Physics Frontier Center in Nonlinear Science

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4 Executive Summary

Over the past two decades, investigations of nonlinear systems have revealed that the simplest laws of nature can lead to bewilderingly complex dynamics, and yet that such dynamics exhibit universal features which are largely independent of the details of the underlying system. Thus, phenomena as disparate as neuronal dynamics and pattern formation in fluids can be studied with the same mathematical tools.

The impact of nonlinear science across the broad spectrum of natural, life, and medical sciences is due to the unity of its fundamental concepts. Investigators of nonlinear phenomena from diverse backgrounds are transforming important problems once considered intractable, or even ill-posed, into promising new fields. Methods developed in the study of nonlinear systems are now being applied at the Georgia Institute of Technology (GT) and Emory University (EU) to such areas as pattern formation, quantum theory, biomotor control, microfluidics, dynamics of neuronal populations, biological fluids, and nonequilibrium transport. These problems cut across many fields, and the progress in solving them requires bringing together researchers from widely diverse fields, such as mechanical, biomedical and electrical engineering, physics, applied and pure mathematics, chemistry, biological and health sciences.

Since the strong nonlinear dynamics program at GT is located at one of the country's leading engineering schools, in close proximity to Emory, the home to one of the country's most eminent medical schools, we are in a unique position to respond to the challenge posed by the complex systems found in engineering and materials, life and medical sciences – recently identified by the National Research Council [1] as one of the six grand challenges for physics. We propose to establish a cross-disciplinary *Physics Frontier Center in Nonlinear Science* (PFCNS) which will bring together faculty, researchers and students in basic sciences, engineering, and medical sciences.

The greatest challenge of modern nonlinear physics is to develop theory and applications of dynamics in systems with many degrees of freedom. We envision a multi-pronged attack on this grand problem through three **cross-cutting MRCs, with nonlinear science as the unifying theme**. The PFCNS cross-disciplinary program will be based on common concepts unifying a broad range of problems of basic science, such as pattern formation, nonequilibrium dynamics, turbulence, classical and quantum chaos. Research and advanced training fostered by PFCNS will impact on a diverse range of applications of nonlinear science to fields such as biophysics, neuroscience, engineering problems involving liquids, interface motion, novel materials, flows at microscales, and nonlinear control, through the three MRCs:

- MRC 1 - **Chaos in classical and quantum systems**: Conceptually new methods, applicable to chaotic as well as mixed chaotic/integrable high-dimensional systems, need to be developed. Teams combining diverse talents will approach the problem from both the experimentally driven (atomic physics, nonequilibrium dynamics, complex materials) investigations of multi-dimensional problems, and by developing new mathematics (high dimensional billiards, periodic orbit theory, wavelet methods) to analyze such problems. The basic mechanisms of chaos in Hamiltonian and dissipative systems and chaos-order transitions in multi-dimensional and infinite-dimensional systems will be addressed both in quantum and classical contexts.

- MRC 2 - **Dynamics of spatially extended systems**: Spatially-extended systems are systems with potentially very many coupled degrees of freedom. The dynamics of such systems can range from ordered (pattern formation near onset) to very disordered (fully-developed turbulence). This MRC seeks to break new intellectual ground by focusing on problems in three broad fields at the interface between these two extremes, (a) pattern formation in technological processes, (b) spatially-extended dynamics of living systems, and (c) theory of spatiotemporal chaos. Cross-disciplinary interaction with technology and biology has tremendous potential for achieving far-ranging impact, both by stimulating development of novel methods of characterizing spatiotemporal complexity, and by applying existing tools of nonlinear science to important problems arising from experimental advances in these fields.
- MRC 3 - **Dynamics of biological systems**: The rapidly evolving fields of biophysics and bioengineering offer opportunities for advances over a broad front. The proposed MRC will focus on investigations of biological systems which lend themselves to dynamical modeling; "many degrees of freedom challenge" in this context refers to modeling of small or large arrays of excitable cells. In one direction, the research interactions will be inspired by advances in physics: what are biological implications of "stochastic resonance" and other surprising consequences of interplay of stochasticity and nonlinear dynamics discovered by physicists? In the other direction, rapid advances by PFCNS experimentalists engaged in neuromorphic engineering of small neural networks in hardware, spatiotemporal imaging of human brain activity, and construction of novel hybrid systems comprised of synthetic neurons coupled to living tissue, will remain a continuous source of challenges for nonlinear theorists.

The innovation we bring to this multi-pronged research effort is **training in cross-cutting methodologies**. The key mission of PFCNS and a significant fraction of its resources will be devoted to integration of diverse research efforts through a common overarching nonlinear science training, seminar, workshop and visitor program. GT and EU have excellent faculty and research infrastructure in nonlinear science, and the appropriate mix of specialties to offer interdisciplinary research training. Nonlinear science training equips students with a set of tools to formulate and solve diverse problems, wherever they might arise: science, engineering, medicine. PFCNS faculty already has considerable experience in initiating cross-disciplinary research projects. The initial topics studied at the start of the PFCNS will of necessity reflect the current interests of the individual faculty members, the PFCNS grant will act as a vehicle for the generation of new interactions, and the development of applications of nonlinear science to new areas. Co-advising of students and research associates will foster training across diverse research groups, alleviating the tendency of the traditional model to turn students into clones of their advisors. PFCNS will stimulate cross-disciplinary research and communication skills through intensive project-based courses, in which small teams investigate topics guided by faculty members with complementary perspectives. Furthermore, PFCNS will generate a highly cooperative and diverse research environment through cross-departmental research seminars, student-run seminars, regional workshops, yearly retreats, and an active visitor program.

Strategic impact and outreach: *Why should PFCNS be based at Georgia Tech?* GT is the leading science and technology institution in the Southeast, with strong state and industrial support. It is a first-rate engineering school, in the process of rapid growth, with PFCNS profiting from the ongoing expansion of the unique GT/EU common biomedical engineering department, the ongoing GT expansion in nanosciences and biosciences, GT's supercomputing facilities, and close proximity of and institutional affiliation with the Oak Ridge National Laboratory, a leading institution of basic and applied research. The PFCNS graduate training and research program will provide a unique common platform bringing together faculty and students across disciplinary boundaries, will establish bridges to other research institutions in the Southeast, will outreach teaching and minority colleges and industrial sites, and stimulate progress in the field nationally and internationally through a visitor program, exchanges and focused workshops. The GT/EU's Atlanta location, with easy access to one of the world's busiest airports, makes it ideal for visitors and workshops, and it already serves as a meeting place for researchers from universities in the South, as well as a site for major international conferences.

The broad range of PFCNS activities, while highly desirable, cannot be sustained by individual grants. The very existence of the proposed program hinges on the availability of cross-disciplinary funding, something that only PFCNS can make possible. The proposed PFCNS program will be instrumental in fusing the faculty from different schools at GT and EU, which will in turn facilitate research training by allowing the PFCNS faculty to recruit, train, and financially support postdoctoral associates and graduate students for the express purpose of pursuing cross-disciplinary research projects in nonlinear systems. In the long run, PFCNS will seed a basic institutional change, with faculty from diverse specialties sharing post-docs and students and building collaborations that will far outlast the PFCNS grant itself.

6 Prior NSF support

Individually, PFCNS faculty have strong funding records, some of which is documented in the "Current and Pending Support" section of this proposal. Here we concentrate on two prior NSF center grants and one Danish Natural Sciences Research Council grant that form the basis for this Center proposal:

The proposed PFCNS director is **P. Cvitanović** (GT Physics). He is currently the Glen Robinson Chair in Nonlinear Sciences and the director of the newly created *Center for Nonlinear Science* [2], a Georgia Tech pilot program that would house the proposed PFCNS.

In the period 1997-2000, prior to moving to GT, P. Cvitanović led the initiative to create a Center for Complex Systems at the Northwestern University, and was the original PI on the **IGERT #9987577**: *Complex Systems in Science and Engineering program* [3], awarded to Northwestern for the period 2000-2004. PFCNS would strongly interact with this "sister" program as well as with the Arizona and Cornell IGERT programs, see sect. 10.

Cvitanović has a considerable experience in running a cross-disciplinary center of PFCNS scope. Cvitanović co-founded and directed (1993-1998) the *Center for Chaos and Turbulence Studies* (CATS) [4] at the Niels Bohr Institute, Copenhagen, a successful cross-disciplinary effort which became one of Europe's leading centers for nonlinear science. CATS was established by the Danish Natural Science Research Council as a "center without walls". The purpose of CATS is to advance research and research training in nonlinear science, and to strengthen the role that nonlinear research in Denmark plays internationally. The Center consists of groups from the Niels Bohr Institute/Nordita, the Chemistry Institute, the H.C. Ørsted Institute, and the Department of Physics, and the Technical University of Denmark. The Center brings together the groups which are actively conducting research and education in nonlinear science, and enables them to share resources more effectively, ensuring broader participation in research projects and offering better training for students and research fellows.

Core funding for the Center in 1993-1998 was 15 million kroner (ca. 2 million US$) over a 5-year period. In addition, the Center received several million kroner annually from private foundations, Danish universities, and the European Union Mobility program, mostly through salary grants for the non-tenured staff. Due to the structure of funding in Europe (low overhead, university graduate research fellowships, and research council post-doctoral fellowships), this level of funding has larger impact than it would have in the US, and CATS housed approximately 15 faculty, 8 post-docs, 45 graduate students, 15 long term visitors, 40 short term visitors, and 5 workshops/conferences in any given year.

