tag string is greater than the number of 1s, the agent is defined as being a member of one group, and vice-versa for the other group. This semantic rule – a mapping of many possible strings into a single group characteristic – is then used to investigate certain distributional properties of that characteristic for the system. Note that the mapping need not be so drastic for such statistical analysis to be performed: one can imagine a rule by which several, rather than half of all, strings were mapped onto a given characteristic (the rule **K** would become a bit more complex but this is not a serious problem). What matters, rather, is the upper limit of this mapping: in no case can a given string be mapped onto more than one characteristic, because in that case the system’s distributional properties would be undetermined.

2.2. Semantically Thin Interactions

In discussing emergence in social systems, it is important to distinguish between two connected but distinct phenomena: repertorial limitations and semantic thinness. It is often argued that everything we know about human beings’ cognitive limitations militates in favor of modeling agents as having sharply limited repertoires of actions open to them. This may well be true (and justified, moreover, by an understandable concern with parsimony), even if, in practice, most persons’ choices seem both wider (3, 4, perhaps many more options open) and narrower (often, we act habitually and do not choose at all) than depicted in standard agent-based models.

However, no matter how large or small the range of choice may be, this has no necessary bearing on the semantics of those choices. In this regard, the question is simply whether a given agent activity has one or more than one meaning for the social system. In Sugarscape-type systems, the first of these options is always the one chosen, i.e., the modeler operates with a thin semantics. Ideally, this option should be a matter of conscious choice rather than of habit or of programming convenience.

In fact, for certain types of social systems, semantic thinness seems plausible as an approximation to reality. (On a strict reading of the ethnomethodological literature discussed in the next section, this thinness should itself be considered as an “achievement” made possible by bracketing much of the thickness of many interactions.) For example, from the standpoint of markets, many interactions map reasonably onto highly limited alternatives: buying or refusing to buy; keeping merchandise or returning it; etc. Similarly, many political interactions have an exceedingly thin semantics: a ballot is either marked for one candidate, another candidate, some third candidate, or not marked at all. (Of course, as we recall, the

mapping rules for this determination are themselves ambiguous and subject to manipulation.) What seems to be the case is that when local interactions take place in an anonymous or semi-anonymous fashion, against the backdrop of a social system characterized by thousands or millions of such interactions, the assumption of thin semantics is not unreasonable.

3. Emergence in Thick Social Systems

3.1. The Semantics of Thickness

Many of the interactions in which we engage are with people whom we either know well or at least expect to have numerous future interactions. This is typically the case in small groups, such as friends, or workplace colleagues, or, shifting to other kinds of agents, regional clusters of national states. In these cases, familiarity makes possible a kind of coded quality to the interactions: the participants know each other well enough to give a completely different meaning to the same behaviors. Such polysemy, to use the technical term, is often quite striking [Winograd 1985]: the same combination of words and gestures can be used in massively different ways. For example, when one friend repeats an expression to another, the expression often takes on a different significance for both interlocutors (and for any other friends who happen to be present) the second time than it did the first; and it may change meaning yet again a third time.

Such polysemy is always a logical possibility in any interaction. However, it is particularly prevalent in a small-group context because in those cases the interactions are often less stylized and more collaborative than in anonymous exchanges. The point about stylization is easy to see (it is important not to conflate it with quasi-ritualistic interactions, such as neighbors who choose to use the same greetings to each other every day); but the point about collaboration is less evident. At issue here is what both ethnomethodologists [e.g., Garfinkel 1967] and conversation analysts [e.g., Sacks 1992] call the achieved quality of interaction. In order for an interaction to be of a particular sort for the participants, each participant has to have his or her background assumptions about the nature of the interaction verified by the others. If, most of the time, this is not problematic, the ease with which that verification can be disrupted indicates just how much work it takes for even routine interactions to “succeed.”

Much the same can be said about conversations. In order for one interlocutor really to converse with another, both have to attend to what the other says and, again and again, say things which are germane (they may be substantive disagreements, but these still are germane) to what has just been said. Given the ease with which new topics can be introduced, this is an achievement of a high order and calls for extensive and continuous collaboration between the speakers.

Seeing interactions in this way highlights the extent to which, at any given moment, the participants in thick interaction have to work together to “fix” the interaction as being of a particular type (e.g., an argument; a game; a brainstorming session). The longer the participants have known each other, and the more they interact in front of others [Simmel 1950], the greater the number of meanings onto

which particular actions can be mapped. It thus follows that to represent these types of local interactions as semantically thin is to distort their significance in ways which fundamentally misrepresent their nature [Schegloff 1997].

3.2. Modeling Thick Interactions

As a technical matter, modeling thick interactions poses several problems. First, however limited the repertoire of agent acts may be, each of those acts can be mapped onto some much larger set of meanings for the social system. To specify this latter is a time-consuming undertaking, requiring either a previously worked out set of categories (e.g., a dictionary of speech acts) or else preliminary empirical work, in a particular setting, aimed at establishing the most standard types of meaning characterizing certain interactions. The second of these options, which is preferable for reasons of verisimilitude, in turn requires an extensive corpus of empirical material.

Second, any agent-based model must of necessity specify transition probabilities for moving from one state to another. The larger the number of meanings, the larger the number of transition probabilities which need to be specified. Unless one knows the particular interaction type well, specifying many of these probabilities is very much a guessing game. Indeed, for many classes of thick interactions, such as face-to-face conversations, a highly detailed, turn-by-turn account, seems out of the question. This is why I have argued elsewhere [Sylvan 2003] that only certain features of conversations (e.g., commitment) can be modeled.

