Project description

1 Participants

Name	Role	Institution	Expertise	Previous IGERT experience
Albion Lawrence	PI	Physics, Brandeis	QFT, strings, cosmo, HEP	None
Bulbul Chakraborty	Co-PI	Physics, Brandeis	Cond mat, Stat phys	None
Blake LeBaron	Co-PI	IBS, Brandeis	Finance, macroecon.	None
Paul Miller	Co-PI	Biology and VCCS, Brandeis	Computational neuroscience	0549390, FP
Daniel Ruberman	Co-PI	Mathematics, Brandeis	Low-dim top, gauge theory	None
Mark Adler	FP	Mathematics, Brandeis	Int Sys, Diff Eqs	None
Yaneer Bar-Yam	FP	NECSI	Complex systems	None
Aparna Baskaran	FP	Physics, Brandeis	Cond mat, stat mech	None
Ruth Charney	FP	Mathematics, Brandeis	Geometric group theory, Topology	None
Irving Epstein	FP	Chemistry and VCCS, Brandeis	Phys chem, complex systems	0549390, Co-PI
Jozsef Fiser	FP	Psychology and VCCS, Brandeis	Computational Neuroscience	None
Michael Hagan	FP	Physics, Brandeis	Biol phys, stat mech	None
Matthew Headrick	FP	Physics, Brandeis	QFT, strings, GR	None
Dmitry Kleinbock	FP	Mathematics, Brandeis	Group theory, Dyn sys, num thry	None
Jané Kondev	FP	Physics, Brandeis	Cond mat, biol phys	0549390, FP
Bong Lian	FP	Mathematics, Brandeis	Alg geom, strings	None
John Lisman	FP	Biology and VCCS, Brandeis	Computational Neuroscience	0549390, FP

Abbreviations

Alg Geom: Algebraic Geometry. **Biol Phys**: Biological Physics. **Cond Mat**: condensed matter physics. **Cosmo**: cosmology. **Diff eqs**: Differential equations. **Dyn sys**: Dynamical systems. **GR**: General relativity. **HEP** High Energy Physics. **Int sys**: Integrable systems. **Low-dim. top.**: Low-dimensional topology. **Macroecon**: Macroeconomics. **NECSI**: New England Complex Systems Institute. **Num thry**: Number theory. **Phys. Chem**: Physical Chemistry. **QFT**: Quantum Field Theory. **Stat Phys**: Statistical physics. **VCCS**: Volen Center for Complex Systems.

2 Vision, Goals, Thematic Basis

The 21st century is witnessing a remarkable expansion of quantitative and mathematical approaches beyond their traditional domains, to all disciplines of the natural and social sciences. Progress in the problems at the frontiers of science – such as climate change, disease epidemiology, the origins of the universe, the emergence of cognition, economic forecasting, the theory of elementary particles, and managing and developing energy resources – requires an understanding of phenomenology *and* a strong foundation in advanced mathematical techniques, the latter to enable quantitative analysis of large datasets and to construct predictive models. The growing role of mathematics has created a need for theorists who can apply their strong mathematical training to diverse problems in new areas.

These mathematical techniques transcend disciplines. Furthermore, the problems in a given discipline increasingly require techniques which are outside of the standard toolkit in any one discipline. We can list many examples which illustrate these observations:

- Dynamical systems theory is central to climatology, social dynamics, economics, neuroscience, statistical mechanics, and more; and it ties together symplectic geometry, analysis, differential equations, group theory, and quantum/statistical field theory.
- Physics insights have led to remarkable advances in low-dimensional topology and algebraic geometry. Field theory techniques allow the formulation and computation of topological invariants. String theory leads to the remarkable phenomenon of mirror symmetry, now a cornerstone of algebraic geometry. String theory ideas underpin Perelman's proof of the Poincaré conjecture [1, 2]. On the other hand, these developments have fed back and allowed physicists to perform highly nontrivial computations in supersymmetric quantum field theory and string theory, which led to a revolution in their understanding of the nonperturbative structure of both.
- The mathematics of dynamical stochastic processes underlies the study of glass dynamics, granular systems, financial systems, climate dynamics, and the geometry of 2d phase transitions via the Schramm-Loewner equations [3]. The last subject involves two-dimensional conformal field theories, which underpin string theory.
- Information theory is central to computational neuroscience; to the study of disordered systems [4]; and to the black hole information problem (*cf.* [5]).
- Supersymmetry (SUSY) plays a central role in modern particle physics and string theory. SUSY and its breaking at low energies provides the leading solution to the "hierarchy problem" (explaining the 15-order-of-magnitude gap between the Planck scale and the scale of electroweak symmetry breaking). Supersymmetry has allowed exact computations in quantum field theory and string theory which has uncovered the nonperturbative structure of both. These exact computations have led to new insights into the topology of four-manifolds. SUSY provides a technique for computing averages over quenched disorder. It also emerges naturally in stochastic processes with Gaussian noise and a conservative force, in which context the glass transition may be associated with supersymmetry breaking [6].

The clear lesson from these observations and examples is that theorists in the natural and social sciences who are in constant contact with problems, methods, and solutions outside of their specialty will gain the deepest understanding of the underlying mathematics in their own field and are in the best position to make key innovations. Furthermore, interaction between scientists in different fields is likely to lead to most rapid progress in problems which themselves transcend a given discipline.

These observations are understood by many researchers. Centers such as the Santa Fe Institute and the Princeton Center for the Theoretical Sciences exist to encourage cross-disciplinary interaction between faculty and postdoctoral scholars through a small set of core faculty and medium-term programs. What is lacking is an educational structure which prepares graduate students to work across disciplines in a productive way. We would also like to create a context which continually encourages serendipitous discovery. The goals are best met by embedding interdisciplinary activities into the everyday life of a research university.