A reviewer might well ask: Cvitanović has done it before, why would he want to do it *again?* A center approach enables research that could not be done otherwise; research that could only have been done through the CATS in the past, and could only be done through a center like the proposed PFCNS in the future. The CATS "Quantum chaos" group was formed by particle physicists, nuclear physicists, condensed matter experimentalists and mathematicians, around the periodic orbit theory program, a program far too ambitious for any one person. The synergy of this "Copenhagen School" has generated a number of important advances: the Dahlqvist-Russberg disproof of the conjectured ergodicity of the $(xy)^2$ potential, K.T. Hansen's work on pruning fronts, H.H. Rugh's proof of the analyticity of Ruelle zeta functions , G. Vattay's work on corrections to the semiclassical trace formulas, A. Wirzba's inclusion of diffraction effects into the periodic orbit theory, and the prettiest application of the periodic orbit theory, D. Wintgen's and G. Tanner's quantization of helium. The team continues the work to this day through the ChaosBook collaboration, a hyperlinked web-based course [6]. The challenge that we now face - developing theory and applications of dynamics systems with many degrees of freedom - will require no less fortuitous combinations of collaborators with different skills.

L.A. Bunimovich is a CoPI and the Director of **GIG #9632032**: *Southeast Applied*

Analysis Center (SAAC), based in the GT School of Mathematics, awarded for the period 1996-2002. Many outreach activities of the PFCNS will continue and extend the initiatives pioneered by SAAC [5]. The goal of SAAC is to stimulate real life applications of applied mathematics and provide support to regional non-research and historically black universities in the Southeast.

One highly successful SAAC program are the *SAAC ambassadors*, who regularly deliver lectures on various forefront topics of modern mathematics in these universities and colleges, and who are greatly appreciated by their faculty and students. Currently we have outstanding some hundred requests to continue these lectures. PFCNS intends to continue and build upon this program by offering lecturers not only in mathematics, but also in physics, biology and chemistry.

SAAC was also successful in establishing working relations and collaborations with other universities in the the Southeast. One of the results of this effort in the recent joint NSF/NIGMS Mathematical Biology proposal (PI Bunimovich) with GT, EU and historically black Morris Brown College participants.

The SAAC post-doc program was exemplary. All SAAC post-docs found academical jobs; R. Latala has been invited to deliver a 45 minute address at the 2002 International Congress of Mathematicians, and B. Guenin was awarded a prestigious prize of the International Society of Computing.

SAAC has contributed significantly to establishing the new GT MS program in Bioinformatics (now in its third year), by developing new courses, through the SAAC seminar in Bioinformatics and Mathematical Biology, and by providing support to bi-annual International conference "Gene Discovery in Silico" which is considered to be one of the (if not THE) best meetings in this area. Another highly successful SAAC activity is running annual "Southeast Probability Days". This meeting regularly gathers about forty active probabilists and statisticians from the Southeast. The next (seventh) conference will be held in April 2002.

7 Major Research Components

We highlight here PFCNS' Major Research Components (MRCs) and the ways in which they are interconnected, with special emphasis on connections that would gain strength and coherence through PFCNS. Throughout the text, the contributing faculty (see sect. 7.D) are indicated by initials; [LAB] stands for L.A. Bunimovich, and so on. The faculty whose primary responsibily is managing a given MRC are indicated in bold type in the "senior personnel" lists.

A Chaos in classical and quantum systems

SENIOR PERSONNEL: ***P. Cvitanović**, **L.A. Bunimovich**, **T. Uzer**, R.F. Fox, R.W. Ghrist, R. Hernandez, A. Shilnikov, E.R. Weeks*

OTHER PERSONNEL: Total of 5-7 research associates and 10-14 graduate students at any given time, of which 2-3 research associates and 4-6 graduate students would be funded by PFCNS.

Overview: This MRC's strategy is two-pronged —combine physics and chemistry experts in applications of quantum mechanics and nonequilibrium statistical mechanics into teams with mathematicians and mathematical physicists working on developing new methods. The goal is to address the same outstanding grand challenge of nonlinear physics: describe classical and quantum chaotic dynamics in dimensions higher than what has hitherto been possible.

Chaotic dynamics of systems with effectively few degrees of freedom is today well understood, and forms the basis for current applications of nonlinear methods to a broad range of fields. However, when the dynamics involves many strongly coupled degrees of freedom, available tools for describing chaos largely fail. Experiments such as the high-resolution spectroscopy of highly excited (so-called "Rydberg") atoms in strong external fields pose both a formidable challenge to theorists and at the same time offer ideal physical laboratories for investigating multi-dimensional dynamics. Developing the theory for these experiments has so far been stymied by the fact that the classical dynamics undergoes a radical change when the number of degrees of freedom exceeds two: beyond that threshold, a wealth of new physics becomes possible. This inability to handle high-dimensional chaos in a systematic way remains a fundamental barrier to the application of the methods of nonlinear science in many disciplines.

Forays into this vast region are still comparatively rare, partly because beyond this divide we lack diagnostic tools comparable in power to the Poincaré surface of section method, and conceptually new methods, applicable to chaotic as well as mixed chaotic/integrable systems, need to be developed. This MRC seeks to break the impasse by putting together teams combining diverse talents in order to approach the problem from two ends: (a) experimentally driven (atomic physics, nonequilibrium dynamics, complex materials) investigations of multidimensional problems, and (b) new mathematics (higher dimensional billiards, periodic orbit theory, wavelet methods) to analyze such problems. Here the cross-disciplinary interaction provided by the center has tremendous potential for achieving far-ranging impact. Thus, one long-range goal of this MRC is to use complex systems studied experimentally in physics and chemistry to stimulate development of novel mathematical physics approaches to describing and utilizing high-dimensional chaos. The second long range goal of this MRC is to identify problems in other fields that could significantly benefit from the application of advances in the theory of high-dimensional dynamics.

The cross-disciplinary focus group on *Quantum chaos in high-dimensional dynamics* brought together by PFCNS will attack a number of experimentally measurable manifestations of quantum chaos where traditional approaches fail. Specific examples include stochastic ionization of atoms in rotating microwave fields, chaotic scattering of electrons, and wave chaos in elastodynamic media. At present, the recently developed phase-space transition state theory of transformations (*e.g.*, chemical reactions), the periodic orbit theory and multi-wavelet methods show great potential, both as diagnostics of chaos in higher dimensions, and as new ways to understand detailed high-dimensional dynamics. Advances here are expected to impact a diverse range of problems, including (to name but a few) the rearrangement reactions of atomic nanoclusters, ballistic electron transport in mesoscopic systems, and the capture of comets and asteroids.

The second focus group on *Chaos and chaos-order coexistence in high-dimensional dynamics* will expand the basic mechanisms of chaos in Hamiltonian and dissipative systems and chaos-order transitions in multi-dimensional and infinite-dimensional systems along several directions. The goal of the first of these directions is the construction of new classes of high-dimensional classical billiards exhibiting chaotic behavior. The second closely related problem is the determination of quantum properties in high-dimensional chaotic billiards. The third is experimentally driven: PFCNS/EU experimental studies of dynamics of complex materials (glasses, foams, colloidal suspensions, granular materials) and the PFCNS numerical studies of chemical nonstationary stochastic dynamics require the development of new methods for effective reduced-dimensionality descriptions of "hybrid" dynamical models.

Why is the PFCNS necessary for the success of this MRC? The proposed PFCNS will provide the kind of support not available from individual grants, but that is vitally important to initiate, stimulate and sustain cross-disciplinary research. Without the PFCNS, both young faculty —afraid to gamble with their tenure decision— and senior faculty —too entrenched in their fruitful but narrow subdisciplines— are unlikely to entertain the radical or risky collaborative projects that will likely be necessary to make advances in high-dimensional dynamics. In particular, the PFCNS will serve as a meeting place for faculty, students and post-docs interested in initiating new cross-disciplinary research directions. PFCNS post-docs will be recruited not for particular faculty but to solve collaborative problems within this MRC. The PFCNS senior faculty not directly involved —but firmly committed to supporting such research initiatives— will nonetheless provide mentoring at the crucial early stages of collaborative projects. Moreover, the PFCNS will offer infrastructure to support the new research directions on high-dimensional chaos through workshops, short-term visitors and long-term visitors both from other nonlinear science research centers, and from institutions which could potentially apply the new methods to outstanding challenges in other disciplines. At present, no other center provides a meeting place for the advancement of the goals of this MRC, and the existence of the PFCNS would thus fill a needed gap.

Background. GT has been at the forefront of classical and quantum chaos research since the very inception of the field, pioneered by (among others) GT researchers J. Ford, L.A. Bunimovich and P. Cvitanović. Instead of using space here to detail the past research of the senior investigators, we pick one recent delightful collaboration (in which, figuratively, Lagrange meets Bohr in Outer Space) as an illustration of how a cross-disciplinary team such as the teams proposed here can solve problems that no individual researcher could have solved alone.

Launched on August 8, 2001, NASA's Genesis spacecraft is currently on a mission to collect solar wind samples. M. Lo of the Jet Propulsion Lab, who led the development of the Genesis mission design, has recruited Caltech mathematician J. Marsden, GT physicist T. Uzer, and West Virginia U. chemist C. Jaffé, to help in the trajectory design. Why? The

Genesis trajectory is by design a highly chaotic orbit of the infamous three body problem, controlled by the Lagrange equilibrium points. The same dynamics controls the motions of comets and asteroids: some of the most dangerous near-earth asteroids and comets follow similar chaotic paths.