Third, whether the interactions in question are dyadic, triadic, or involve still more participants, the interactions are chained together as sequences. For example, consider a diplomatic interaction in which one state makes a proposal to several of its allies. The latter need to respond, but then, in the next "turn," any of the states (including the most recent responders) can follow up on the response. Ignoring face-to-face interactions, even diplomatic exchanges carried out in written form often go on for anywhere from 5 to 20 turns. Modeling approaches (e.g., argument analysis [Rescher 1977]) do exist for capturing this back-and-forth but have not yet been extended to a multiplicity of agents engaging in many chained interactions.

3.3. Complexity and Emergence

Let us now return to the more general question of social systems linked to thick base interactions. What precisely is the nature of these systems? To begin with, recognize that small groups are quite different from populations. For participants, groups of which they are members have a real significance lacking in populations. Within groups, it is possible to enjoy prestige or be ashamed, to fight with others or to socialize. Such group-oriented activities and emotions are simply not possible in the context of a population: the latter is not of any social or affective relevance to most individuals. For example, one can feel embarrassment over one's behavior in front of friends or colleagues; to do so with respect to strangers, or with people whom one expects never to meet, is much harder. In other words, groups are relevant as such in ways not possible for populations.

This in turn means that when groups act (as, say, a group of friends going to the movies or a group of states going to war), these actions are of relevance to their members. Note that the members need not themselves all join in the group's action, at least in the same way (for example, small states may not be have naval vessels to send to a blockade); what matters is that the group's activities are important to the members, very much in the same way as the above point about significance and emotions.

Taken together, these two points mean that groups serve as the filter through which thick interactions are meaningful. The meaning of such interactions is precisely the collaborative categorization (e.g., as prestigious, as immoral, as a power-play, as a grudging acquiescence) of the sequence of actions comprising them by the participants, the latter acting as knowledgeable and bona fide members of a group. In this sense, the significance for the group of its members' thick interactions is identical to the significance of those interactions to the participants. Hence, thick local interactions are already emergently complex, and there cannot be additional socially relevant features to groups. (Obviously, one can still perform statistical calculations on semantically identical interactions, but this is not of any social significance for the participants.) Complexity in thick social systems is organized all the way down; or, one might say, local-ness is present all the way up.

One implication of this argument is that social systems fall into two classes. Both are self-organizing and complex by almost any definition; but their characteristics and the types of models they call for are very different. To treat groups as if they were populations is unfortunate from the standpoint of both groups and populations; it flattens out much of the analytical – and political – and moral – intricacy of social life.

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Chapter 40

Comparing the dynamics of stomatal networks to
the problem-solving dynamics of cellular computers

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1 Introduction

Is the adaptive response to environmental stimuli of a biological system lacking a central nervous system a result of a formal computation? If so, these biological systems must conform to a different set of computational rules than those associated with central processing. To explore this idea, we examined the dynamics of stomatal patchiness in leaves. Stomata—tiny pores on the surface of a leaf—are biological processing units that a plant uses to solve an optimization problem—maximize CO_2 assimilation and minimize H_2O loss. Under some conditions, groups of stomata coordinate in both space and time producing motile patches that can be visualized with chlorophyll fluorescence. These patches suggest that stomata are nonautonomous and that they form a network presumably engaged in the optimization task. In this study, we show that stomatal dynamics are statistically and qualitatively comparable to the emergent, collective, problem-solving dynamics of cellular computing systems.

2 Stomatal Networks

Stomata are pores on the surfaces of leaves that permit the exchange of gases between the inside of the leaf and the atmosphere. In most plants, stomata are between 30 and 60 μm long and occur at densities between 50 and 200 per mm^2 . Figure 1 shows an image of a typical stomatal network. A stoma (singular) consists of two guard cells that change their shape, as a result of changes in internal water content via osmosis, thereby creating a pore of variable aperture. Gases diffuse through the open stomatal pores. For example, CO_2 enters the leaf, permitting photosynthesis to occur. At

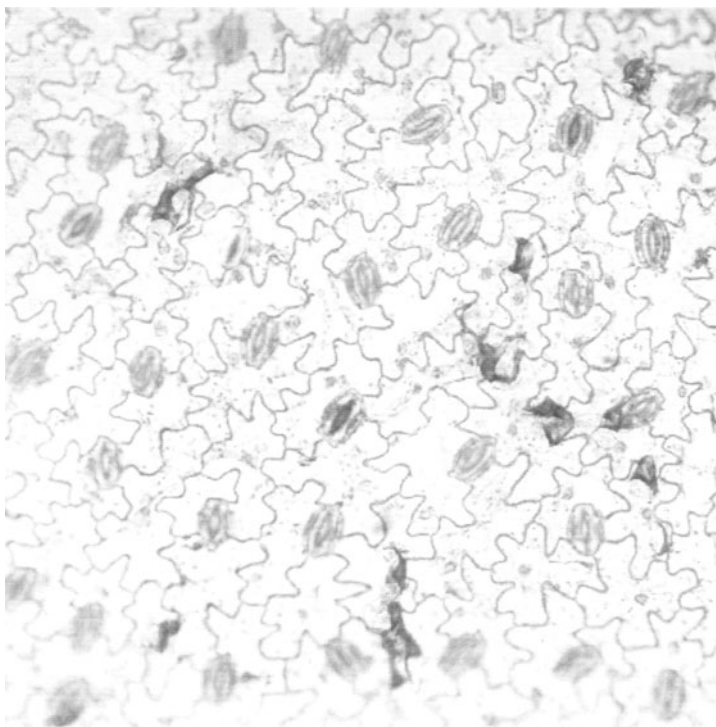


Figure 1: Stomatal Network. The image (taken with a confocal microscope) shows stomata (the bean-shaped structures) separated by epidermal cells on the surface of a *Vicia faba* leaf. In this figure, the stomatal pore apertures are about $2\text{ }\mu\text{m}$ wide.