This IGERT proposal, therefore, redesigns the education and training of future theorists to generate a cross-disciplinary experience, while maintaining their elite core-discipline training. We propose to create a network of faculty and graduate students across the natural and social sciences, connected by research rotations, breadth requirements in advanced coursework, shared seminars, and intensive summer institutes. Through these, the students will acquire facility with problems and approaches outside their discipline, and perhaps as importantly, develop a shared language so that they can best access needed expertise outside their field, or collaborate across disciplines. The constant contact between theory faculty and students in the program should provide fertile ground for innovation.

Our hope is that the IGERT will be the seed for lasting institutional changes at Brandeis. Thus, we propose to re-engineer components of the Brandeis curriculum to serve a more interdisciplinary approach to science. Our goal is also to create a lasting network of faculty, linked by a variety of shared mathematical techniques, who are trained to deliver this new curriculum.

Brandeis is ideally positioned to launch this effort. The Provost and the Board of Trustees have approved an integration of the sciences into a Division of Science. The Division will allow Brandeis to streamline and coordinate its offerings for undergraduate and graduate programs, and it will facilitate attempts to generate new interdisciplinary initiatives. This development follows a research-driven, highly interdisciplinary culture within the sciences. Brandeis occupies a unique position as a small, high-quality research university, with less than 3500 undergraduate and approximately 2000 postgraduate students. The small size has catalyzed an unusually collegial and interactive atmosphere with low barriers between disciplines, as evidenced by Brandeis' success in competing with much larger research universities for competitive interdisciplinary grants (e.g. NSF-MRSEC, HHMI-QB, NSF-IGERT, NSF-FRG). Brandeis has also had great success in leveraging these grants to consolidate interdisciplinary research and teaching efforts. There are long-standing ties between mathematics and physics, between physics and chemistry, and between the physical and life sciences. This proposal uses graduate education and research to continue this integration in a new direction, by focusing on theoretical research and by tying together the natural and social sciences.

The educational goal of this IGERT is to create a generation of students who are prepared to pursue careers in academia, industry, finance, and public policy, in which they face a broad spectrum of problems rooted in different fields of science. In this regard, the New England Complex Systems Institute (NECSI), located nearby in Cambridge, MA, is an ideal partner. The NECSI has been a pioneer in socially relevant applications of advanced mathematical methods, including policy responses to the economic crisis (influencing actions by the Financial Services Committee), healthcare policy (advising the Centers for Disease Control and Prevention), international development (advising the World Bank and Asian Development Bank), and military organization and transformation (advising multiple branches of the US and Canadian military and military engineering organizations). Co-PI Blake LeBaron and Faculty Participant Irv Epstein are both co-faculty at NECSI, so there is already a natural connection. We have therefore partnered with the New England Complex Systems Institute (NECSI) to provide education, internships, and potential research projects for our students.

Our proposed training program builds on existing disciplinary research and education efforts. The students will still generally pursue their primary education within their home departments, and choose their PhD advisor from this department. This will provide depth and a solid foundation to their education. Our intent is to provide structure that *complements* students' traditional disciplinary instruction. Since theoretical research often progresses on shorter time scales than laboratory research and it is hard to predict all potential interdisciplinary opportunities, our program is broad in scope. A broad education is possible and necessary because a set of closely related mathematical themes and structures that recur in the theoretical sciences and in our research: complex systems; stochastic processes; quantum and statistical field theory; and geometry and topology. We describe these themes and how they connect to the IGERT disciplines below.

Our program will create a unique environment in which students receive a broad education in theoretical science which is nonetheless tied to their core discipline through these recurring structures. While there are exciting opportunities at many institutions for students to work on specific problems on the boundary between disciplines, our proposal ensures that students are fully trained in their core discipline while acquiring a broad knowledge base.

Before continuing, we wish to remind the reader that the IGERT rules specify a 3-page limit for references. We use citations to point at existing results or approaches or to bolster a statement that is not obvious or widely known, and regret that we cannot give credit where it is due.

3 Major Research Efforts

The proposal is structured around four broad scientific themes, described in §3.1 below. Each faculty member is currently involved in two or more of them. These themes represent mathematical frameworks and techniques which recur in a variety of settings, and they are highly connected with each other. By focusing on interdisciplinary education through these themes, the students and faculty can best broaden their knowledge base without sacrificing depth in their own disciplinary subject. Following this, we list a set of specific interdisciplinary research projects in §3.2, which arise naturally from existing research at Brandeis, and which connect these themes.

Brandeis has had great success in interdisciplinary collaborations. We have received a MRSEC grant, which includes many of the investigators here (Baskaran, Chakraborty, Epstein, Hagan, Kondev), tying together physics, chemistry, and the life sciences. Other investigators (Epstein, Kondev) are participants in the highly successful Quantitative Biology IGERT grant. Lawrence and Lian have recently received an FRG in generalized geometries, together with researchers at Harvard and at Texas A&M.

Previous interdisciplinary funding has been strongest in the connection between the physical and life sciences, and this has paid off in research, education, and student recruitment at Brandeis. We intend this proposal to be a catalyst for generating new connections based on more general theoretical and mathematical congruences in the natural and social sciences.

3.1 Major research themes

1. Complex systems. (Adler, Bar-Yam, Baskaran, Chakraborty, Charney, Epstein, Hagan, Kleinbock, Kondev, Lawrence, LeBaron, Lisman, Miller.)

The study of complex dynamical systems arises in many areas of physics, chemistry, biology, neuroscience, and economics. Techniques such as the renormalization group, developed in the context of field theories, and other tools for analyzing phase transitions, can be applied widely to study complex systems that are far from equilibrium. These include Belousov-Zhabotinsky (BZ) reaction systems and active neural circuitry.