In what would have been a surprising turn of events for anyone but N. Bohr, the identical type of chaotic orbits that govern the motions of comets, asteroids, and spacecraft, are being traversed by highly excited Rydberg electrons on the atomic scale. The near-perfect analogy between the atomic and celestial mechanics implies the transport mechanism for both systems are virtually identical: On the astronomical scale, transport takes the spacecraft from one Lagrange point to another, until it reaches its desired destination. On the atomic scale, transport refers to the electron initially being trapped around the atom and then escaping by ionizing, never to return. The orbits used in celestial mechanics to design space missions turn out to also determine the ionization rates in atoms or rates of chemical reactions in the case of molecules! Such connections between micro and macroworlds are not only of great intellectual interest, but have important implications for engineering in the aerospace and chemical industries. And the solution of this problem is greatly enriched by the collaboration of this *ad hoc* group of chemists, physicists, and mathematicians. The presence of the PFCNS at GT and EU would ensure that such groups would be formed frequently and that they would persist long enough to advance the field.

Focus group: Quantum chaos in high-dimensional dynamics

GT has been at the forefront of research into quantal manifestations of classical chaos for over two decades. The research has been particularly fruitful on "Rydberg" atoms in which an electron is promoted to such a high energy state that it almost becomes a classical object. Rydberg atoms and molecules represent an extreme form of matter: They can be as large as a fine grain of sand, can outlive excited states of ordinary atoms by many orders of magnitude, and at the same time they are extremely sensitive to certain perturbations. They are ideal physical laboratories for investigating multi-dimensional dynamics.

The PFCNS cross-disciplinary framework will enable us to put together a team whose goal is to solve a number of open challenges in quantum chaos posed by the recent and planned experiments: ionization of Rydberg states in rotating microwave fields, the chaotic scattering of Rydberg electrons, applications of novel wavelet methods to analysis of the dynamics of multi-dimensional systems, and closely related "wave chaos" phenomena that arise in studies of elastodynamic resonators [7]. The track record so far is that such problems have been successfully solved only through collaborative efforts of atomic physicists, chemists, nonlinear dynamicists and mathematicians. This is scenario is currently employed by CNS: TU and plasma spectroscopist E. Oks (Auburn U.) are combining their expertise in atomic physics with the renormalization-theory expertise of the CNS Ford Fellow C. Chandre, and the geometrical expertise of S. Wiggins (Bristol U.), to solve a number of problems - detailed below - that each of the investigators alone would not be able to solve.

Most early knowledge about quantum chaos can be traced back to two fundamental experiments, both of which were performed on Rydberg atoms [8]: The first one concerns quasi-Landau oscillations in Rydberg atoms placed in strong magnetic fields (the quadratic Zeeman effect, also known as the diamagnetic Kepler problem) and the second is ionization of Rydberg atoms in linearly polarized strong microwave fields. The interpretation of the quasi-Landau oscillations in terms of a particular periodic orbit of the Hamiltonian – an elementary example of Gutzwiller trace formula [8] – ushered applications of classical mechanics to a wide variety problems, which until that time had been considered the exclusive domain of quantum theory–a very fruitful approach from which we are still benefitting. The interpretation of the microwave ionization problem remained a puzzle to atomic theory until its stochastic, diffusional nature was uncovered through the theory of chaos.

The classic experiments in quantum chaos have been understood through models with two or fewer degrees of freedom. However, a number of recent experiments have broken new ground in the dynamics of multi-dimensional chaotic systems. Among these are the high-resolution spectroscopy of Rydberg atoms in crossed static electric and magnetic fields [9], and the microwave ionization of hydrogen using elliptically polarized radiation [10]. Developing the theory for these experiments is an outstanding challenge of nonlinear dynamics.

Chaotic ionization of electrons in microwave fields: In recent experiments probing multidimensional chaotic systems, a strong static electric field is added parallel to a linearly polarized microwave field of comparable strength [11]. These detailed experiments [11] show ionization yield curves which are rich with regular oscillatory features and signatures of resonance transitions. Since the fields are strong enough to render the standard time-dependent perturbation theory useless, a new approach is needed to sort out the many transitions that arise from the interplay of the strong static fields and the dressed states created by the strong microwave field. The CNS group has recently shown that most of the experimental observations can be satisfactorily understood in terms of multi-frequency transitions driven by a single-frequency microwave field between Floquet (or quasi-energy) states [12].

Unlike the linear and circular polarization cases, the elliptically polarized case [10] supports no constants of motion, and explores all three space dimensions – too many for the Poincaré surface of section method to be of any use, and is therefore an ideal quantum chaos experiment to which the time-frequency wavelet transform methods [13] can be applied. Indeed, there is still no satisfactory classical mechanical treatment of this problem, and we intend to find the sources and mechanism of chaos using the time-frequency wavelet transform, to be explained below.

Chaotic scattering of electrons in three dimensions: Quantal evidence for chaotic scattering in the crossed-fields problem was soon confirmed by classical calculations showing that the ionization times for the electron showed fractal structure. By concentrating on the threshold ionization dynamics [14], the CNS group was able to identify the classical mechanism that explains this and related observations for energies below, at, and above threshold. In particular, it was found that the transition to chaotic scattering is caused by a critical point in the Hamiltonian flow (the Stark saddle point), which in turn arises from a velocity-dependent, Coriolis-like force in Hamilton's equations [9]. The CNS group has shown that there exists a "transition state" in the planar atom in crossed electric and magnetic fields problem [14] . The fundamental importance of the transition state is that it represents a state of no return. By means of this object, the coordinate space is partitioned into two regions: one corresponds to atomic states, while the other corresponds to ionized states.

Until very recently, neither the theoretical understanding nor the computing power was adequate to explore phase-space transport beyond two degrees of freedom. In two degrees of freedom, there is a distinguished periodic orbit whose projection into coordinate space connects two relevant branches of the equipotential surfaces. This unstable periodic orbit is called "periodic orbit dividing surface" because it bounds a surface separating reactants and products. Recently a CNS/Bristol team has generalized this solution by constructing hypersurfaces of no return in the *phase space* of strongly coupled, multi-dimensional systems [15]. The solution leads naturally to the multi-dimensional generalization of a two-dimensional saddle point and its associated separatrices. Indeed, the advances in dynamical systems theory [16], in particular the concept of "normally hyperbolic invariant manifolds" [17], anchor rigorously the notion of a "barrier" in phase space of the classical theory of chemical reactions in nonlinear dynamics.

The PFCNS group will apply these ideas to a wide variety of physical problems, since transition state is a general feature of many dynamical systems, provided that the system can evolve from "reactants" into "products". The transition state method, therefore, is not confined to chemical reaction dynamics, but it also controls rates in a multitude of interesting systems, including the rearrangements of clusters, the ionization of atoms [14], conductance due to ballistic electron transport through microjunctions, and the capture of comets and asteroids [18] (described above in the introduction to this MRC).

Wavelet methods: Much of our understanding of nonlinear systems is based on their Fourier spectra, and especially the resonances between different modes of the system (KAM theorem, Fermi resonances in molecules, Laskar's work in celestial mechanics). Frequency analysis of quasi-periodic systems shows that the motion can be trapped in nearly quasi-periodic resonance zones. These successes suggest that snapshots of a chaotic system in terms of frequencies [13] could provide key information about dynamics also in multi-dimensional settings, where the conventional methods of analysis fail us. The recent work by the CNS group demonstrates that one can take snapshots of a chaotic system in terms of its time-varying (instantaneous) frequencies. One of the goals of this focus group will be to develop wavelet methods which would allow us to zoom into segments of chaotic trajectories with arbitrary frequency resolution.

Focus group: Chaos and chaos-order coexistence in high-dimensional dynamics

Chaos theory deals with systems with complex dynamics. Therefore it is especially important to have a rich collection of physical systems which can be fully (best of all, rigorously) investigated and thus provide a firm foundation for intuition required to deal with complicated, "real" systems. In Hamiltonian dynamics *billiards* form such distinguished class of physical systems. Besides the role they play in optics, acoustics, classical mechanics, statistical mechanics, etc., billiards are a very useful testing ground for new approaches in quantum chaos.

In Hamiltonian systems there are two basic mechanisms of chaos: dispersing and defocusing. The first one has been discovered by Hadamard, Hedlund and Hopf in geodesic flows on surfaces of constant negative curvature, and by Sinai in billiards with dispersing boundaries. The billiards whose boundaries are focusing (such as circles, ellipses, spheres, ellipsoids, surfaces of positive curvature) were believed not to exhibit full chaos until Bunimovich discovered in 1974 that Hamiltonian systems can reach chaos by another mechanism, "defocusing", whereas for sufficiently long free paths "focused" beams start diverging. All of the original examples were two-dimensional and for some 25 years a question whether the mechanism of defocusing can also wreck chaos in higher dimensions remained wide open. The trouble lies in a well known optics phenomenon, astigmatism, caused by wide variations in the strength of focusing along different reflection planes. Recently the CNS group [19]-[21] has proved that the mechanism of defocusing can generate chaos in any dimension for a particular class of billiards. The PFCNS team will attack this problem from two directions. The first one deals with classical chaos: the goal is to extend the class of high-dimensional billiards with chaotic behavior, employing the boundary focusing components of constant positive curvature. The guiding conjecture is that focusing components of the boundary must be also absolutely focusing.

The second natural problem is to study quantum analogs of high-dimensional ($d > 2$) chaotic focusing billiards. Recently T. Papenbrock introduced a provocative mechanical model of nuclei [22], a model equivalent to a high-dimensional focusing billiard. Numerical experiments show that these billiards are chaotic, and the quantum chaos investigations [23] of these systems indicate very interesting behavior. The PFCNS group will will study a much larger class of such multi-dimensional systems and develop rigorous foundations for their quantum-chaotic properties, properties so far only suggested by numerical investigations.

Generic Hamiltonian systems are neither integrable nor chaotic; their phase space is a mixture of integrable islands and chaotic components. Even though this behavior was proven to exist for a generic Hamiltonian systems and was found in numerous computer experiments (the standard map is the best known example), there are no rigorously investigated examples of physical systems with such behavior. Recent developments [24] suggest that it should be possible to exploit such *mixed phase-space* properties to design systems for which the energy of a source (such as a beam of light) is arbitrarily nonuniformly distributed across the configuration space, opening up a wealth of applications, such as in the stochastic cooling of atoms [25].

