

CSUMS Research Project Opportunities

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1 Microbiological Simulations

Current research in nanotechnology seeks to develop microscopic devices to perform specialized medical tasks within the human body, such as delivering drugs to specific targets (such as tumors) or to perform robotic repair work. Such devices may need to “swim” through the bloodstream as part of their function. Much research has been done on how various organisms swim, and one prevalent theme is that the mechanisms (and underlying physics) depends crucially on the length scale of the organism. Fish and sharks swim in very different ways than bacteria because the former move at high Reynolds number while the latter move at low Reynolds number [1], and the relevant forces of interaction with the fluid are quite different in the two regimes. Another important transition happens at the micron scale, below which thermal fluctuations (responsible for Brownian motion [2]) become significant. Swimming in the presence of thermal fluctuations has not been much explored thus far, but Prof. Kramer and collaborators have developed a computational method based on the immersed boundary method [3] for simulating microbiological and microphysical systems where thermal fluctuations play an important role [4, 5]. This method has thus far been applied to study some model systems of intermediate complexity, such as the osmotic pressure exerted by polymer knots confined in a membrane and the speed of transport of a basic molecular motor model [5]. More sophisticated simulations of molecular motors and organelles are contemplated by Kramer and his collaborators, and undergraduates could participate in advancing this research through studies of particular components of such models, particularly the swimming process.

One such example would be the simulation of simple swimming models similar to “Purcell’s swimmer” [6–8], consisting generally of three limbs which move in a periodically prescribed fashion. An important recent variation is a swimmer with an extended linear shape which moves by extending and retracting bead-shaped components [9]. While not as efficient as Purcell’s swimmer, it is more amenable to analysis [10] and may be more relevant for the design of artificial devices that need to swim through narrow tubes like blood vessels. Recent studies have examined how the movements of these simple swimmers should be designed to optimize the swimming efficiency (at low Reynolds number) [11, 12]. The immersed boundary method would allow the study of the effects of flexibility in the limbs [13] and the effects of thermal fluctuations [14]. Because the swimmer models involve the application of active forces, which have been implemented in the deterministic [3] but not the stochastic version of the immersed boundary method, this work would also provide some insight within the context of a simple system into how to model more sophisticated molecular motors such as actin polymerases, which require active force components to model the influence of unresolved chemical interactions (such as ATP hydrolysis).

Fundamental questions students could address with the computations and analysis include: How do thermal fluctuations affect swimming efficiency of specified stroke patterns, particularly those that are optimal in the absence of thermal fluctuations? What stroke patterns optimize swimming efficiency in the presence of thermal fluctuations?

In this project, students would need to familiarize themselves first with the general code (available through http://www.cims.nyu.edu/~paulatz/computational_projects/projects.html) which integrates the underlying differential equations for the fluid and structural degrees of freedom, and develop some portions pertaining to the specific force models for the structures they are simulating. The undergraduates would also be expected to write shorter pre-processing and post-processing codes to set up and analyze statistical quantities of the simulated systems. Mathematical techniques required for the analysis and modeling include differential equations, probability theory, perturbation theory, optimization theory, and fluid mechanics.

2 Stability and Resilience in Ecological System Models

The continued expansion of the human population and its resource consumption has made more urgent the consideration of human activities on the Earth's ecosystem. Disturbances might, beyond their direct effects, precipitate further catastrophic shifts to alternative states of the ecosystem that are less resilient and affect the environments capacity for water purification, carbon storage, and soil renewal [15]. Such indirect impacts mediated by organism populations and their two-way interaction with the environment can be studied through ecosystem models consisting of systems of differential equations for variables describing the environmental condition and the size of important organism populations [16]. Student teams conducting research in this area of Rensselaers CSUMS program would develop both analytic models and computer simulations aimed at improving our understanding of the stability and resilience of ecological systems under the supervision of Prof. Peter Kramer and ecological modeler Prof. Brad Lister in the Department of Biology at Rensselaer. The student projects would advance the state of existing ecosystem models consisting of systems of differential equations of Lotka-Volterra type [17] by incorporating various features which would make the models more realistic and/or allow new scenarios to be explored.