2. Stochastic processes. (Adler, Bar-Yam, Chakraborty, Epstein, Fiser, Hagan, Headrick, Kondev, Lawrence, LeBaron, Miller.)

Stochastic processes are ubiquitous in systems consisting of a large number of interacting entities, whether they be biological molecules inside a cell, neurons in the brain, granular materials, or the financial market. They are an important part of problems in random matrix theory and are useful probes of geometry and topology. Through Schramm-Loewner equations, they have made a striking and important appearance in studying the geometry of phase domains in two-dimensional systems at a second-order phase transitions [3]. Such systems are described by 2d conformal field theories which are also central to string theory.

3. Quantum and statistical field theory. (Chakraborty, Headrick, Kondev, Lawrence, Lian, and Ruberman.)

Quantum and statistical field theories describe large numbers of fluctuating degrees of freedom, as encoded in a weighted ”path” integral over equilibrium or dynamical configurations. The weighted sum over configurations can implement quantum superposition; thermal averaging; coarse-graining in a deterministic system which is highly sensitive to initial conditions; or an optimization protocol in some computational system. The renormalization group, developed in the context of field theory, can be applied as well to other contexts such as asymptotic methods for solving differential equations [7]. Finally, many important mathematical problems such as the computation of topological invariants can be written as quantum field theory computations, to powerful effect.

4. Geometry and topology. (Chakraborty, Charney, Hagan, Headrick, Kleinbock, Kondev, Lawrence, Lian, Miller, and Ruberman.)

The theory of general relativity ushered in a new era in the interaction of physics and geometry. Gauge field theories have led to an especially fruitful interaction between geometers and topologists on the one hand, and theoretical physicists on the other. Much of this concerned extended field configurations in quantum field theory; solitons, instantons, and topological defects [8]. Topologically nontrivial field configurations such as topological defects are important in condensed matter physics and biological physics [9] as well as in particle physics. String theory has revolutionized enumerative geometry [10] and low-dimensional topology. Finally, symplectic geometry is at the heart of studying Hamiltonian dynamics, an important subset of complex dynamical systems.

3.2 Research problems

In this subsection we list a set of broad, interdisciplinary programs and specific projects attached to them. This is not meant to be an exhaustive list; it would be neither possible nor desirable to do so. Research in the mathematical sciences ranges from well-laid out, multi-year programs as is common in mathematics, to rapidly-evolving opportunistic research (on the time scale of months) as is common in string theory. The reader will note that the projects below cover only a subset of possible disciplinary overlaps. For lack of space we chose them to reflect especially strong existing contacts. As the program goes forward, we anticipate new research connections will open up and boundaries will further dissolve. We will point out a few possibilities latent in existing disciplinary research programs at the end of this subsection.

3.2.1 Emergence of Synchronization in an Ensemble of Oscillators (A. Baskaran, B. Chakraborty, I. Epstein, J. Lisman and P. Miller)

Synchronization is a powerful driving force in nature [11]. The spectacular displays of flashing fireflies emerges through self-organization of their individual, internal clocks. The functioning of heart pacemaker cells relies upon synchronization. Engineering applications rely, for example, upon the synchronization of coupled chemical oscillators, and laser networks. Brandeis has a long history of studies of chemical oscillations [12] and oscillations in networks of neurons [13, 14]. Synchronization has been studied extensively using the tools of complex dynamical systems. Our proposal centers on adding on the techniques of statistical field theory and stochastic differential equations.

Whether and how perfect synchrony emerges out of an interacting population of individual oscillators, often in a noisy environment is a fascinating question that has been the subject of intense research. The work of Kuramoto [15] marked a turning point in the field by offering an exactly solvable model that exhibited synchrony as the strength of the coupling between oscillators was increased beyond a critical value. The work of Strogatz and Mirollo [16] has led to mathematically precise statements about conditions that are necessary and sufficient for perfect synchronization. In the context of physical systems whose functions rely on synchronization, the existence or lack of perfect synchrony is less relevant than the emergence and spatial organization of clusters of oscillators that do synchronize. Understanding the emergence of these structures and the associated length and time scales which are typically much larger than the microscopic scales associated with individual oscillators is also a more difficult problem [16].

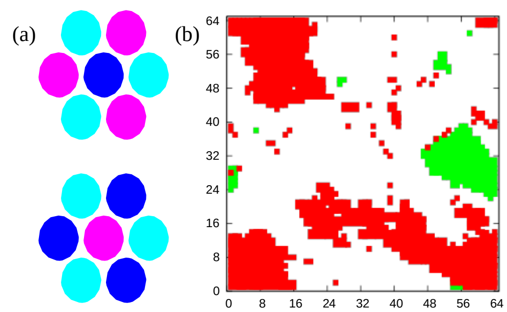

Figure 1: Arrays of repulsively coupled Kuramoto oscillators on a triangular lattice organize into domains with opposite helicities in which phases of any three neighboring oscillators either increase or decrease in a given direction. Fig. (a) illustrates these two helicities in which cyan, magenta and blue vary in opposite directions. In Fig. (b), white and green regions represent domains of opposite helicities. The red regions indicate the frequency entrained oscillators, which are predominantly seen in the interior of the domains.

The study of synchronization has mostly relied on the analysis of systems of coupled, nonlinear differential equations. Such studies have led to a mature understanding of the effects on synchronization of (a) interaction range [17], (b) time-delay coupling [18], (c) type of oscillator (relaxation vs non-relaxational) [19], and (d) excitatory vs inhibitory coupling [17]. The complexity of the nonlinear dynamical systems encountered in “real-world” synchronization problems has, however, limited numerical studies to a small number of oscillators, adopting a mean-field limit, or neglecting stochasticity arising from a noisy environment or intrinsic randomness in the oscillator frequencies. It has, therefore, been difficult to characterize the behavior that emerges on scales much larger than an individual oscillator. An alternative approach that has been gaining prominence is to understand synchronization by exploiting the analogy between cooperative behavior of oscillators and phase transitions and critical phenomena in condensed matter systems [16, 17].