the same time, water vapor escapes. Excess water loss can have serious detrimental consequences for a plant, so plants are faced with a problem: under a given set of environmental conditions, how open or closed should the stomatal pores be? Plants solve this problem on a daily basis by solving what has been formalized mathematically as a constrained optimization problem [5].

Traditionally, the constrained optimization model of plant biology treats

stomata as autonomous units that respond independently to such environmental stimuli as light, CO_2 , humidity, and H_2O stress. In the traditional formulation, the model predicts that, as long as environmental changes are sufficiently slow, stomatal conductance, g (determined primarily by aperture), varies as environmental conditions change such that $\partial A / \partial G \propto \partial E / \partial g$ (where A is the rate of CO_2 uptake and E is the rate of water loss). It also predicts that the spatial distribution of g should be essentially uniform when environmental conditions are spatially uniform, varying only because of small structural differences in stomata. It has been shown, however, that groups of tens to thousands of stomata can behave drastically differently from stomata in adjacent areas even when environmental conditions are the same everywhere [20, 3, 13, 14].

This spatially heterogeneous behavior is called stomatal patchiness. Stomatal patchiness can be dynamic, with complicated and apparently unpredictable spatial and temporal variations appearing over the leaf surface. Figure 2 shows an example of stomatal patchiness with constant, spatially uniform environmental conditions. The figure, taken in the near infrared, is of chlorophyll fluorescence. Under carefully controlled conditions, chlorophyll fluorescence can be interpreted in terms of stomatal conductance [8, 12, 21]. Stomatal patchiness is inconsistent with the constrained optimization model. Nevertheless, it has been observed in over 200 species [3]. Experiments have demonstrated that stomata can interact locally via hydraulic forces mediated by the epidermal cells between the stomata. Such forces may provide a mechanism for producing and sustaining the coordinated, stomatal behavior observed in patchiness [10, 15, 17].

Stomatal patches are often initiated by changing external humidity. In experiments that we have conducted where an abrupt, spatially uniform

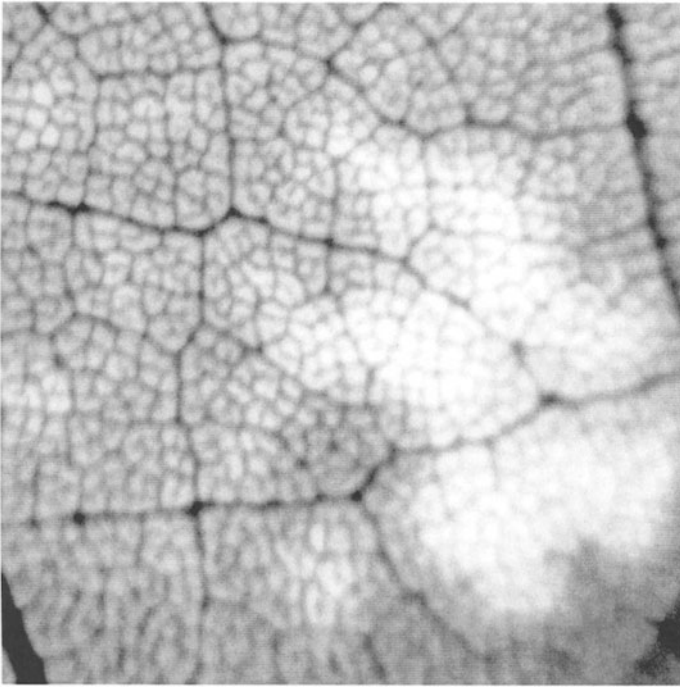


Figure 2: Patchy stomatal conductance. In this chlorophyll fluorescence image of a Cocklebur (*Xanthium Strumarium*) leaf, open stomata appear as dark areas and closed stomata appear as light areas (the veins do not contain stomata). The area shown is 2.54 cm $\times$ 2.54 cm, and contains over 100,000 stomata.

humidity decrease is applied to the leaf, we observe a variety of stomatal responses. In each case, the experimental region of the leaf starts in what appears to be a uniform steady state, with stomata approximately uniformly open. As a result of the applied humidity drop, stomata tend to close. How this closing is achieved, however, is remarkably variable. Often, all stomata tend to close more-or-less uniformly. In these cases, no patches are observed. Sometimes patches form for a brief period, then quickly disappear. In rare instances, patches persist for hours and display rich dynamics. Which of the behaviors occurs in any one experiment is never predictable. The variability we observe suggests that stomatal dynamics is exquisitely sensitive to microscopic conditions that we cannot directly control—a situation that is reminiscent of space-time systems with self-organizing dynamics [1]. We presume that, in our experiments our plants start with a roughly uniform g_i , predicted by constrained optimization. After we lower the humidity, our plants presumably seek out a new, optimal g_f . We are interested in how the transition from g_i to g_f occurs, and the role (if any) patches play in it.