By resilience we mean the degree to which an ecosystem returns to its previous state following perturbations, to which all ecosystems are continually subjected. For example, disease and parasitic infections may sweep through a community, or alien predators or competitors may invade and displace or kill off the native species. Physical disturbances, such as hurricanes, fires, and droughts, can occur over a range of different frequencies, severities, and spatial scales. Under certain conditions, ecosystems can be pushed beyond their limits of resilience and undergo catastrophic shifts into alternative states or chaotic fluctuations. Ecologists have identified a growing number of such catastrophic shifts including desertification in China, dead zones in the Gulf of Mexico, the loss of woodlands in Africa, and the collapse of the Bering Sea food web. Global warming, introduction of alien species, massive deforestation, and the extermination of top predators are pushing many ecosystems towards the edge of collapse. As a natural extension of their work on model ecosystems, students will investigate the effects of various simulated perturbations on ecosystems with different web architectures [18] (including migration of a species between spatial locations [19, 20]), different numbers of species and different levels of information flow. The perturbations will include varying the key environmental variables mentioned above (temperature, pH, nutrients, and moisture),

deleting varying numbers of species from the simulations (i.e. simulating the impact of extinctions), and introducing alien species.

2.1 Stochastic Models for Environmental Perturbations

Typically for a fixed set of environmental variables, the ecosystem can be described a phase portrait with certain stable states, unstable states, limit cycles, chaos, and other dynamical features. As the environmental variables change, so will the phase portrait, and certain environmental changes could create structural changes, such as change of stability of a steady state or the introduction or disappearance of a chaotic regime [18]. Typical stability studies would investigate how the phase portrait of the ecosystem changes as the environmental parameters are varied. This would be adequate if the environmental parameters were simply moved and fixed at new values. But in reality, the environmental variables will fluctuate due to natural and human causes, typically in highly unpredictable ways [21–23]. One question is how well the dynamics of an ecosystem with stochastically fluctuating environmental variables can be inferred from phase portraits with fixed environmental values. Particular interesting cases are those in which the environmental fluctuations move the system between phase portraits with qualitative differences (change of stability of steady states, presence/absence of chaos, etc.) Also of interest is the question of predictability – how does uncertainty about the future conditions of the environment affect the uncertainty of the behavior of the ecosystem. Does unpredictability become amplified or stabilized by the ecosystem dynamics? Current research is also finding interesting ways in which migration of populations affects their resilience to disturbances [19, 20]. Mathematical techniques that could be used in this research include dynamical systems analysis, catastrophe theory, and probability theory.

2.2 The Effects of Information Flow and Decision Making on Ecosystem Dynamics

Living organisms base their strategies largely on the auditory, visual, chemical, and tactile information they receive from their environment. For example, a seed-eating rodent will choose where to forage in a forest based partially on its past experience of where seeds and predators are likely to be found. Existing models of animal behavior assume that the rodent in fact has perfect information about the probabilities of encountering seeds and predators. Since behavioral decisions affect birth and death rates, inclusion of the role of available information will consequently have an impact on population abundance.

Students can investigate the effects of information and decision making on multi-species ecosystems via stochastic dynamic models of individual behavior [24] which are based on optimizing fitness measures based on the information that an organism possesses about its environment. We can begin with relatively simple examples to develop the conceptual approach. We may have a single predator species and a single prey species in a habitat with several patches. Each patch may have variable levels of predators and food, and the prey population will make decisions about which patch to visit based on its past experience with encountering predators and food (rather than the true levels of predator and food in each patch).

For social organisms, one can include the ability for individuals to communicate their experience to others. As a particularly striking example, we may consider foraging strategies for ant colonies.