In this research problem we will adopt a two-pronged approach to develop theoretical tools that will help unfold the emergent phenomena in coupled oscillator systems. On the one hand we will use numerical analysis of models for real oscillator systems including spiking neurons and Belousov-Zhabotinsky (BZ) reaction systems to identify and characterize the emergent behavior. On the other hand, we will adapt and extend the well developed tools of condensed matter physics to build systematic coarse-grained theories for simple phase oscillator systems in order to identify mechanisms and governing principles associated with the emergence of synchronization. The feedback between the two approaches will be bi-directional, with the system specific explorations providing the targets for the minimal model coarse-graining efforts and the mechanisms identified within the minimal models explored in the detailed system specific implementations. The Epstein group at Brandeis has been a leader in experimental studies of oscillating systems, and these ongoing experimental studies [20, 21] provide unparalleled opportunities for theorists to develop and test model predictions.

General framework for emergence of synchronization.

Coupled oscillator systems exhibit striking similarities to the well studied spin glass system. In spin glasses, a state of “frozen” spins with non-trivial spatial organization emerges on scales much larger than molecular scales. Frustration, a concept that captures the inability of the microscopic entities (spins, oscillators) to simultaneously satisfy the demands of competing interactions is key to understanding the physics of spin glasses. Generically, oscillators coupled through short-range interactions will be frustrated when placed on random networks. There is a significant body of work exploring the effects of frustration on synchronization [22], however they have mostly been studied using the tools of dynamical systems. A simple example of frustration is phase oscillators [15] placed on a triangular lattice, which interact with nearest neighbors via a repulsive coupling. There are explicit realizations of this system, for example, in microfluidic arrays of droplets containing chemicals that generate the BZ reaction [21]. Our numerical studies of this model show domains of synchronized oscillators that coarsen (grow) for intermediate values of the interaction strength. At larger values of the the coupling strength, the system freezes into domains of synchronized oscillators, a feature reminiscent of spin glasses (see Figure 1).

We will adapt and extend techniques of replica symmetry breaking [23], field theories of stochastic differential equations [23], and supersymmetric hamiltonians [23] developed in the context of X-Y models of spin glasses to a system of repulsively coupled Kuramoto phase oscillators to characterize the emergence of synchronization. We will use this theoretical framework to address the following specific questions: (i) The relationship between phase and frequency synchronization, which often play different roles in a collection of neurons for example, (ii) Minimal requirements of the connectivity and nature of coupling, necessary to obtain synchronization and the role that the topology of the underlying network plays in this emergent phenomenon. (iii) The evolution of the characteristics of a cluster of synchronized oscillators as a function of coupling strength. (iv)The influence of other noise sources. (v) The effect of time delay, such as in diffusively coupled oscillators, on synchronized domains or axonal and synaptic delays between coupled neurons.

Specific realization - Neural networks

A topical problem of interest in neuroscience is the suggestion that neurons responding to the same item can be ‘bound’ via synchronization of their action potentials (spikes) [24]. We will investigate how such binding can arise from adjustments in connections between neurons arising from correlated spikes and assess the importance of correlational structure (*i.e.* small-world or not) in the random network for allowing synchrony to arise in a subset of neurons [25]. Moreover, it has been suggested that short-term memory of multiple items is based on the separate synchronization of subsets of coupled neurons [14], whereby each subset spikes in phase in one single high-frequency (40-80Hz) cycle, of the many such cycles that arise at different phases within a slower (6-10Hz) cycle (see Figure 2). Whether such selection of multiple subsets of neurons by means of multiple discrete phases of firing within a slow carrier wave can arise from a heterogeneous population of initially ungrouped neurons is unknown. We shall address the question by extensive simulations of the neural systems combined with the analysis and simulations of networks of phase-oscillators mentioned above.

Specific realization -Chemical Oscillators

An interesting recent result in coupled chemical oscillators comes from the Epstein-Fraden group at Brandeis [21]. In experiments performed on 2D, hexagonal arrays of BZ microdrops they observe a multitude of patterns. The coupling between droplets is inhibitory, and they would ideally like to synchronize with neighboring oscillators in antiphase relation. This is, however, not realizable on the hexagonal array, and the droplets respond to the geometrical frustration by synchronizing into a state with neighboring oscillators being $2\pi/3$ out of phase. At stronger coupling, however, a new pattern emerges in which there is a $\sqrt{3} \times \sqrt{3}$ lattice of silent droplets that do not oscillate. Each of these silent droplets is surrounded by 6 droplets that are oscillating in antiphase relation. Our preliminary studies of coupled phase oscillators show frozen domains (Figure 1) with domain boundaries containing neighboring oscillators that are π out of phase. Adding amplitude variations to the model could relieve the frustration and create the state observed in experiments at large coupling, and that would indicate that geometrical frustration is primarily responsible for the changing patterns. We will also carry out simulations of the BZ equations in this geometry in order to investigate the effects of diffusive coupling, the relaxational nature of BZ oscillators, and the disorder in coupling strengths arising from disorder in the geometrical array on the emergence of synchronization. These results will be used to build increasingly sophisticated theoretical models to understand phase and frequency synchronization in the BZ microdroplet arrays.