Either purely deterministic dynamical systems or stochastic random process are traditionally employed to model physical, chemical and biological phenomena and processes. A theory of either is very rich, and our intuition about evolution of such systems is well developed. This intuition is based on explicitly solvable simple examples and physically transparent (but nontrivial) systems. In the theory of stochastic processes the examples are sequences of identical independently distributed random variables (Bernoulli shifts), random walks, etc. In dynamical systems theory such explicit models include toral automorphisms, one-dimensional quadratic maps, billiards, etc.

Many physical problems are *hybrid systems* in the sense that their dynamics is neither purely deterministic nor purely random but rather a combinations of both. This holds for disordered systems, chemical kinetics, and theoretical problems of computer science (Turing machines with many heads and/or many tapes). Complex materials such as glasses, foams, colloidal suspensions, and granular materials with liquid-like structures and solid-like properties studied experimentally at microscopic level by the CNS/EU group by means of confocal microscopy in both static and dynamic settings [26, 27], offer a rich set of challenges for "hybrid" systems theory. Further inspiration can be garnered from the CNS group numerical studies of *nonstationary stochastic dynamics*. In some cases, the dynamics of reduced-dimension coordinates describing an effective solute may induce nonlinear responses in the effective solvent. In *spatially heterogeneous solvents*, models have been developed using the generalized Langevin equations with space-dependent friction. When the solute is sufficiently concentrated, the collective solute dynamics can be modeled by a time-dependent self-consistent friction [28, 29].

The time evolution of such systems is often quite counter-intuitive [31]. Traditionally one considers either a small random perturbation of a deterministic system, or by adding a small advection component to a diffusion process. Such small perturbations do not address the hard problem, the behavior of hybrid systems whose evolution is governed by deterministic and stochastic components of comparable strength. There exist very few (if any) comprehensive investigations of such hybrid systems. Recently a breakthrough has been achieved in the studies of one class of such systems, known either as the "Lorentz lattice gas cellular automata" or the "Many-dimensional Turing machines". Let a light (particle, signal, wave, spike, animal, etc.) move on some graph. there is a scatterer (scattering rule, protocol etc.) which determines where this propagating object will go after visiting a given vertex. If the scatterers are randomly distributed, the dynamics is a deterministic walk in a random environment. The moving object can in turn affect the environment by changing the state of a visited vertex. Then one can study not only motion of a single particle (like in the classical Lorentz gas) but also dynamics of many moving objects which interact indirectly, by changing the environment in which another objects also move. This challenging high-dimensional systems is also a natural high-dimensional representation of a Turing machine because each vertex can be thought of as an infinite tape with a (deterministic) protocol which prescribes how environment should change in a given vertex. This model happens to be the central concept of the new branch of theoretical computer science called "collision based computing" [30]. Deterministic walks in random environments also have applications in statistical physics, chemical kinetics, environmental studies, neuronal dynamics, etc.

Consider now walks in "rigid" environments [31] where one introduces a parameter r of environmental's rigidity into a general deterministic walk in a random environment, with the environment of a vertex changing after rth visit to this vertex. It turns out that such walks are completely solvable models on one-dimensional lattices. Moreover, they exhibit the three possible types of diffusive behavior: normal, sub- and super-diffusion. All these types of behavior are deterministically generated, demonstrating the interplay between symmetry properties of a lattice and the types of scatterers which form the environment [32]. Another unexpected phenomenon exhibited by random lattices is localization [33], analogous to the Anderson's localization in condensed matter physics. This research will continue in several directions: studies of walks in environments with nonconstant rigidity, studies of models with many particles and continuous limits of these models.

While in the context of quantum theory Hamiltonian systems play a special role, dissipative systems are at least as important as models of fluid, chemical and neuronal dynamics. It is increasingly clear that it is quite unlikely that hyperbolic attractors appear in models which have anything to do with real systems, and PFCNS group will therefore focus on pseudo-hyperbolic attractors in high-dimensional systems, where "pseudo" stands for chaotic attractors with homoclinic tangencies but without stable periodic orbits. Another open multi-dimensional challenge in dissipative dynamics is the description of "hyperchaos", i.e. chaos with more than one unstable directions. This situation is relevant for a large variety of applications. Another direction for the PFCNS teams is study of bifurcations in slow-fast systems which appear in neural (individual and group) dynamics. The PFCNS would team the Georgia State University mathematician with the EU experimentalists in order to investigate a fourteen-dimensional neuron model [34].

B Dynamics of spatially extended systems

SENIOR PERSONNEL: ***M. Schatz, R. Grigoriev, G.P. Neitzel****, L.A. Bunimovich, P.A. Cvitanović, S.P. DeWeerth, W.L. Ditto, K. Wiesenfeld*
OTHER PERSONNEL: Total of 4-6 research associates and 8-11 graduate students at any given time, of which 1-2 research associates and 2-3 graduate students would be funded by PFCNS.

Overview:

Spatially extended systems are systems with potentially very many coupled degrees of freedom. The dynamics of these systems can range from ordered (pattern formation near onset) to very disordered (fully-developed turbulence). While the methods of nonlinear science have achieved a certain "universal" (in the spirit of equilibrium critical phenomena) understanding of low-dimensional behavior in spatially extended systems, current tools for describing these systems fail when the dynamics are high-dimensional, involving many spatial and temporal degrees of freedom. This inability to handle spatiotemporal complexity presents a fundamental barrier to the application of the methods of nonlinear science in many disciplines.

This MRC seeks to break new intellectual ground by concentrating efforts in three focus groups: (a) Pattern Formation in Technological Processes, (b) Spatially Extended Dynamics in Living Systems, and (c) Theory of Spatiotemporal Chaos. Cross-disciplinary interaction in technology and biology has tremendous potential for achieving far-ranging impact. Many important problems in technology and biology involve dynamics that are typically in spatiotemporally complex regimes. Thus, one long range goal of this MRC is to use studies of problems in these fields to stimulate development of novel methods of characterizing and classifying spatiotemporal complexity. At the same time, the methods and approaches of nonlinear science are still relatively unknown in many areas of technology and biology. Thus, a second long range goal of this MRC is to applying existing tools of nonlinear science to important problems arising from advances in technology and biology.

The recent establishment of the GT/EU Center for Nonlinear Science has already helped initiate the kind of cross-disciplinary research envisioned under this MRC, as described in detail below. Patterns in technology are being explored by means of optical methods of multipoint manipulation developed at the CNS for hydrodynamics experiments; these methods are providing the means for conducting a wide range of novel experimental studies that include exploration of dynamics and control of coating flow (a fundamental manufacturing process) and application of pattern formation methodologies to microfluidics, the science and technology of microscale fluid mechanics for biological and chemical applications. Spatially extended dynamics of arrythmias in cardiac tissue in vivo is a compelling problem that pushes development of new experimental and theoretical approaches for characterizing spatiotemporal complexity.

The planned PFCNS provides the kind of support, not available from individual grants, that is vitally important to stimulate, sustain and broaden such cross-disciplinary research on spatially extended systems. Firstly, the PFCNS provides support for the critical mass of personnel (students and postdocs) needed for work on new cross-disciplinary research directions at the crucial preliminary stages when such work lacks the track record needed to attract support from more conventional sources. Secondly, the PFCNS will support the cross-pollination of ideas for new research directions on spatially extended systems in technology and biology by using short-term (e.g., workshops) and long-term (e.g., resident scholars) visiting opportunities to attract to the PFCNS researchers from universities, national laboratories, and industrial research centers. These visitors are expected to benefit from PFCNS interaction by acquiring new approaches to unsolved problems in their disciplines. At the same time, the research environment at the PFCNS will be invigorated by visiting researchers who provide fresh problems that push the current frontiers of our understanding of spatially extended dynamics.

Focus group: Pattern Formation in Technological Processes

Dynamics and Control of Coating Flow: Coating is a technological process of great significance, with applications ranging from electronics and optics to automotive and airspace industry. A typical coating application involves a two step process: first the substrate is coated with a layer of solution, then the solvent is left to evaporate, leaving a layer of solute on the surface of the substrate. The main difference between various coating techniques is in the way the initial liquid coating is produced. For instance, dip-coating technique is used for optical fiber coating [39], and (anti)reflective optical coatings of lenses and mirrors. Similar techniques are used to produce hydrophobic [40] and hydrophilic coatings. Spray coating is used to produce sol-gel coatings of TV screens [41] and, more routinely, for painting. Spin coating [42] which was originally developed for microelectronics applications has also found numerous applications in the optical industry.

Most types of coating techniques (e.g., dip-, spin-, or blow off coating) involve forced spreading of the liquid onto a substrate, where the external forcing is provided by gravity, inertia, viscous drag, or imposed gradient in surface tension. Regardless of the type of forcing, the process of driven spreading shows a generic feature: for some parameters the solid-liquid-gas contact line exhibits a transverse (fingering) instability [43]. The instability is believed to arise due to the increased mobility of the capillary ridge forming near the contact line [44] and manifests itself in the formation of fingers and troughs advancing with (in general) different velocities.

Another type of instability arises when the liquid coating starts to evaporate [45]. Surface tension gradients arising from variations in temperature (thermocapillarity) or concentration (solutocapillarity) can combine with the normal pressure of the escaping vapor on the liquid-gas interface to destabilize the liquid layers of uniform thickness. The ultimate fate of this latter instability is eventually determined by the properties of the substrate: if it is non-wetting, the film will generally rupture [49], producing a pattern of dry spots, a phenomenon often referred to as de-wetting or reticulation. Otherwise it may remain continuous but spatially nonuniform. For instance, during spin-coating, instability manifests itself in a pattern of radially oriented lines of thickness variation, or striations [48] (see Figure 1).