3 Cellular Computer Networks

An artificial cellular computing system consists of individual units, cells, usually arranged in a regular one- or two-dimensional lattice. Each cell is connected to some subset of other cells in the system. The states of the cells are updated simultaneously according to a deterministic rule. Depending on the degree of connectivity and the treatment of time, space, and state, a cellular computer can be categorized as a neural network (NN), a coupled map lattice (CML), a cellular neural network (CNN), or a cellular automaton (CA) (see Table 1).

Table 1: Cellular Computer Networks. A categorization of different artificial cellular computer types based on their connectivity and treatment of space, time, and state. C=continuous; D=discrete; E=extensive; L=limited.

Model Type	Space	Connectivity	Time	State
Neural Network	D	E	C	C
Coupled Map Lattice	D	E or L	D	C
Cellular Neural Network	D	L	C	C
Cellular Automaton	D	L	D	D

Cellular computing systems can perform global computational tasks. Depending on the degree of connectivity, the completion of that task can be non-trivial. For example, the performance of a global computation by an extensively connected network, where at any moment each cell has access to information from the entire system, is relatively simple. On the other hand, the same task performed by a strictly locally connected network, where at any moment each cell has access to a very limited amount of information from the entire system, is difficult. If the global behavior is not explicitly defined by the deterministic behavior of individual network units then the computation is said to be emergent [6]. It has been shown that, in some locally connected CA that perform emergent computation, the global task is accomplished by patches of information coherently propagating over large distances [7]. In these example systems (in which information is processed strictly locally), global computation is achieved because distant regions of the system can communicate via coherent patch propagation.

An instructive example of this is the density classification task performed by a two-state CA [9, 7, 19]. In one version of this task, the CA starts

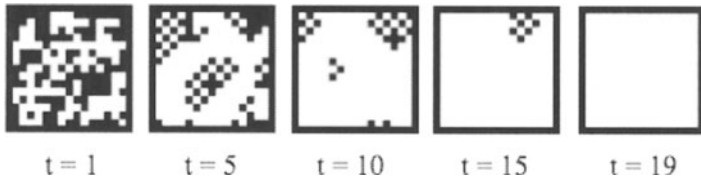


Figure 3: Density Classification by a 2D CA. The configuration at $t=0$ for this 15 by 15 lattice is a random distribution of 1s (white) and 0s (black) with $> 50\%$ of 1s. As time progresses the CA evolves to a steady state of all 1s, indicating that 1s were initially in the majority.

with any initial distribution of 0 and 1 states. The density of this initial configuration is said to be classified if the CA eventually evolves to a state of all 1s if the initial configuration had more 1s than 0s, and to all 0s, otherwise. Figure 3 shows an example of a two-dimensional CA performing density classification. In this CA, each cell shares information with only a few of its nearest neighbors, yet the system as a whole manages to correctly assess that 1 was initially the majority state. No cell individually performs the density classification task in the CA shown: the global result emerges from the strictly local interaction of the component cells. Note that, shortly after the CA in Figure 3 begins to evolve, patches form and move coherently across the CA space.

In general, the farther the initial density is from 0.5 the more quickly and more accurately a density classifier CA will perform the classification task. For densities close to 0.5, the task becomes more difficult, though some CAs still perform fairly well even under these circumstances. We have made an exhaustive study of the behavior of very good 1D and 2D density

classifier CAs for initial densities near 0.5. In our study, we start each time with exactly the same macroscopic initial density but with different microscopic configurations. In the vast majority of instances, these good classifiers quickly achieve a correct steady state. Much less frequently, the CAs take an inordinately long time (if ever) to reach steady state. The difference between two initial configurations that lead to rapid and protracted transients can be as little as two cells. Which initial configurations produce long transients is never predictable. In other words, density classifier CAs exhibit sensitive dependence on the microscopic details of their initial configurations.

4 A comparison of stomatal networks and cellular computer networks

Our discussion of stomatal networks and cellular computers identifies a number of suggestive similarities. Both are able to perform sophisticated global tasks even though distantly separated parts of the respective systems are not directly connected. Both show evidence of extreme sensitivity to microscopic system details. Both manifest dynamic patchiness, which, in the case of cellular computers, at least, is the mechanism by which global problem solving is accomplished. One wonders whether these similarities are merely accidental or if there are deeper, more quantitative connections between stomata and cellular computers [11, 16].

To probe this question, we have closely examined some of the statistical properties of the dynamics of these two different kinds of networks. Because stomata have continuous aperture states that change asynchronously and continuously in time, while CAs have discrete states that change synchronously in discrete time, statistical similarities in their dynamics are not

expected *a priori*. On the other hand, both stomata and CAs that compute appear to harbor the same kind of collective behavior that has been observed in simulations of self-organized critical systems [2]. Taking a cue from such simulations, we have calculated Fourier spectra, Hursts rescaled range (R/S) statistics, and event waiting distributions for both stomata and for several 1D and 2D density classifier CAs.