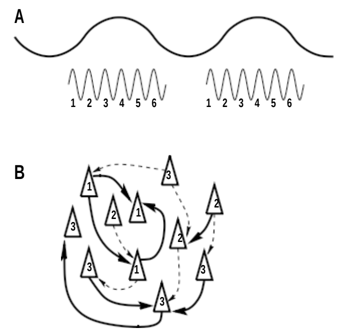

Figure 2: Neural activity synchronized on multiple subcycles of a lower frequency oscillation. A. Nested cycles: separate numbers correspond to spiking of separate subgroups of neurons. B. Examples of random connections between neurons (triangles) with inset number referencing the subgroup. Learning mechanisms are expected to produce stronger connections between cells of the same subgroup, increasing their likelihood to synchronize with each other. Inhibitory connections are present but not shown.

3.2.2 Emergent physics of soft active materials (Y. Bar-Yam, A. Baskaran, B. Chakraborty, M. Hagan)

Soft active materials are inherently out of equilibrium systems composed of many interacting units that consume energy and collectively generate motion or mechanical stresses. Specific realizations include bacterial suspensions, the cell cytoskeleton, living tissues and nonliving systems, such as vibrated layers of granular rods and particles in a fluid propelled by self-catalytic reactions. These are complex materials that exhibit a wide range of phenomena including long-range order in two dimensions [26], anomalously large number fluctuations [27], enhancement of order due to activity [28], pattern formation on mescoscopic scales, and a variety of rheological and mechanical properties, including active thinning and thickening [29–31], spontaneous flow and oscillations [32], spontaneous contractility and active stiffening [33]. Understanding the mechanisms that give rise to these properties will enable nano-engineered smart active materials with tunable mechanical and rheological properties and wide-ranging applications in materials science. The proposed research combines tools from complex dynamical systems, statistical field theories and geometry and topology to analyze patterns in active matter.

From a research perspective, active materials have been subjected to extensive theoretical analysis, but our understanding of them remains limited in two aspects. First, theoretical explorations that undertake minimal studies that uncover global dynamical mechanisms which describe the general classes of observe phenomena have been few. Second, theoretical studies of active materials outnumber experimental investigations by approximately 100/1, and controllable experimental model systems have been challenging to develop. Hence, the connection between theory and experiment remains incomplete. We at Brandeis are uniquely qualified to begin bridging this gap in two ways. First, we will bring together diverse expertise ranging from non-equilibrium statistical mechanics to numerical analysis and computer simulations to address the challenges here. Secondly, our investigations will be driven by and closely coupled to experiments on a model system in which molecular motors drive suspensions of microtubules or actin being performed in the Dogic lab at Brandeis (these experiments are funded by the Brandeis NSF MRSEC). This model systems can be tuned to exhibit the wide spectrum of observed behavior in active materials, ranging from liquid crystal physics to that of active elastomers.

We will develop a program to address two major problems in these systems: 1) Pattern formation in active materials and 2) The influence of boundaries on the physics of active materials.

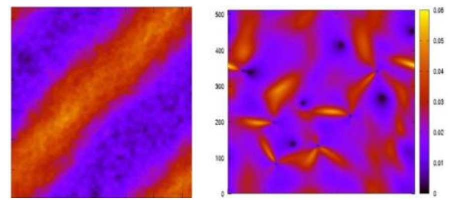

Figure 3: Plots of the nematic order parameter characterizing orientational ordering in an active nematic obtained from a preliminary numerical solution of a simple coarse grained theory. Left panel : Stripes of ordered regions alternating with regions of orientational disorder with the white arrow showing the direction of nematic ordering within the stripe. Right Panel : The formation of -1/2 defects in the system that are precursors to asters. The two patterns occur in different regions of parameters including activity density and noise intensity.

Pattern formation.

Non-equilibrium pattern formation can be precursors to biological functionality in many *in vivo* bio-materials. A systematic understanding of microscopic mechanisms governing pattern formation in active materials is crucial to be able to control the phenomena, both to make designer materials and better understand their biological relevance. We will develop a systematic program to uncover minimal global mechanisms underlying pattern formation in active fluids. The most fruitful starting point for this study is a coarse-grained hydrodynamic description for the conserved and broken symmetry variables in the system. Depending on the region in parameter space, the simplest of such equations exhibit complex patterns (see for example Figure 1). We will study these canonical coarse grained theories using the systematic tools developed in the context of non-equilibrium pattern formation in fluid systems [34] including amplitude equation techniques and hydrodynamic mode-mode coupling. We will use the systematic approach to explore a wide parameter space including : (i) The nature of the orientational ordering in the system, polar vs apolar. (ii) The change in the underlying patterns as determined by the degree of activity in the system. (iii) The role of the medium and the interactions induced by it in the emergent pattern formation. (iv) The influence of the details of the microscopic interactions among the particles on the emergent patterns.

Our approach will include tri-directional feedback among analytical and numerical differential equation techniques and computer simulations of reliable microscopic models. While we seek to understand pattern formation in active systems in general, we will directly compare our results to the Dogic lab experiments on motor driven suspensions of microtubules, which have already demonstrated a variety of patterns that depend on temperature, solution conditions, and motor concentrations.

Influence of boundaries.

In equilibrium fluid systems the intrinsic scale separation between molecular interactions and macroscopic observables allows the influence of boundaries to be accounted for by simple boundary conditions in systems of differential equations. To date, hydrodynamic theories for active matter systems have followed the same protocol. However, systems of topical interest today (bacterial suspensions, collections of artificial microswimmers and nanobots) do not enjoy this scale separation, and thus theories that describe them must account for the effects of boundaries more robustly. We propose to extend the traditional numerical and analytical tools of nonequilibrium statistical mechanics to do so. A key ingredient in understanding how to extend these tools will be rigorously coarse-graining microscopic theoretical and computational models for motor driven microtubules in the vicinity of walls. This endeavor will build on microscopic models for pairwise interactions between motor-driven filaments. We will perform mathematically rigorous coarse graining procedures (e.g. force matching or the Boltzmann inversion method) to establish a connection between the physical ingredients of the system (i.e. microtubules and kinesin) their interactions, and models at different levels of resolution. At the same time we will employ heterogeneous multiscale methods to rigorously connect microscopic models to hydrodynamic equations that describe large-scale system behavior. We will address using the above techniques both direct contact interactions with the wall and medium mediated long range interactions. This analysis will also feed back into the pattern formation studies by identifying the theoretical starting points for exploring pattern formation in channel geometries and other configurations of direct experimental relevance.