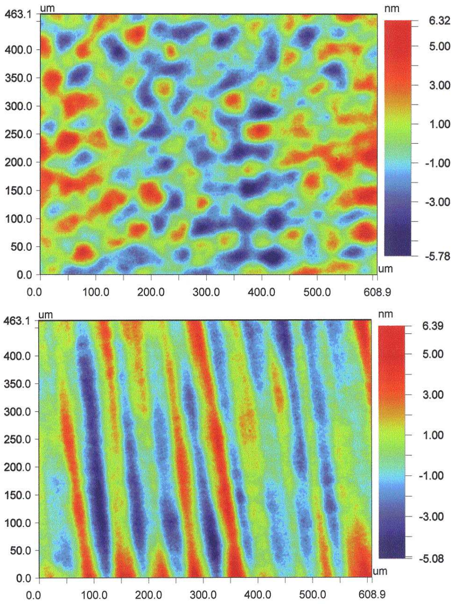

Figure 1: Thickness profile of an evaporating liquid layer on the surface of a disk spinning at 2000 RPM in the center (top) and 2cm away (bottom) (Courtesy D. P. Birnie, U. Arizona).

Both fingering and evaporative instabilities can crucially affect the quality of produced coatings, so understanding the governing mechanisms and devising methods to suppress them is fundamentally and practically important. A number of CNS faculty are actively involved in related research. The studies of thermal convection in thin layers [49, 50, 51, 52] and liquid bridges [53] and control of interfacial instabilities [45, 54] represent only a few of the examples of the previous and current work. On-going research on coating flows is focused in two main directions: dynamics and control of driven contact lines and thermo- and soluto-capillary instabilities of thin liquid layers.

Perhaps the most familiar example of fingering instability is provided by the formation of drip rivulets that can occur when vertical surfaces, such as household walls, are painted. Although the case of gravity-driven spreading is relatively well studied, the problem of surface-tension-gradient-driven spreading has received comparatively little attention [46]. This latter case is important because experimental approaches developed for manipulating thermocapillary convection (described below) could find use in technological applications, so a much deeper understanding of the fundamental physics of the contact line instability is necessary to both exploit and suppress it. Our theoretical analysis [47] suggests that the presence of capillary ridge determines the stability in this case as well. Experimental study of the fingering instability will exploit the unprecedented capabilities of multipoint thermal actuation to manipulate the dynamics of the coating flow.

The effectiveness of thermocapillary-based optical manipulation of dynamics has been demonstrated in several previous experiments on free surface flows. The imposed thermal profile was used as a tool for probing and controlling instabilities leading to pattern formation. In work on surface-tension-driven Bénard convection, selected patterns were imposed as initial conditions using a computer-controlled optical heating from an infrared laser. In one case, imposing patterns with designed imperfections permitted, for the first time, quantitative measurement of the dynamics of penta-hepta defects, which are the most common disordering mechanism in hexagonal patterns found in a wide variety of physical systems [52]. In a second case, effective closed-loop control was achieved for the suppression of thermocapillary convection waves by using infrared temperature measurements coupled with feedback via optical heating by an infrared laser [55].

Our preliminary experiments show that variations in the thermal profile imposed in response to the contact line distortion can be used to actively suppress the instability in an all-optical setup (see Figure 2). These experiments also raise a number of questions regarding the optimal choice of the spatial structure of the applied perturbations. These questions can only be answered by taking into account the full dimensionality of the physical space (local changes in the temperature of the liquid film produce fluxes in the direction of the spreading as well as transversely to it) as well as the non-normality of the evolution operator (the standard linear stability analysis provides a poor description of the dynamics). To find the answers more efficiently the theoretical analysis will be tightly integrated with the concurrent experiments. These studies will also address the question of whether the proposed techniques can be used for controlled patterning of the coating flow.

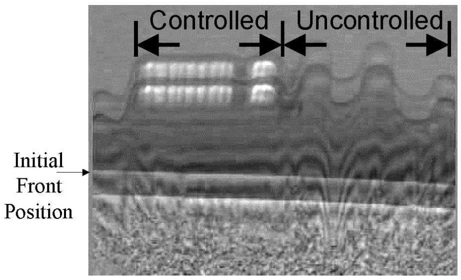

Figure 2: Optically controlled spreading of a thin liquid film on a solid substrate. The formation of "fingers" (right side of figure) can lead to nonuniform coating. Small temperature-induced surface-tension (thermocapillary) gradients, applied optically (left side of figure), can suppress the instability, permitting the spreading front to remain flat and to spread uniformly.

Although the problem of controlling evaporative instabilities in pure liquids is now rather well understood [45], essentially all liquids used in coating applications are mixtures whose properties sometimes differ rather dramatically from those of pure liquids. The studies involving complex (multi-component) liquids have barely scratched the surface. The major difficulty in describing the complex liquids is the fact that all physical properties become functions of relative concentrations of different components, immediately increasing the dimensionality of the problem. Additional complication is produced by the presence of components that tend to segregate near the interface (e.g., surfactants). In order for the results of experimental and theoretical studies to advance the state of knowledge in practically relevant cases, these difficulties have to be addressed.

Combined theoretic and experimental approach will also be used for the study of the dynamics and control of thin layers of multiple-component volatile liquids. The theoretical description will be built by generalizing the approach developed for pure liquids by RG and it will be extensively tested experimentally in the laboratory of MS with the experiment and theory providing continuous feedback for each other. The experiments will start by providing experimental validation for the theory [45] developed for the case of pure liquids and then move on to the more complicated case of binary mixtures and solutions. Both RG and MS will interact extensively with the materials science group at the U. of Arizona (D. P. Birnie, D. E. Haas), which has expertise in the studies of spin-coating involving complex liquids.

Microfluidics for Biological and Chemical Applications: Miniaturization in electronics has spurred many advances in solid state physics and numerous wonders of technology. Similarly, the goal of miniaturizing biological and chemical processing ("Labs-on-a-Chip") is stimulating both science and technology in the field of microfluidics. To perform genetic assays, chemical synthesis or water quality tests on a chip-sized device requires the ability to manipulate a large number of tiny fluid samples. At present, there is no broad agreement on the best methods for controlling fluid flow at the microscale [56]. Techniques drawn from studies of spatially extended systems, which, at first glance, are seemingly unrelated to microfluidics, have, in fact, the potential for providing new approaches for this emerging area.

Lack of reprogrammability/reconfigurability is a major shortcoming of most current microfluidic devices. Microfluidic chips today are constructed with lithographic techniques inspired by microelectronics. However, unlike semiconductor manufacture, where the resulting devices (e.g., CPUs) can be readily reconfigured for many tasks, lithography in microfluidics etches the devices into a fixed configuration that is typically capable of performing only a single very specific assay. (If microcomputers had developed this way, a new chip would have to be plugged in with every software installation!)

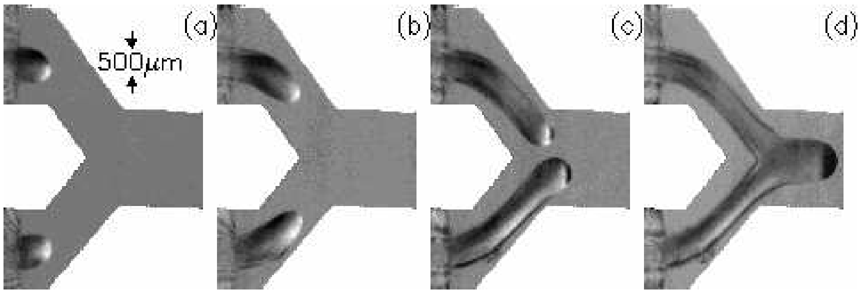

Figure 3: Optically controlled thermocapillary driving of microstreams on a FEATURELESS horizontal glass substrate is shown in a sequence of time lapse images. A spatially varying temperature is imposed optically on the substrate, inducing surface-tension gradients that (a) draw two 500 μm wide silicone oil microstreams from reservoirs, (b) turn the microstreams toward one another, (c) merger the microstreams, and (d) drive the merged stream.

The possibility of using dynamics rather than geometry for microfluidics is suggested by the work on coating flow described earlier. Preliminary experiments demonstrate that optically-induced thermocapillarity can confine and transport microflow on a substrate that is mechanically and chemically featureless (Fig. 3). In other words, no etching of pipes or hydrophillic/hydrophobic surface treatments are required to channel the flow. Instead, the fluid is confined and guided by a combination of "self-containment" by capillary forces along with dynamically adjustable thermocapillary forces imposed by the illumination. Liquids in microdroplet form may also be driven optically on liquid substrates. In Figure 4, the focused beam of an infrared laser is rastered along the liquid substrate near the droplet and the beam heats the interface by direct absorption. The resulting thermocapillary flow produces an interfacial motion away from the laser spot that carries along the droplet at speeds of up to a few centimeters per second. Again, no pipes or patterning are required to contain the flow; the microdroplet is self-confined by its own surface tension.