As the ants explore their environment, they leave trails with chemical signals which indicate to other ants whether they have found food. One can then set up a design problem to optimize the strategy by which ants follow chemical signals. For example, if they always follow a trail, they may get to the food after other ants have eaten it all. So it may pay for the ants to sometimes explore new ground. Through optimizing mathematical models for animal behavior, one sometimes arrives at a strategy close to that which emerged naturally, and then one obtains some insight into why the animal behaves the way it does. When one finds a more optimal strategy than that found in nature, it can be useful in the design of artificial systems and algorithms for solving engineering problems.

The research objective here is largely methodological – how can one incorporate the flow of information within an ecosystem into mathematical models? Some ideas can be drawn from the economic [25, 26], epidemic [27], and dynamical systems literature [28]. This question is already worthwhile being explored on very simple systems, and can lead later to the even more challenging question of how a mathematical model with information flow formulated at the organism level can be coarse-grained into a population level model (such as Lotka-Volterra). Consequently, creative modeling ideas will be central to this research, as will techniques from dynamical systems, probability theory, optimization theory, and stochastic programming.

2.3 Interaction of Food Web Structure and Dynamics

Recent research has shown that food webs, like human social networks, have a small-world structure [29–31], with only one to three links separating the majority of species. Like many complex networks, food webs moreover tend to have a scale free architecture dominated by a small number of hub species that are highly connected to other species in the system [32–34]. While these findings have stimulated a resurgence of interest in food webs, comparatively little is known about how the small world, scale-free structure of ecosystems affects their dynamics [35]. Students will investigate various aspects of this problem by modeling ecosystems with different network architectures using algorithms developed by Barabasi [36]. For example, model ecosystems with small and large degrees of separation can be compared with regard to how quickly and to what extent changes in one part of the web are transmitted to other parts of the web (e.g. information or disease [37]). In a similar fashion, students will compare model ecosystems with different degrees of clustering, different numbers and kinds of hub species, and different slopes for the power laws that describe network architecture.

An important research direction would be to study food web networks which evolve dynamically in response to predator-prey interactions and other ecological interaction laws. Of particular interest would be to investigate how the properties of the dynamically evolving network responds to the ecological interaction laws. Can the small-world and scale-free properties observed in food web networks be obtained naturally through realistic interaction rules? How does the network architecture [18, 38] respond to changes in the rules (amount of predation, level of migration, contact with new species, etc.) [39]? How resilient are the resulting networks to disturbances or catastrophic events [40, 41]?

Probabilistic rules for the network evolution are rather natural given the coarse-grained representation of the populations. An interesting variation would be to study how the dynamics of the spread of a disease depend on the network properties of social contacts [37, 42]. Again, the

network could evolve dynamically in response to the spread of the disease to reflect quarantines, fear, etc. Students could incorporate probabilistic dynamics (relevant for diseases that begin with a relatively small number of people) and examine how the results compare to deterministic models.

2.4 Evolution of Fitness Characteristics in Interacting Populations

The previous topic is concerned with modeling macroevolution – the flourishing or extinction of species in response to their placement in the food web network. Recent papers have also explored mathematical models for microevolution of fitness characteristics within a population. The members of the population are generally tagged by some genetic sequence which determines their fitness properties – in the models the genetic string is relatively short (several bits). Of course if a species evolves in a fixed environment, it will likely tend to evolve characteristics toward an optimal fitness with respect to that environment. More interesting is the case of interacting species where the genetic sequences in the various species may evolve toward a diverse range of fitness characteristics to exploit niches, rather than all species moving toward the same optimal target which could create intense lethal competition.

Particular questions of interest include: How does the structure of the food web network affect the genetic evolution of species in the network? In particular, how does the diversity of the species which result depend on the network structure? How does the overall fitness of the ecosystem, perhaps viewed as resilience to disturbance, depend on its architecture. How are these answers affected if the ecosystem has spatial variations (which could be simply represented in the model through a few spatial patches with varying environmental characteristics)? A more ambitious research program would allow the food web network to evolve dynamically (as above), but the questions posed are already interesting to address in a static food web network.