The intellectual merit of this research problem in the context of this theory IGERT is as follows. First, the nature of research in the field of active materials is highly interdisciplinary as it lies at the interface of soft condensed matter theoretical physics and Biology and hence allows involved students to see the cross-disciplinary relevance of their theoretical work. Next, the tools required to carry out the above research program namely amplitude equations, nonlinear analysis and fluid dynamic numerical methods are traditionally not part of the physics curriculum and are at the cutting edge of techniques to study emergent behavior today. Hence, this will prepare students to address a variety of problems over and beyond the specific ones outlined here.

Applying concepts in active matter to research in ethnic violence.

NECSI has also demonstrated through research on ethnic violence, that social systems can also, at times, be analyzed using concepts of active matter. In particular, the geographical distribution of populations appears to follow a pattern formation process similar to chemical phase separation, and ethnic violence can be predicted based upon a model that analyzes the geographical distribution of the population. Test of this model have been able to predict the locations of violence in the former Yugsolavia and India at a level of 90% or greater, a remarkable accomplishment for social systems prediction [35]. Thus the mathematics of collective behaviors of non-equilibrium sytems can be extended even to social systems and policy concerns about how to prevent violence. This work will be expanded to additional social system behaviors and regions of the world.

3.2.3 String theory, quantum field theory, and low-dimensional manifolds (M. Headrick, A. Lawrence, and D. Ruberman)

Research in topology over the last 30 years has shown that low-dimensional manifolds exhibit very different phenomena from their cousins of dimensions at least 5. Concepts from quantum field theory have been instrumental in studying these manifolds. In dimensions 2 and 3, geometric ideas pioneered by Thurston were supplemented by the work of Perelman on Hamilton's Ricci flow to establish a powerful classification scheme; Perelman's work was largely motivated by string theory and two-dimensional quantum field theory. In dimension 4, while some portion of the high-dimensional surgery theory extends to give results about classification up to homeomorphisms, the smooth theory is dominated by methods of gauge theory, originating in quantum field theory.

We propose three projects which lie in this intersection of physics and mathematics, both within an established area of interdisciplinary work and in relatively unexplored areas. Taken together, these projects touch on all of the research themes described above: not only geometry and quantum field theory, but stochastic processes and dynamical systems, themes central to the other projects here. Therefore, these projects will benefit from being embedded in the IGERT program.

Spacetime singularities and Ricci flow.

Ricci flow is a flow equation for the metric on a manifold M : $\partial_t g_{ij} = -R_{ij}$, where R is the Ricci tensor, a measure of the curvature of M . It appears as the one-loop renormalization group (RG) flow equations for a nonlinear sigma model with target M , where t is the logarithm of the RG (length) scale. This flow is a powerful tool in modern mathematics and physics. For example, Headrick and collaborators have used it to efficiently generate numerical solutions to Einstein's equations for static geometries [36, 37].

In his proof of the geometrization conjecture [1,2], Perelman established precisely what kinds of singularities of three-manifolds form during Ricci flow, and under what circumstances. This could have a powerful impact on our understanding of quantum field theories. The diverging curvatures at these singularities correspond to diverging couplings in the underlying quantum field theory. This one-loop divergence is generally the sign of new, non-perturbative phenomena: the *physical* RG flow, which includes higher-loop and non-perturbative effects, must remain non-singular. The best-understood case is that of a two-dimensional sigma model with target space S^{N-1}, also known as the $O(N)$ model. This target space shrinks to a point under Ricci flow; physically, instantons generate a mass gap. This is the two-dimensional analogue of the phenomenon of confinement in four-dimensional gauge theories. The other types of singularities which develop under Ricci flow involve the collapse of a lower-dimensional submanifold, such as an S^2 inside a three-manifold; these singularities have been less well-studied by physicists. For finite-time singularities, mathematicians implement a surgery and continue the Ricci flow.

We wish to study whether this surgery has an interesting physical underpinning in the RG flow of two-dimensional quantum field theories with such target spaces. There are hints that the answer is yes. In related cases, Adams *et. al.* [38] and Headrick and Wiseman [39] argued that a localized form of "confinement" at this singularity leads to a change of target-space topology, much like surgery. We intend to study a wider set of examples to show that such localized confinement occurs more generally, and that the topology change is precisely the surgery the mathematicians implement to avoid singularities in Ricci flow [2, 40]. This phenomenon would significantly generalize the notion of confinement, with potential implications for gauge theories in four dimensions. It would also imply an even closer relationship between sigma-model RG flow and Ricci flow than previously suspected.

This project, at the intersection of geometry, topology, and quantum field theory, would require both a mathematician's understanding of Perelman's insights and a physicist's understanding of the renormalization group flow and nonperturbative dynamics of nonlinear sigma models.

String theory and the geometry and topology of three-manifolds

String theorists have concentrated largely on backgrounds with vanishing or positive scalar curvature (with the notable exception of anti-de Sitter spacetimes). Here we describe proposed work on the physics of string theory in negatively curved backgrounds, which intersects with current deep problems in mathematics.