Tools developed from studies of other spatially-extended systems can be used to address important issues in dynamics-based microfluidics. For example, studies of pattern formation in the classic Bénard thermal convection problem have shown that thermocapillary-induced instability can lead to topological changes, *e.g.*, break-up and rupture of the liquid [49]. These effects are well-modeled by both linear and nonlinear theory in the convection problem [57]. Similar mechanisms are expected in thermocapillary-driven microfluidics and can potentially be used to split microstreams or microdroplets for metering purposes. As a second example, studies of spatially-extended fluid systems have demonstrated the phenomenon of chaotic advection, in which a passive scalar (e.g. concentration) in the flow can exhibit complex behavior even in cases when the velocity field of the flow is not chaotic [58, 59, 60]. In many cases, chaotic advection can be described using methods developed for understanding chaos in Hamiltonian systems [58]. Implementing chaotic advection in microfluidics should beneficially enhance mixing, which otherwise is usually dominated by slow molecular diffusion. Chaotic advection has been implemented in geometry-based microfluidics [61] and can be implemented in dynamics-based microfluidics by suitable temporal/spatial modulation of the thermocapillary driving of the microflow.

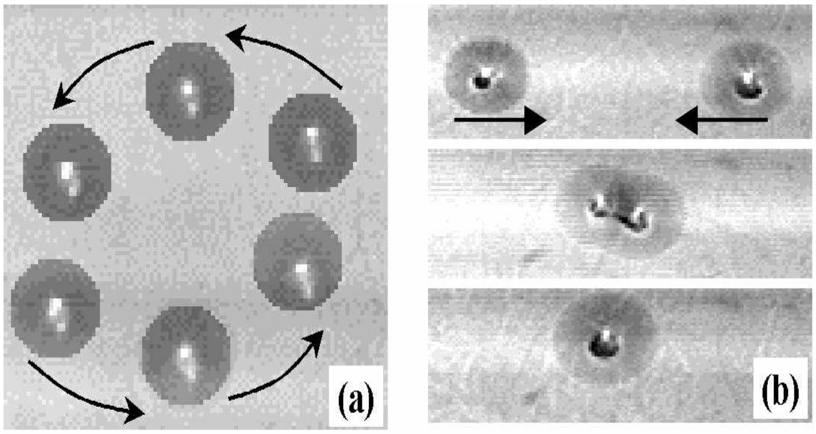

Figure 4: Optically controlled thermocapillary guiding and merging of 300 nanoliter insulin droplets suspended on a perfluorocarbon liquid substrate. A single droplet is driven in a repeated elliptical trajectory, as shown in the multiple exposure image in (a). A time sequence of images shows the merger of two droplets (b).

A recently formed partnership between GT/EU CNS (involving MS, RG, GPN) and Yerkes Regional Primate Research Center/Emory School of Medicine has proposed to explore the potential of dynamics-based microfluidics for use in biomedical applications. This partnership, which joins expertise in pattern formation, hydrodynamics, and genetics, will explore the scientific and technological issues related to developing a reprogrammable/reconfigurable PCR (Polymerase Chain Reaction) analyzer for the identification and detection of infectious agents.

Focus group: Spatially Extended Dynamics in Living Systems

Sudden cardiac death is the leading cause of death in the industrialized world with the majority of such tragedies due to ventricular fibrillation (VF). VF is a frenzied and irregular heart rhythm disturbance that quickly renders the heart incapable of pumping blood and hence sustaining life. Instead of contracting regularly and uniformly, the ventricles writhe and fibrillate at a frequency some ten times faster than the normal heart rate. Understanding these self-sustaining dynamics and the mechanisms responsible for their initiation is crucial for developing effective and reliable defibrillation techniques. The presently existing techniques are based on "resetting" the heart with a strong electrical discharge and have large failure rates.

Although at first sight the dynamics of the heart tissue during VF seem to be very irregular, it is not random and possesses a high degree of spatial and temporal coherence, indicating that it is governed by a deterministic process [62]. The dominant approach toward characterizing this dynamics has been based on the studies of simplified models of excitable media that all share with the heart the functional properties of excitability and refractoriness. The generic feature of such models is that their dynamics are dominated by travelling waves. In particular, reentrant spiral waves, seen in numerical solutions of three-dimensional simplified models of cardiac tissue for a long time were believed to occur during ventricular tachycardias. However, experimental detection of such reentrant waves in fibrillating mammalian ventricles has been difficult.

Recent experiments conducted by WLD and collaborators [63] suggest that spiral waves are rarely observed. In the early stages of VF, the dynamics is dominated by transiently erupting rotors (source structures surrounding the core of rotating spiral waves). This activity is characterized by a relatively high spatiotemporal cross correlation. During this early fibrillatory interval frequent wavefront collisions and wavebreak generation are also dominant features. In the contrast, the later stages (chronic VF) are characterized by patterns which are much more complex and are less correlated in both time and space, while the epicardial rotors are no longer observed.

Despite this complexity, some spatial correlation remains, indicating the presence of spatially coherent structures (CS). Identification of such CS was suggested as a general way to reduce the dimensionality of spatiotemporally complex dynamics. This approach which was originally developed in the context of fluid turbulence [64] has found numerous applications in other areas, most notably characterization and control of chemical reactions [66, 67]. During the early stages of VF in the heart tissue CS can be associated with rotors. Even though the spiral wave may break down just outside the core, the rotors can be easily identified as the points of phase singularity, or topological defects around which the excitation wave propagates in clockwise or counterclockwise direction. High degree of spatial and temporal coherence can be exploited to design implantable defibrillators, which are capable of quickly detecting VF.

The origin of coherent structures present at the later stages is presently unknown, which makes defibrillation during chronic VF especially challenging. However, this is precisely the regime that should be targeted by clinical defibrillation techniques, since by the time VF is detected in most patients the earlier stages will be over. The lower degree of coherence indicates that the dynamics is characterized by a larger number of degrees of freedom, making it harder to analyze and control.

An additional difficulty is associated with the fact that presently no general techniques exist capable of suppressing spatiotemporally chaotic behavior in systems of complexity comparable to that of the heart tissue. One promising approach is currently under investigation by RG and MS (from theoretical and experimental standpoints, respectively). The main idea is to simplify the description of the dynamics by factoring out the degeneracies associated with translational degrees of freedom and performing statistical analysis on the reduced data set using the proper orthogonal decomposition (POD) to identify the coherent structures (Fig. 5), their position, and orientation, which will allow the construction of a reduced-order model. Such a model can be used for the purpose of designing a control algorithm for defibrillation in both the early and later stages of VF.

Presently this approach is developed using Rayleigh-Bénard convection (RBC) as a model system displaying spiral defect chaos (SDC). RBC represents the typical features of spatiotemporally complex dynamics in general, such as chaos in both the temporal and spatial domains, and interaction of coherent structures at different length scales. The regime of SDC has particularly many features similar to the dynamics of the heart tissue. The main attraction of SDC is, however, that it is considerably more tractable than the fibrillatory dynamics: its effective dimensionality is much lower, while the availability of a quantitative weakly nonlinear description in terms of amplitude equations provides the opportunity to model certain aspects of SDC analytically. In addition, the dynamics of this system can be easily controlled on a very fine scale via optically-imposed multipoint thermal actuation (see discussion above).

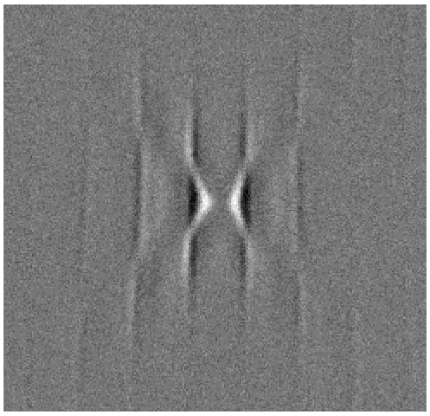

Figure 5: The fastest growing mode of the instability leading to roll breakup in Rayleigh-Bénard convection.

The typical application of POD [66] uses time averaging in the absence of external stimuli to extract coherent structures containing the effective degrees of freedom from the chaotic signal. This approach is inherently flawed for two reasons. First of all, (approximate) translational invariance produces degeneracy in the position of coherent structures, smearing them over the whole domain [65], rendering the dimension of the embedding space produced by POD too large to be useful. Second, any external stimulus (a requisite ingredient in any control, or in this case defibrillation, technique) will knock the system out of its attractor, rendering the description of the unperturbed dynamics largely irrelevant. Both of these problems can be solved by changing the way in which statistical sampling is performed. By replacing the time average with an ensemble average performed for a collection of different initial conditions produced by imposing local perturbations, a set of localized coherent structures is obtained, yielding a reduced-order model whose dimensionality is independent of the system size.

The theoretical and experimental studies envisioned within this proposal will look at implementing the above approach in the context of VF. RG will be responsible for modeling and theory. The methodology will be tested experimentally on convective systems in the laboratory of MS at GT and the results and techniques will be adapted for application to the dynamics of heart tissue under the direction of WLD, with experiments conducted at the clinical facility of the University of Alberta. The experimental studies will concentrate on two main directions: reconstruction and visualization of fibrillatory dynamics in three dimensions, and characterization of the effects of spatially and temporally localized external stimuli on the dynamics.

Since the ventricles are relatively thick, the influence of the third dimension cannot be neglected, if an accurate description of the dynamics is to be constructed. Since the proposed approach assumes that the data used to extract coherent structures faithfully (and uniquely) represents the state of the system, the availability of three-dimensional imaging with adequate spatial and temporal resolution is crucially important. Equally important, reconstruction and visualization of the dynamics of heart tissue in three dimensions is necessary for gaining additional insights into the mechanisms leading to the initiation and evolution of VF and for construction of more accurate mathematical models. For instance, since the heart tissue is almost transparent to intense radiation of appropriate frequency, optical tomography using voltage-sensitive dyes can be employed for three-dimensional reconstruction.