Data for stomatal networks were obtained from chlorophyll fluorescence images (512×512 pixels) from three different experiments during which extended dynamical patchiness occurred. We examined (512 entry) intensity time series for each of 50,000 randomly chosen pixels in our data sets. From these we calculated Fourier spectra and a summed power spectrum. The same data were used to calculate the Hurst R/S statistic. We defined an event as an unusually large change in pixel intensity (for a more detailed description see [18]) and calculated the distribution of time between successive events at each pixel.

The same statistics were calculated for 1D and 2D density classifier CAs. A good density classifier typically reaches steady state in a time that is too short to produce reasonable statistics. Thus, to protract the dynamics, we injected low amplitude white noise in the form of occasional random state flips. This perturbation introduces spurious high frequency variations in the dynamics, so care has to be taken to filter out its effects. Event waiting times were extracted from examples of unusually long, but unperturbed, transients. We defined an event in these studies as a change in patch type at a cell, specifically, as a time series of 1111 followed by a 0, or 0000 followed by a 1, or 1010 followed by a 0, or 0101 followed by a 1.

A summary of the statistical results is presented in Table 2. The spectral densities, $S(f)$, of the dynamics of all three network types (stomata,

Table 2: Statistical Summary. A summary of the statistical properties of stomatal networks and locally connected density classifying CAs that exhibit patches during the problem-solving process. P_F is the exponent of the power law expression $S(f) \propto f^{-P_F}$ fit to the Fourier spectra. H is the exponent of the power law expression $R/S \propto d^H$ where R/S is Hurst's rescaled range statistic and d is the time delay. P_W is the exponent of the expression $F_W \propto W^{-P_W}$ where F_W is the frequency of the waiting-time and W is the waiting-time. ** insufficient data to calculate this statistic.

System	P_f	R^2	H	R^2	P_w	R^2
Stomatal Network	1.94 ± 0.10	0.99	0.60 ± 0.03	0.94	1.15 ± 0.21	0.93
1-D CA	1.98 ± 0.12	0.99	**	**	1.77 ± 0.23	0.91
2-D CA Case 1	1.99 ± 0.11	0.99	0.54 ± 0.02	0.99	2.22 ± 0.14	0.96
2-D CA Case 2	2.16 ± 0.12	0.99	0.60 ± 0.05	0.96	1.96 ± 0.11	0.97
2-D CA Case 3	1.91 ± 0.12	0.99	0.44 ± 0.05	0.96	2.73 ± 0.24	0.92
2-D CA Case 4	1.84 ± 0.17	0.99	0.35 ± 0.08	0.96	2.35 ± 0.19	0.93

1D and 2D CAs) have extended regions that are well fit by a power law, $S(f) \propto f^{-P_F}$, with exponents $P_F \sim 2$. The Hurst exponent, H , of the power law expression $R/S \propto d^H$ (where d is the time delay) should be related to the spectral density exponent by $P_F = 2H + 1$. The calculated values of P_F and H for the 2D CAs we examined and for our stomatal networks fit this relationship well. The waiting time frequency distributions for the three network types are fit well by a power law, $F_W \propto W^{-P_W}$. In studies of self-organized dynamics, it is found that the value of P_W depends sensitively on the specific details of the system [4]. It is therefore not surprising that P_W for stomatal networks and density classifying CAs might be different. What is surprising is that these distributions are all power laws. The results presented here are strong evidence that stomatal networks and cellular computers are dynamically close cousins.

5 Conclusion

Plants plausibly achieve an optimum stomatal aperture for a given set of environmental conditions. When a plant is presented with a difficult problem (e.g., an abrupt change in humidity), groups of stomata can form collective dynamical patches, contrary to the constrained optimization model of plant biology. We argue that the qualitative and quantitative features of stomatal patches are essentially indistinguishable from those found in locally connected cellular computers that perform global computational tasks. This leads us to conjecture that the reason so many plant species exhibit stomatal patchiness may be that, through their stomata, plants are performing a sophisticated kind of problem solving that is similar to emergent computation. Unambiguous resolution of this conjecture awaits the development

of sharper tools than now exist for quantifying computation, especially as it exists in natural systems.

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Chapter 41

A New Approach to Ecological Risk Assessment: Simulating Effects of Global Warming on Complex Ecological Networks

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1. Introduction

1. 1 Ecological Risk Assessment

The field of Ecological Risk Assessment (ERA) has been under development since the 1970s. Early ERA borrowed basic concepts from human health risk assessment (HRA) methodology [NAS 1983]. However, because of the nature of an ecosystem, there is a fundamental difference between HRA and ERA. In an HRA, the only receptor is a single human being and the concerned endpoints are always associated with human health issues, such as the risk of cancer. In ERA, however, entire populations, communities and ecosystems are at risk, and ERA must rigorously assess these more complex and larger scaled concerns. Many investigators have attempted to develop a new paradigm for ERA that can deal with this intrinsic distinction. Currently, a six-step framework is now widely used by the U.S. EPA and its contractors. This new paradigm is characterized by: (1) receptor identification, (2) hazard identification, (3) endpoint identification, (4) exposure assessment, (5) dose-response assessment and (6) risk characterization [Lipton *et al.* 1993, Suter 1993]. The six-step framework identifies receptors at risk, possible hazards related to certain receptors, and chooses appropriate assessment and measurement endpoints [Suter 1990]. While the additional receptor and endpoint identifications improve on the

traditional framework, single-species laboratory toxicity tests typically estimate ecological responses simply by predicting an environmental concentration associated with a certain stressor divided by the no-observed effect concentration (NOEC) for that stressor. This “Hazard Quotient” (HQ) approach ignores interactions between species that are critical to the functioning of communities and ecosystems.