Milnor [41] and Margulis [42] show that there is a direct relationship between the geometry and topology of negatively curved low-dimensional manifolds: negative sectional curvature implies exponential growth of the fundamental group. The Selberg trace formula, a basic theorem in the study of chaotic dynamical systems, relates the spectrum of the Laplacian on the surface (which is dictated by the geometry) to the growth of geodesics on that surface. On the other hand, the geodesics can be broken up into elements of the fundamental group, and counted by counting independent elements of the fundamental group. These elements can be mapped to random walks in a lattice whose directions are equal to generators of the fundamental group; such walks have an exponential growth rate is bounded by the number of such generators.

This fact has direct implications for string theory. Negative curvature enhances the "effective central charge" of string backgrounds, which counts the exponential growth of string states and is a good operational definition of the spacetime dimensionality of a string background [43, 44]. This growth is related to the number of independent winding states, which is mapped (at lowest order in the string loop expansion) to states in the fundamental group. In the case of Riemann surfaces, it was shown by Lawrence and collaborators that string theory on a small genus-g Riemann surface was precisely equivalent to string theory on a $2g$-dimensional torus. This circle of ideas sits nicely in the intersection of quantum field theory, stochastic processes, dynamical systems, and the the geometry and topology of low-dimensional manifolds. There are many avenues for future research, of which we mention two here.

The argument given in [44] is closely related to T-duality, which typically operates on manifolds with nontrivial first homology group, exchanging the momentum and winding of strings about the homology cycles. In the Riemann surface case, the generators of the fundamental group are associated with elements of the first homology group. However, one does not always need a first homology group for T-duality to work. For example, T-duality operates on toroidal orbifolds such as T^4/Z_2 (the orbifold limit of a K3 surface), via an operation on the covering space. In our case, we are interested in studying the string spectrum on target spaces which are homology three-spheres. An important conjecture of Thurston's, the Virtual Positive Betti Number Conjecture [45], states that a rational homology three-sphere with infinite nonabelian fundamental group has a multiple cover with nonzero first homology group. We intend to study the implications of this theorem for string theory on homology three-spheres. It is possible that this study will provide an avenue for proving Thurston's conjecture. This will require a strong grasp of Thurston's geometrization program and a real physics-based understanding of string theory.

A second question involves the entropy of black holes whose horizon is a compact, negatively curved manifold H . Such black holes can be embedded into spacetimes with negative cosmological constant; string theory on these spacetimes is equivalent to gauge theory on $H \times$ R, where R denotes the time direction [46, 47]. Emparan [46] has pointed out that such black holes have finite entropy even at zero temperature. Our proposed project is to derive this entropy from the dual gauge theory. Preliminary research indicates that this will require a sophisticated understanding of geometry and topology as well as of gauge field theories.

Quantum field theory and four-manifold topology

Gauge field theories, developed to describe the fundamental forces in particle physics, are a powerful tool in the study of four-dimensional manifolds. This tool has been sharpened by exact results derived by physicists working in the areas of supersymmetric field theory and string theory. Here we describe ongoing research which makes use of these results, and which would benefit from collaboration between mathematicians and physicists.

Ruberman has been engaged in a long-term project [48, 49] with N. Saveliev (U. Miami) and more recently [50, 51] with T. Mrowka (MIT) on gauge-theoretic invariants of manifolds with the homological type of $S^1 \times S^3$, and the relation of these invariants to the classical Rohlin invariant. Much of this work uses results based on Seiberg and Witten's solution of the vacuum dynamics of string theory, a solution which also began a revolution in the nonperturbative understanding of string theory.

Defining invariants of such manifolds is challenging because the standard arguments that are used to exclude singularities in the configuration space require that the characteristic number b^2_+ be positive, whereas it vanishes in this case. Ruberman and collaborators have resolved this in two different ways, one using Yang-Mills gauge theory, and more recently using Seiberg-Witten theory, yielding invariants λ_{YM} and λ_{SW} . The Seiberg-Witten invariant λ_{SW} contains, as a counter-term, the index of the Dirac operator on a non-compact spin manifold with a periodic end. Such operators occur in many geometric situations, and Ruberman and collaborators are actively working on a general index theorem analogous to the Atiyah-Patodi-Singer formula. In the 4-dimensional setting, the index theorem will be used to study the Seiberg-Witten invariant for the poorly-understood class of non-Kaehler complex surfaces.

The two invariants defined have different useful properties; λ_{YM} vanishes if the fundamental group is **Z**, while λ_{SW} reduces modulo 2 to the Rohlin invariant. Current research focuses on showing that the two invariants are the same and have additional properties with respect to orientation-reversing symmetries. These results would resolve two long-standing questions in topology: the existence of an exotic $S^1 \times S^3$ detected by the Rohlin invariant, and the high-dimensional triangulation conjecture. The conjectural equality $\lambda_{YM} = \lambda_{SW}$ can be approached either by the original physical arguments of Seiberg and Witten [52] or via the more mathematical technique of the PU(2) monopole cobordism [53]. In either approach, a key point to understand is the meaning of the index-theoretic counterterm. In the case of a product $S^1 \times M^3$, the counterterm may be expressed in terms of η-invariants [54], which are well-known in string theory due to their role in the analysis of anomalies.

A student working on these projects would be greatly served by combining a mathematical background in the topology of four-manifolds and the mathematical approach to gauge theories, with a deep understanding of nonperturbative results in supersymmetric quantum field theories.

3.2.4 Coherent trading behavior and instability in financial markets (Y. Bar-Yam, A. Baskaran, B. Chakraborty, and B. LeBaron)

This section builds off the themes of complex systems and stochastic processes from section 3.1. Financial markets have a clear overlap with many complex systems driven by large numbers of interacting components, yielding nontrivial macro level dynamics. The statistical patterns found in many financial time series show certain stochastic signatures which are familiar to many in various teams on this proposal. Our goal is to pool our knowledge and students with expertise in different areas to gain better understanding of important questions about financial markets.