The study of the response of the heart tissue to external stimuli represents another important ingredient of the proposed approach. The inherent degeneracy in the position (and possibly orientation) of coherent structures coupled with their localized spatial structure, demands the ability to apply localized perturbations to suppress the instabilities leading to VF. Novel ways to apply temporally and spatially localized perturbations will be developed based on the idea of optically activated electrical, thermal, or chemical stimuli. Different methods will be tested experimentally and the best technique will be identified and compared with the conventional technique of delivering electrical stimuli via implantable electrodes. The analysis of the response to such perturbations will be used to construct a reduced order model for designing new defibrillation methods.

PFCNS would enable the integration of presently separate individual efforts by MS, RG, WLD, and the clinical group at the University of Alberta (K. Kavanagh, P. Penkoske) to study the dynamics of VF and enable the transfer of the expertise developed in controlling spatiotemporally complex dynamics in convective systems to the problem of designing reliable and efficient defibrillation methods. This is an extremely complicated and ambitious goal, which cannot be achieved on the level of individual collaborations. The success requires a collaborative effort involving specialists with the expertise in the areas of physiology, cardiology, spatiotemporal dynamics, and control. Without such a highly centralized approach the progress will be limited to incremental advances having little bearing on the ultimate goal – saving lives.

Focus group: Theory of spatio-temporal chaos

The GT experimental group of M. Schatz has a unique skill; they are able to *design* a large repertoire of initial spatio-temporal patterns by their multipoint thermal actuation technique (described above). If the dynamics is spatio-temporally chaotic, such patterns are unstable and quickly fall apart - and this instability is precisely what fascinates the mathematical physicists which PFCNS will team up with this experimental group.

In explorations of modern field theories (classical Yang-Mills, gravity, hydrodynamics, Ginzburg-Landau systems) the dynamics tends to be neglected, and understandably so, because the wealth of their solutions can be truly bewildering - the strongly nonlinear classical field theories are turbulent, after all. If one is to develop a theory of a spatially extended systems that are chaotic, one needs to determine, classify, and order by relative importance the solutions of nonlinear field theories. Such systematic exploration has so far been implemented [68, 69] only for one of the very simplest field theories, the 1-d Kuramoto-Sivashinsky system [70]. This research is still in its infancy, but it has lead to a working hypothesis the PFCNS plans to explore: For any finite spatial resolution, the system follows approximately for a finite time a pattern belonging to a *finite* alphabet of admissible patterns, and the long term dynamics can be thought of as a walk through the space of such unstable patterns. The *periodic orbit theory* [35] provides sophisticated mathematical machinery that converts this intuitive picture into a precise calculation scheme. The patterns singled out by the theory can be created and tested by MS's technique. The PFCNS team is currently the only one which possess both experimental and theory expertise to carry this program to fruition.

Computer simulations of classical field theories are of necessity discretized in space as well in time. They inspired research into Lattice Dynamical Systems (LDS), systems of spatially interacting local units, with each unit in itself a dynamical system, *e.g.* a nonlinear oscillator. So far, studies of LDS have lead to a mathematically rigorous definition of space-time chaos, and proofs of its existence for lattices of weakly interacting local chaotic systems [71]. Another important advance was the discovery that that the appearance of coherent structures can be understood as a "thermodynamic formalism" phase transition [72], and existence of such phase transitions was proven for weakly interacting LDS [73]. It is an experimental and numerical fact that LDS and "reaction-diffusion" systems exhibit complex spatial patterns. The traditional perturbation theory cannot be applied to these important phenomena. The great challenge here is to develop a mathematically well-founded theory, not only for its intellectual merits, but also because the problems faced here might be well beyond what can be simulated by the conventional numerical methods.

C Dynamics of biological systems

SENIOR PERSONNEL: ***R.L. Calabrese****,* ***K. Wiesenfeld****,* ***S.P. DeWeerth****, G.S. Berns, R.J. Butera, Jr., W.L. Ditto, S.M. Potter, R.F. Fox, L.A. Bunimovich, P. Cvitanović, M. Schatz, R. Grigoriev*
OTHER PERSONNEL: 1-2 research associates, 3-5 graduate students funded by PFCNS each year: 3-4 research associates, 6-8 graduate students funded by other grants

Overview: The rapidly evolving fields of biophysics and bioengineering offer excellent opportunities for research advances over a broad front. At the same time, the interdisciplinary nature of the Center provides an unusually attractive environment to tackle selected problems in these fields. PFCNS seeks to capitalize on and strengthen existing ties between GT and EU in these fields. Our combined effort in this area brings together researchers from several GT units (biology, physics, and mathematics), the EU School of Medicine, and the recently established joint GT/EU School of Biomedical Engineering. This unit was formed in 1997 as a unique academic entity that evolved out of a need to formalize collaborative research efforts and provide an innovative educational forum between GT and EU. This academic unit reports to both the College of Engineering at GT and the School of Medicine at EU. The School of Biomedical Engineering takes advantage of the strong traditions of each institution, enabling the School to define new degree programs that integrate a rigorous grounding in life sciences and engineering, with real world experience in industry and clinical medicine.

The proposed MRC will focus specifically on investigations of biological systems which lend themselves to dynamical modelling. In this respect the tools we will use include both traditional ones applied to new problems, and newer tools that are themselves under continual modification and development. In the former category sits modelling via nonlinear stochastic differential equations and nonlinear time series analysis of very large, complex spatiotemporal data sets, while the latter includes modelling of neuronal systems in VLSI hardware, as well as hybrid systems which are part living tissue and part electronic circuitry.

The emphasis on dynamical modelling nevertheless allows us to consider problems that range in size and scope from subcellular processes to single cell, interneuronal, and whole organ levels. The phenomena share a common thread, complex, often chaotic and/or stochastic dynamics. Each of the projects described in the following have in place both experimental and theoretical components. The environment provided by PFCNS and its shared activities is expected to greatly enhance the number and quality of these interactions.

The planned PFCNS provides the kind of support, not available from individual grants, that is vitally important to sustain the inherently cross-disciplinary research on biological systems envisioned here. PFCNS will provide a stimulating environment for new research directions in biophysics and bioengineering by supporting cross-disciplinary post-docs, students, short-term (e.g., workshops) and long-term (e.g., resident scholars) visiting opportunities to attract to the PFCNS researchers from universities, national laboratories, and industrial research centers. These visitors are expected to benefit PFCNS interaction by acquiring new approaches to unsolved problems in their disciplines. At the same time, visiting scholars will invigorate the PFCNS research environment by providing fresh problems and sometimes fresh approaches that push back the current frontiers of dynamics in biophysics and bioengineering.

The research under this MRC falls into two focus groups, described in more detail below. The first addresses problems of spatiotemporal dynamics in neurobiological systems. The spatial aspect arises through interactions of individual parts, in this case neurons. The fundamental scientific questions and the tools we use to adress them depend on whether the number of interacting elements is small or large. When only a few elements are involved, the specific dynamical character of individual parts is important, and one seeks rather complete information about the effects of parameter variation and feedback control. It is here that analog VLSI and hybrid circuit methodologies are especially powerful. When the number of interacting elements is large, in our case ranging from several thousands (in neural tissue samples) to trillions (whole brain studies), the central problem is different as one looks for large scale emergent behavior. Here, it is imperative to develop new methods for identifying structure within huge sets of spatiotemporal data. The expertise of our research teams is well suited to tackling these challenges.

Focus group: Spatiotemporal dynamics of neurobiological systems

The projects within this focus group take advantage of the truly unique composition of the PFCNS team, which includes researchers from engineering, neuroscience, physics, and mathematics. Theoretical methods from nonlinear systems mix with technologies of analog VLSI electronics, high speed data acquisition and processing, fast optical imaging, and functional magnetic resonance imaging. For this focus group, the epicenter for these efforts is the Coulter Department of Biomedical Engineering, a joint venture between the GT College of Engineering and the EU School of Medicine.

A primary focus of this department and the associated Laboratory for Neuroengineering is the study of neurobiological systems combining the tools and techniques of engineering and the quantitative sciences. The associated faculty are all involved in research efforts that cross these boundaries, and can provide a conduit between the PFCNS and the neuroscience research being conducted at EU.

The Coulter Department combined with the EU Graduate Neuroscience Program provides expertise in a number of areas of neuroscience. Already, the formation of the GT Center for Nonlinear Science has begun to enhance interactions between these bioscientists and bioengineers, and nonlinear dynamicists in the physics and mathematics departments. The formation of the PFCNS will enhance that relationship and facilitate the long-term development of this cross- disciplinary research development.

The projects in this focus area fall into two categories. The first category is the *nonlinear dynamics of small networks* of neurons. In particular, this entails exploring the dynamics of individual cells and the coordination of their dynamics in the formation of small neuronal circuits. The second category deals with *large assemblages of neuronal elements.* Large networks cannot be studied on a cell-by-cell basis, but instead are explored through the analysis of the collective dynamics of populations of cells. A theme which pervades all projects in both categories is the use of dynamical techniques in conjunction with cutting-edge instrumentation to explore the behavior of neurobiological systems. It is no exaggeration to say that we seek to answer questions that could not be addressed to any serious extent without this unique combination of tools.

Small Assemblies of Biological and Simulated Neurons: Brain functions such as information processing, memory formation and motor control often involve *oscillatory neuronal networks*. In investigating the cellular mechanisms, biologists have frequently resorted to small networks, typically from invertebrates. These networks are unique in that indivdual cells with known properties are visually identifiable, and the nature of the connectivity within such networks can often be determined on a cell-to-cell basis. Detailed data permits the development of *biophysically-based models* to study the dynamics and function of such oscillating networks. Mathematical modeling has been particularly useful in gaining insights into how such oscillations are generated and how they contribute to nervous system function.

More recently, a method known as the dynamic current clamp technique permits the interaction between real-time computational models and in-vitro cellular experiments. An alternative technique is the development of analog very large-scale integrated circuits (aVLSI) that possess dynamics similar to the computational models. PFCNS participants have significant experience with both techniques [74, 75].