1.2 Shortcomings and Challenges of Current Ecological Risk Assessment

As noted above, the major shortcoming of any ERA is that it ignores most, if not much, of ecology. Ecology focuses on relationships among species and interactions among species and the environments they live in. A well-developed ERA should focus on the structure (e.g., food-web structure) and function (e.g. biomass production or decomposition) of communities and ecosystems [Burger and Gochfeld 1992]. However, due to the ecosystem complexity and limited information, ERA in practice typically focuses on toxicity at smaller scales of biological organization, such as physiological mechanisms of toxicity and the responses of discrete endpoints in a single species to toxicant exposure [Preston 2002]. This approach to ERA employs a linear, reductionist and determinist paradigm that considers risks to each species to be independent of one another and determined by “causal” relationships inferred between input and output, such as dose and response [Kastenberg 2002]. Another major shortcoming is the absence of predictive tests [Holdway 1997] stemming from simplistic methods employed in the ERA. One prevalent method relies on single-species acute and chronic toxicity test data obtained in the laboratory to predict population impacts of environmental stressors in the field. However, such predictions are not field tested. Also, little if any effort is expended on understanding how estimates of toxicity vary among different environmental contexts. Prediction of long-term population-level effects in the field by applying data from short-term laboratory experiments may be particularly problematic due to the large discrepancy between the spatiotemporal scales of the experiments and the predictions they generate [Martinez and Dunne 1998]. Ecotoxicologists have been facing the challenge and working on developing a more holistic approach to ERA. Both the exceedence profile (EP) [Solomon and Takacs, 2001] and the potentially affected fraction (PAF) methods illustrate a relationship between the proportion of species affected and the likelihood that their response concentrations to certain toxicant will be exceeded. The strength of the PAF method is that it considers multiple-species, instead of single-species in an ecosystem. However, species interactions, especially those that depend on species exposed to higher than NOEC levels, are not addressed well. Some mesocosm studies have estimated effects of toxicants on small-scale ecosystems. These mesocosm studies can observe both direct and indirect effects on multiple species and inform ERAs beyond information derived from laboratory single-species toxicity data. However, the mesocosm studies are almost always conducted after toxicant releases and are applied to specific species and areas, such as lakes. This limits more general understanding of ecological risks to wide varieties of ecosystems and species.

We propose a novel and more holistic *in silico* complement to ERAs that simulates the structure and dynamics of complex ecological networks to generally estimate and predict the risk under environmental stressors, such as global warming to

entire communities including species' extinction risks. So far, such holistic effects of global warming that account for species' interactions have been poorly studied. In this paper, our main objective is to examine the persistence of community structure and species under a warmed climate and to provide a more synthetic, integrated, and holistic model to help decision makers and the public learn more about ecological risks associated with environmental stressors.

2. Approach

2.1 Food-web and Trophic Dynamics Models

Our *in silico* approach combines models of food-web structure [Williams and Martinez 2000] and trophic predator-prey dynamics [Yodzis and Innes 1992] with competitive consumption of multiple limiting abiotic resources by producer species [Tilman 1982, Huisman and Weissing 1999]. A detailed description of the synthetic model is given in Brose et al. (in press). Here, we briefly describe the model's basic components including the "niche model" of network structure and the bioenergetic model of feeding and consumer growth dynamics.

The network structure of the food webs are constructed by the stochastic "niche model" that uses species richness (S) and directed connectance (C , number of directed feeding links divided by S^2) as input parameters. The niche model hypothesizes that food-web structure is a result of a particular arrangement of a one-dimensional community niche space where all species and their diets are located as described in Figure 1.

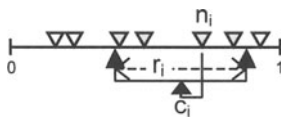


Figure 1. Niche model diagram. S (trophic species richness, here $S = 7$, shown by inverted triangles) and C (connectance) are set at the observed values for the empirical web being modeled. The niche model assigns each of S species a uniformly random "niche value" $0 \leq n_i \leq 1$ that establishes each species' location in the community niche. Each species is then assigned a beta distributed feeding range $0 \leq r_i \leq 1$ with a mean equal to connectance ($C=L/S^2$). Each i th species consumes all species within its r_i which is placed on the niche by choosing a uniformly random center (c_i) of the range between $r_i/2$ and n_i . The species with the lowest n_i is assigned $r_i = 0$ so that each "niche web" has at least one basal species. All other species that happen to eat no other species are also basal species.

Following previous works [McCann and Yodzis 1994, McCann and Hastings 1997, McCann et al. 1998, Brose et al. 2003], we use a bioenergetic consumer-resource model for the species' consumptive interactions that has been recently extended to n species [Williams and Martinez 2001]. The rate of change in the biomass, M_i of species i changes with time t is modeled as:

$$\frac{dM_i(t)}{dt} = G_i(R) - x_i M_i(t) + \sum_j^n (x_i y_{ij} \alpha_{ij} F_{ij}(M) M_j(t) - x_j y_{ji} F_{ji}(M) M_j(t) / e_{ji}) \quad (1)$$

where $G_i(R)$ describes the growth of producer species; x_i is the mass-specific metabolic rate; y_{ij} is species i 's maximum ingestion rate of resource j per unit metabolic rate of species i ; α_{ij} is species i 's relative strength of consuming species j , which is equal to the fraction of resource j in the diet of consumer i when all i 's resources are equally abundant, normalized to one for consumers and zero for producers, and e_{ji} is the biomass conversion efficiency of species j consuming i . We used a type II functional response, $F_{ij}(M)$ that indicates the flow of biomass from resource j to consumer i .