References

- [1] Henry C. Fu, Thomas R. Powers, and Charles W. Wolgemuth. Theory of swimming filaments in viscoelastic media. *Phys. Rev. Lett.*, 99:258101, December 21 2007.
- [2] Peter Kramer. Brownian motion. In Alwyn Scott, editor, *Encyclopedia of Nonlinear Science*, pages 78–81. Routledge & Kegan Paul, London and New York, 2005.
- [3] Charles S. Peskin. The immersed boundary method. *Acta Numerica*, 11:479–517, 2002.
- [4] Paul J. Atzberger and Peter R. Kramer. Error analysis of a stochastic immersed boundary method incorporating thermal fluctuations. Submitted to *Mathematics and Computers in Simulation*, 2006.
- [5] Paul J. Atzberger, Peter R. Kramer, and Charles S. Peskin. A stochastic immersed boundary method for fluid-structure dynamics at microscopic length scales. *J. Comput. Phys.*, 224(2): 1255–1292, June 10 2007.
- [6] Ali Najafi and Ramin Golestanian. Propulsion at low Reynolds number. *J. Phys.: Condens. Matter*, 17:S1203–S1208, 2005.

- [7] J. E. Avron, O. Kenneth, and D. H. Oaknin. Pushmepullyo: an efficient micro-swimmer. *New Journal of Physics*, 7:234, 2005.
- [8] R. Dreyfus, J. Baudry, and H. A. Stone. Purcell’s “rotator”: mechanical rotation at low Reynolds number. *Eur. Phys. J. B*, 47:161–164, 2005.
- [9] Ali Najafi and Ramin Golestanian. Simple swimmer at low Reynolds number: Three linked spheres. *Phys. Rev. E*, 69:062901, 2004.
- [10] David J. Earl, C. M. Pooley, J. F. Ryder, Irene Bredberg, and J. M. Yeomans. Modeling microscopic swimmers at low reynolds number. *J. Chem. Phys.*, 126:064703, 2007.
- [11] J. E. Avron, O. Gat, and O. Kenneth. Optimal swimming at low reynolds numbers. *Phys. Rev. Lett.*, 93(18):186001, October 29 2004.
- [12] Erik Gauger and Holger Stark. Numerical study of a microscopic artificial swimmer. *Phys. Rev. E*, 74:021907, 2006.
- [13] Rémi Dreyfus, Jean Baudry, Marcus L. Roper, Marc Fermigier, Howard A. Stone, and Jérôme Bibette. Microscopic artificial swimmers. *Nature*, 437(6):862–865, October 2005.
- [14] Ramin Golestanian. Force generation due to fluctuations of media and boundaries. *Modern Physics Letters B*, 18(24):1225–1237, 2004.
- [15] Brad Lister. The resilience of ecological systems. Module produced with Thomson Learning, Inc., June 2006.
- [16] R. M May. *Stability and complexity in model ecosystems*. Princeton University Press, Princeton, 1973.
- [17] Peter Turchin. *Complex population dynamics: a theoretical/empirical synthesis*, volume 35 of *Monographs in Population Biology*. Princeton University Press, Princeton, NJ, 2003. ISBN 0-691-09021-1.
- [18] Gregor F. Fussmann and Gerd Heber. Food web complexity and chaotic population dynamics. *Ecol. Lett.*, 5:394–401, 2002.
- [19] John E. Franke and Abdul-Aziz Yakubu. Periodic dynamical systems in unidirectional metapopulation models. *J. Difference Equ. Appl.*, 11(7):687–700, 2005. ISSN 1023-6198. American Mathematical Society Special Session on Difference Equations and Discrete Dynamics.
- [20] Abdul-Aziz Yakubu and Michael J. Fogarty. Spatially discrete metapopulation models with directional dispersal. *Math. Biosci.*, 204(1):68–101, 2006. ISSN 0025-5564.
- [21] T. Coulson, E. A. Catchpole, S. D. Albon, B. J. T. Morgan, J. M. Pemberton, T. H. Clutton-Brock, M. J. Crawley, and B. T. Grenfell. Age, sex, density, winter weather, and population crashes in soay sheep. *Science*, 292:1528–1531, 2001.
- [22] Nils Chr. Stenseth and Kung-Sik Chan. Nonlinear sheep in a noisy world. *Nature*, 394:620–621, August 13 1998.