Quantitative measures and model taxonomy.

Financial markets generate many interesting features which share common properties with physical systems. Stock returns display near power-law tails and persistent volatility. The persistence in volatility is close to long memory, with no clear time scale. These features of financial market pose many challenges to physical scientists. For example, there are no robust theoretical frameworks for systems with multiplicative noise which closely follow some of these properties of stock returns. As in physical systems, some self-organizing feature of the system is working to align behavior, generating reliable macro level phenomena. In the world of agent-based finance (which spans both social and physical scientists) the generation of models that reproduce these "stylized facts" has not been difficult. There are now many models which demonstrate that the interaction of reasonable trading strategies give similar macro dynamics. Among the most recent surveys to this work are, [55–57]. Also, [58] present the case for this style of modeling in economics and finance. What we would like to do is to see if there are any analogies between these simple financial systems and some of the other models described here that might allow us to begin to separate out some of their behavior, and better understand a general taxonomy of model classes. Experience with physical systems has shown us that establishing universality classes leads to the identification of the essential driving forces behind collective behavior.

As a second step, it will be important to move beyond simply replicating qualitative features. We would like to push the statistical technologies to determine how precise we can be about these power laws, and how confident we are of their existence. This would include both return power laws (spatial), and the persistence/memory power laws (temporal). The key question is not whether these features are ubiquitous to most financial series, but what are the estimated values, and how precise we can be about these estimated values. Then one can see if any of the model classes generate features which would be empirically falsifiable. Also, it will be important to tie all of this to the latest empirical methodologies in finance that utilize high frequency trading data to separate discrete jump components from continuous Brownian components in stock return dynamics as in papers such as [59, 60]. If these fitted separations are indeed true, then they may form a useful new noise platform to feed into agent-based models. If both the noise structure and the model structure are correct then we should get a final outcome which aligns well with the empirical features already mentioned.

It is possible that there are some properties which are clearly generic across all these classes of models. The agent-based modeling world has long conjectured this to be true, but has never really reached an understanding on this. Being able to find the deeper connections is obviously a general goal of several of the research groups on this project, and our skill and student overlaps will work toward finding these common results across fields.

The dynamics of high frequency trading systems.

Electronic trading systems now dominate trades in most financial assets. Not only are the mechanisms for matching buyers and sellers automated, but many of the orders generated come from machine based strategies designed to find patterns in very high frequency data. Research has begun to show that a simple electronic trading mechanism based on a limit-order book, where offers to buy and sell are submitted and displayed to other traders, combined with relatively simple trading strategies is capable of generating many stylized features in financial time series as in [61–63]. These features again depend on some form of endogenous synchronization across trader behavior. The synchronization aspects of trading behavior can be approached using some of the same tools that have been discussed in §3.2.1. Applying some of the previous testing frameworks to models of high frequency trading dynamics will be a second important test of the reliability of different types of agent-based models to generate financial market features.

A second direction we would like to explore is to extend the single trading hub model. Modern equity trading systems now operate with many trading hubs. In other words the previous problem now involves multiple order book locations. Even though the basic stability and integrity of modern financial systems depend on this structure, their dynamics is still not well understood. We will again apply our framework to the analysis of this problem. The problem is now made more complicated by the fact that strategies must deal not just with buy and sell orders, but where to send these orders. This is a difficult problem, and has yet to be addressed in the agent-based finance world. We are particularly interested in how heterogeneity of order processing at the various hubs impacts the system dynamics. This research is relevant to understanding the dynamics driving financial market instabilities such as the "flash crash" of May 2010 which is described in [64]. During a brief period on that day, U.S. equity markets became extremely unstable, with prices moving far from rational stock valuations.

The “flash crash” has led to a flurry of activity by the Securities and Exchange Commission (SEC) to restore confidence in the financial markets, including the addition of various untested, ad-hoc ”circuit breaker” rules. The importance of quantitative analysis of the high speed dynamics in relation to regulatory actions to ensure stability of the markets is recognized. This recognition includes the importance of scientific analyses for future regulatory action. The New England Complex Systems Institute has already played a key role in advising the House Financial Services Committee and has been invited to present analyses to the SEC, [65, 66]. NECSI also has tbytes of transaction level market data. These relationships, the experience in bridging between scientific studies and policy, and the available data, will serve as a foundation for the program of education and research.

3.2.5 Further possibilities

Many aspects of the existing disciplinary research programs of the IGERT faculty could either extend to interdisciplinary programs or progress substantially as a result of contact with IGERT faculty in other disciplines. These will generate new interdisciplinary alliances beyond the ones described above.

Prof. Adler works in random matrix theory and integrable systems, and complex systems and stochastic differential equations. His work in random matrix theory involves studying infinite dimensional diffusions, viewed as the limit of finite dimensional stochastic processes like the Dyson process on the spectrum of random matrices. Of particular importance are universal processes, and constructing the partial differential equations satisfied by the transition probability. Integrable systems play a big role in this process, and there are strong connections to techniques applied in string theory. Connections also exist with stochastic equations that appear in financial models.

The ”information problem” is the question of how black hole formation and evaporation is consistent with quantum mechanical unitarity, or the preservation of information (*cf.* [5] and references therein). Profs. Headrick and Lawrence are studying aspects of the black hole information problem from the point of view of information theory and of stochastic processes, which could provide a fruitful point of contact with the neuroscience faculty in this proposal.

Prof. Lawrence studies supersymmetry and supersymmetry breaking in quantum field theory and string theory. This connects to studies of disordered systems [6] and to the use of supersymmetric Hamiltonians in §3.2.1.

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