2.1 Climate Change and Metabolic Rates

In this study, we consider a single environmental stressor, temperature change due to a warmed climate, by focusing on the effects increased temperature on species' metabolic. Earth's climate has warmed by approximately 0.5 °C over the past 100 years [Pollack *et al.* 1998], and global warming is an ongoing process. The Intergovernmental Panel of Climate Change (IPCC) (2001) has projected the mean global surface air temperature to increase by 1.4 °C to 5.8 °C from 1990 by 2100, with the magnitude of the increase varying both spatially and temporally. Coastal ocean temperature increases are expected to be slightly lower than the IPCC projected increases for land, but are still expected to rise measurably. This increase in temperature causes increases in species' metabolic rates [Gillooly *et al.* 2001]. Given that these metabolic rates define the species' expenditure of energy on maintaining themselves – their cost of life – we hypothesize that increased metabolic rates might severely impact their extinction risks.

Gillooly *et al.* (2001) proposed that species' metabolic rates depend on their body-sizes and temperatures in a highly predictable manner. The metabolic rates, B , scale with body mass M as $B \propto M^{3/4}$ so that their mass specific metabolic rate equals $B/M \propto M^{-1/4}$. Temperature governs metabolism through its effects on rates of biochemical reactions. Reaction kinetics vary with temperature according to the Boltzmann's factor $e^{-E/kT}$, where T is the absolute temperature (in degrees K), E is the overall activation energy, and k is Boltzmann's constant. When considering both species' body mass and temperature dependence of the whole organism, the metabolic rate can be derived by

$$B = B_0 M^{3/4} e^{-E/kT} \quad (2)$$

In Equation (2), B_0 varies according among taxonomic groups and metabolic-state-dependent normalization constant, and M is the body mass of an individual [West *et al.* 1997, Gillooly *et al.* 2001]. T is the body temperature of organisms, at which different biochemical reactions occur. For ectotherm species – invertebrates and ectotherm vertebrates, T is nearly equal to the environmental temperature [Savage *et al.* 2004]. Equation (1) fits metabolic rates of microbes, ectotherms, endotherms, and plants in temperatures ranging from 0° to 40°C [Gillooly *et al.* 2001]. When the temperature T changes from T_1 to T_2 , metabolic rate B will change from B_1 to B_2 , and the proportional change in metabolic rates, ΔB , can be derived by

$$\Delta B = \frac{B_2(T_2)}{B_1(T_1)} = \frac{B_o M^{3/4} e^{-E/kT_2}}{B_o M^{3/4} e^{-E/kT_1}} = \frac{e^{-E/kT_2}}{e^{-E/kT_1}} = e^{\frac{E}{k} \left(\frac{T_2 - T_1}{T_2 T_1} \right)} \quad (3)$$

We assume that body mass is the same before and after the temperature change. ΔB depends on $\Delta T = T_2 - T_1$, and the initial temperature T_1 . Therefore, if T_1 and ΔT are known, equation (3) can be used to predict metabolic rates.

2.2 An Example for Community Risk Assessment

We simulate the response of *in silico* species and complex ecological communities to global warming and the subsequent increase of the species' metabolic rates as an example in order to demonstrate the framework for community risk assessment we proposed in the previous section. Numerical integration of 30-species invertebrate food webs including eight producer species and 135 trophic interactions (connectance = 0.15) over 2000 time steps yields long-term predictions on community-level effects. The model parameterization assumes invertebrate species, predators that are on average ten times larger than their prey, and producer species with a relative metabolic rate of 0.2 in model cases without global warming effects. The sensitivity of the simulation results to these assumptions will be studied elsewhere. In particular, we address changes in persistence, i.e. extinction risk, for species in general and for producer species (species without prey), consumer species (species with prey) and omnivores (species feeding on multiple trophic levels). Furthermore, we study changes in food-web structure in terms of connectance (links/species²). To study the effects of global warming, we compare numerical integration results averaged over 50 replications with and without increases in metabolic rates that are subsequently indicated by the subscripts 'warm' and 'const', respectively. For instance, proportional change in species extinction risks, ΔR due to global warming are calculated as

$$\Delta R = 1 - \frac{R_{warm}}{R_{const}} \quad (4)$$

where R is species richness. R_{warm} is the species richness after a temperature increase and R_{const} is the species richness in the benchmark case in which the global temperature remains constant at its currently observed values. The proportional changes in the other dependent variables are calculated similarly.

To help understand our model framework, we examined the model's sensitivity to temperature change. Three climate change scenarios are studied: the anticipated "best-case scenario" minimally increases global temperature by 1.4 °C, the "average-case scenario" increases global temperature by 3.6 °C, and the "worst-case scenario" increases global temperature by 5.8 °C. Based on these three scenarios and equation (4) with $E/K = 9.15$ for multicellular invertebrates [Gillooly *et al.* 2001], proportional metabolic rate changes are evaluated in Table 1. Simulations concern a thirty-species invertebrate food web living in an area with a 0 °C average annual temperature.