- [23] B. T. Grenfell, K. Wilson, B. F. Finkenstädt, T. N. Coulson, S. Murray, S. D. Albon, J. M. Pemberton, T. H. Clutton-Brock, and M. J. Crawley. Noise and determinism in synchronized sheep dynamics. *Nature*, 394:674–677, August 13 1998.
- [24] C. Clark and M. Mangel. *Dynamic State Variable Models in Ecology: Methods and Applications*. Oxford University Press, New York, Oxford, 2000.
- [25] Janusz Miśkiewicz and M. Ausloos. Delayed information flow effect in economy systems. *Physica A*, 382:179–186, 2007.
- [26] Patrick de Fontnouvelle. Information dynamics in financial markets. *Macroeconomic Dynamics*, 4:139–169, 2000.
- [27] Franco Bagnoli. Risk perception in epidemic modeling. *Phys. Rev. E*, 76:061904, 2007.
- [28] X. San Liang and Richard Kleeman. A rigorous formalism of information transfer between dynamical system components. II. Continuous flow. *Phys. D*, 227(2):173–182, 2007. ISSN 0167-2789.
- [29] D. J. Watts and S. H. Strogatz. Collective dynamics of 'small-world' networks. *Nature*, 393(6684):440–442, June 4 1998.
- [30] M. E. J. Newman, A. L. Barabasi, and D. J. Watts, editors. *The Structure and Dynamics of Complex Networks*. Princeton University Press, Princeton, 2003.
- [31] Brad Lister and Carl McDaniel. Food webs: Small worlds in the entangled bank. Ecology 8: Community Structure module, Thomson Learning, Inc., April 17 2006.
- [32] Albert-László Barabási and Eric Bonabeau. Scale-free networks. *Scientific American*, 288: 60–69, May 2003.
- [33] Jose M. Montoya and Richard V. Solé. Topological properties of food webs: from real data to community assembly models. *Oikos*, 102:614–622, 2003.
- [34] Jose M. Montoya and Richard V. Solé. Small world patterns in food webs. *j-theor-bio*, 214(3): 405–412, February 7 2002.
- [35] Robert M. May. Network structure and the biology of populations. *Trends Ecol. Evol.*, 21(7): 394–398, jul 2006.
- [36] Albert-László Barabási and Réka Albert. Emergence of scaling in random networks. *Science*, 286(5439):509–512, 1999. ISSN 0036-8075.
- [37] Robert M. May and Alun L. Lloyd. Infection dynamics on scale-free networks. *Phys. Rev. E*, 64:066112, 2001.
- [38] Carlos J. Melián and Jordi Bascompte. Complex networks: two ways to be robust? *Ecol. Lett.*, 5:705–708, 2002.
- [39] Andreas Pusch, Sebastian Weber, and Markus Porto. Generating random networks with given degree-degree correlations and degree-dependent clustering. *Phys. Rev. E*, 77:017101, 2008.
- [40] Réka Albert, Hawoong Jeong, and Albert-László Barabási. Error and attack tolerance of complex networks. *Nature*, 406:378–382, July 27 2000.

- [41] Réka Albert and Albert-László Barabási. Statistical mechanics of complex networks. *Rev. Modern Phys.*, 74(1):47–97, 2002. ISSN 0034-6861.
- [42] N. H. Fefferman and K. L. Ng. How disease models in static networks can fail to approximate disease in dynamic networks. *Phys. Rev. E*, 76:031919, 2007.