Table 1. Proportional metabolic rate change for three climate change scenarios

Temperature Increase	Proportional Metabolic Rate Change*
1.4 °C	0.017%
3.6 °C	0.044%
5.8 °C	0.070%

* We assume an initial temperature of 0 °C.

3. Quantitative Results and Discussion

The mean values of our dependent variables for the benchmark case ($\Delta T=0$) and each climate change scenario are given and compared in Table 2 and Table 3. For example, with a 5.8 °C temperature increase, 0.2 species die out after 2000 time steps due to the temperature increase in the invertebrate food-web. Total species richness among all scenarios ranges from 24.3 to 23.5 and the proportional change in species extinction risks due to warming (ΔR) ranges from -2.36% to 1.1% under the projected global temperature increases of 1.4 °C to 5.8 °C, respectively. The number of links decreases, then increases from a baseline of 92.3 links to 94.9-88.9 links. The richness of top species ranges from 2.0 to 2.4 and the proportional changes in extinction risks for top species (ΔTop) ranges from 25.2% to 11.1%. The richness of basal species remains at the original number, 8 despite the temperature increases of 1.4 °C to 5.8 °C. In other words, all producer species typically survive the climate warming. Connectance varies from 0.161 to 0.162 as the temperature increases. With global temperature increases of 1.4 and 3.6 °C, species richness are greater than the benchmark species richness. In the worst temperature increase scenario, species richness drops down below 23.7, which indicates a proportional change in species extinction risk, 1.11%.

Table 2. Output parameters from the simulations for three climate change scenarios

Temperature Increase	Species Richness	Connectance (Link/Species ²)	Links	Top**	Basal**
0.0 °C*	23.7	0.163	92.3	2.7	8
1.4 °C	24.3	0.161	94.9	2.0	8
3.6 °C	23.8	0.162	91.8	2.4	8
5.8 °C	23.5	0.161	88.9	2.2	8

* The benchmark case, ** Top = top species richness and Basal = basal species richness.

Table 3. Comparisons between three climate change scenarios and the benchmark case

Temperature Increase	ΔR^* (%)	ΔTop^* (%)	ΔBasal^* (%)	ΔConn^* (%)
1.4 °C	-2.36	25.2	0	1.85
3.6 °C	-0.34	11.1	0	1.21
5.8 °C	1.10	18.5	0	1.56

* ΔR = proportional change of species richness, ΔTop = proportional change of top species richness, ΔBasal = proportional change of basal species richness and ΔConn = proportional change of connectance.

From the above data analysis, we hypothesize that small temperature increases may favor the species richness. However, beyond this range, temperature increases can decrease biodiversity and increase species' extinction risks. In order to understand

better, we simulated the responses to varying the possible change of metabolic rates by 0.01% to 1% based to the temperature range from 0°C to 40°C used in equation (2).

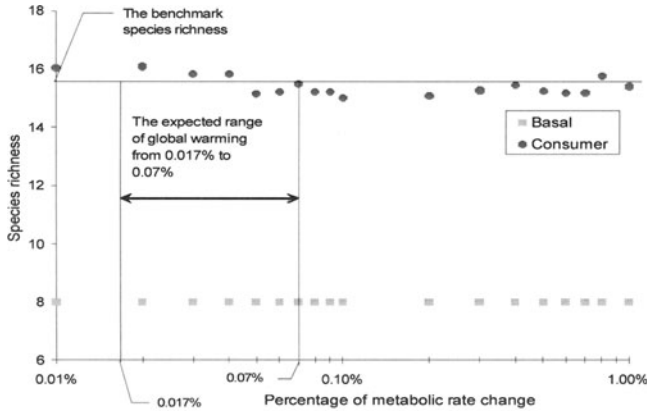


Figure 2. Effect of metabolic rate on species richness for basal (producer) and consumer species with a metabolic rate change range from 0.01% to 1% after 2000 time steps

Figure 2 gives the tendencies of species richness with varying the metabolic rate changes from 0.01% to 1%. The trend in species richness basically suggests that global warming presents very little if any extinction risks to consumer species due only to temperature effects on metabolic rates. Basal species such as plants appear unaffected by increases in metabolic rates while such temperature increases affect consumer's abilities to persist.

Here, we propose a generic framework for estimating and predicting community risks that may be extended to address many other risks such as those posed by toxics in the environment combined with global warming. We have examined how a warmed climate in terms of metabolism change, affects biodiversity and species' extinction risks. Surprisingly, a warmed climate in terms of metabolism change makes minor effects on biodiversity and species' extinction risks, which is not as what we expected. We will explore how different mechanisms, such as assimilation efficiency will affect different ecosystems due to climate change and other stressors. In this paper, we have more simply explored how an invertebrate ecosystem may respond to a warmed climate. However, this is more a description and exploration of our methods rather than a specific prediction of future events. In order to make such predictions, further research will examine more specific food webs, such as invertebrate, ectotherm vertebrate and endothermic vertebrate food webs parameterized for more specific habitats including terrestrial and marine systems in tropical, temperate, and polar climates. Results from these future studies may help scientists to understand, and society to decide, which geographic areas and which habitats and species are most at risk and in need of the most urgent attention and action. Temporal predictions of ecosystem response to external perturbations should be very valuable for predicting

and understanding ecological risks associated with climate change and other anthropogenic effects on ecosystems.

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