The objective of this theme of research is to investigate the use of *hybrid-systems* models as a tool to analyzing and understanding the dynamics of small neuronal networks. Such hybrid systems are fundamentally experimental systems, yet the real-time simulation component offers complete specificity of parameters and complete observability of internal processess. Our efforts in this category will focus on two fundamental issues: *mechanisms of half-center oscillations* and *mechanisms of spike-synchronization*. An underlying theme in both lines of inquiry is to apply what is already know from a bifurcation analysis of computational models to investigate the dynamics of the experimental system.

The leech heartbeat *central pattern generator* (CPG) is an oscillatory neural network, which is one of the best described in terms of morphology, connectivity and dynamics. The heartbeat CPG consists of a set of seven segmentally repeated pairs of inhibitory heart (HN) interneurons located in the first seven segmental ganglia. Such oscillators made up of mutually inhibitory neurons or groups of neurons are often referred to as *half- center oscillators* [76]. A central challenge is to understand exactly how synchronization between the individual elements of the oscillatory pair occurs. To address this we will begin by improving existing dynamical models so as to account for recent experimental results. The models assume that the HN cells in isolation were not capable of rhythmic bursting oscillations in the absence of synaptic coupling to other cells. We now know that isolated HN cells are capable of rhythmic oscillations. A bifurcation analysis of the model (see Fig. 6) illustrates that the parameter regime where individual cells are capable of intrinsically bursting is quite small.

By incorporating real-time simulations with experiments on single HN neurons, we will be able to modify HN cell conductances and test whether or not the diagram above is a true representation of the dynamics of the individual HN cells. We will then proceeed to study mechanisms of sychronization between HN neurons, using both real-time simulations and are aVLSI models of HN cells (see Fig. 7a).

In a parallel project, the goal is to understand the fundamental dynamical mechanism underlying spike synchronization. *Synchronization of spiking neurons* is a fundamental process in both the generation of rhythmic patterns as well as inforamation processing and representation. In the simplified case of two coupled neurons, conventional wisdom has it that excitatory synapses, as well as gap junctions (electrical coupling) lead to in-phase synchrony, while inhibitory synapses lead to anti-phase synchrony. However, recent computational and theoretical work has shown that such generalizations are questionable in their generality. It has been demonstrated that inhibitory synaptic coupling can lead to synchrony, excitatory coupling can be destabilizing, and the gap junctional coupling does not always lead to synchrony and can cause anti-phase synchrony to occur [77, 78]. While experimental evidence and computer simulations strongly support a role for inhibitory synapses serving to sychronize neural networks, neither this phenomena nor most of the others shown here have been conclusively demonstrated experimentally. (One notable exception is ref. [79].)

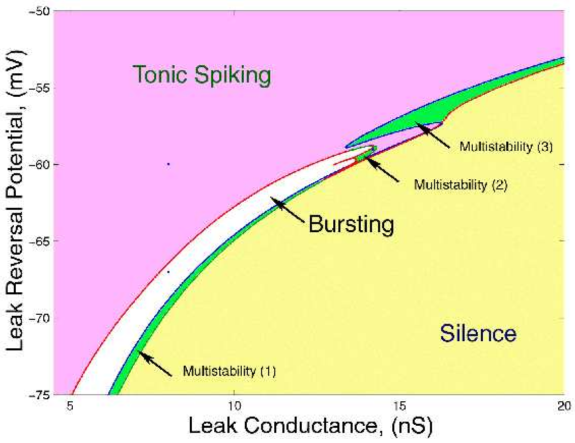

Figure 6: Bifurcation diagram of a single model HN cell showing different dynamical oscillatory modes.

Using our hybrid systems, we will couple pairs of neurons from the buccal ganglia of the pond snail Helisoma Trivolvis. This animal was chosen since the buccal ganglia is a symmetrical pair of clusters of neurons, this it is possible to identify a pair of neurons with similar electrophysiological properties. Our real-time simulation methodologies [80] enable us to simulate the kinetics of fast synapses at rates up to 40 kHz. The first step is to artificially couple pairs of neurons using this approach to study how the dynamics is altered as the sign and kinetics of the coupling are varied. We will also study the effect of electrical coupling.

The results of these experiments will yield in vitro bifurcation diagrams that can be used to describe the parameter-coupling regimes of the experimental system and attempt to validate earlier theoretical work on neuronal synchronization with a real experimental system. The Fig. 7b illustrates data from Butera's laboratory, coupling a simulated spiking neuron running in real-time with a single neuron from the pond snail. The top panel illustrates in-phase synchrony between the in vitro and simulated neuron (cross-correlation to right). The bottom panel demonstrates anti-phase synchrony under a different set of synaptic parameters. Further efforts will aim to extend previous work studying the syncronization dynamics of aVLSI neurons to hybrid systems of aVLSI neurons and in vitro neurons.

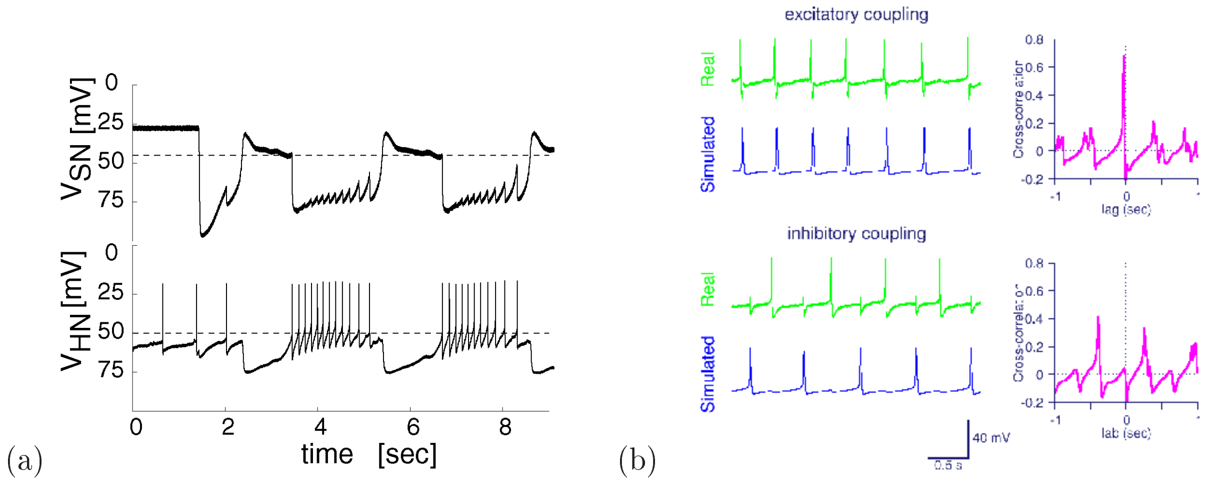

Figure 7: a) aVLSI HN cell (top) coupled to in vitro HN cell (bottom). b) In-Phase (top) and anti-phase (bottom) coupling between a real (green) and simulated (blue) invertebrate motoneuron. Cross- correlations shown to right.

Large Networks of Vertebrate Neurons: We will concentrate on two projects that involve very large collections of neuronal elements. In one, the system consists of cultured networks of thousands of mammalian neurons. In the other, the system is the human brain. These are admittedly ambitious projects that are at the far frontier of what might be possible. Nevertheless, they represent an important component of the PFCNS scope in tacking new problems that require new methods as well as cross-disciplinary thinking.

The first project will study the collective dynamics of ensembles of neurons with *neural dynamical computing* in mind. Everything that mammalian brains do, they do by the co-operation and interaction of many cells. We aim to discover how information is represented and stored in a distributed fashion in living neural networks, and how it is used to control behavior [81].

Most electrophysiology has been done using one or a few micropipette electrodes. By recording neural activity optically, using voltage-sensitive dyes (or fluorescent proteins), we will learn how activity propagates through the excitable medium of a cultured network of several thousand mammalian neurons. We designed and built a unique high-speed CCD camera for this purpose [82] (see Fig. 8a). It represents a significant advance in resolution over commonly used photodiode arrays, and is unmatched in sensitivity by commercially-available high-speed imagers. This allows us to image individual action potentials in many cells, without averaging, which is necessary if we wish to observe the role of noise or dynamics that vary from trial to trial. We developed a breakthrough in neural culture [83] that has enabled us to grow primary neuronal cultures for well over a year, on multi-electrode array substrates (see Fig. 8b). This allows us to record spontaneous or elicited neural activity from 60 electrodes (a few hundred cells) and to stimulate them non-destructively. We developed a feedback system in which the network's own activity (motor output) influences its stimulation (sensory input) via a simulated animal, the Neurally Controlled Animat [84]. With this tool, we have observed a wide variety of chaotic and patterned dynamics in cultured networks, on time scales ranging from milliseconds to months.

A major bottleneck for this research is that we are swamped with too much data, and insufficient analytical tools to find the underlying structure in these patterns. This is precisely where close collaboration with theorists in nonlinear dynamics may lead to advances in elucidating the structure of the dynamical landscape of these nets, in multi-dimensional activity space. And more relevant to human brains, how we can alter these dynamics with feedback stimulation to model perception, learning, memory, and other basic properties common to all neural systems. It is likely that the mesoscale dynamics that we uncover with these new tools (both hardware and theoretical) will be applicable to those in living animals, including humans. By using a reduced preparation of a few thousand cultured neurons (with glia), we have the unique ability to observe activity and changes in every single cell that forms part of the net, to follow activity all the way from the bottom up. And by using the net to control the behavior of simulated (or mechanical) animals, we can demonstrate the relevance of our findings to the top-down neuroscience community as well as utilize living neurons in devices like biosensors and nonlinear biocomputers.

(a)

(b)

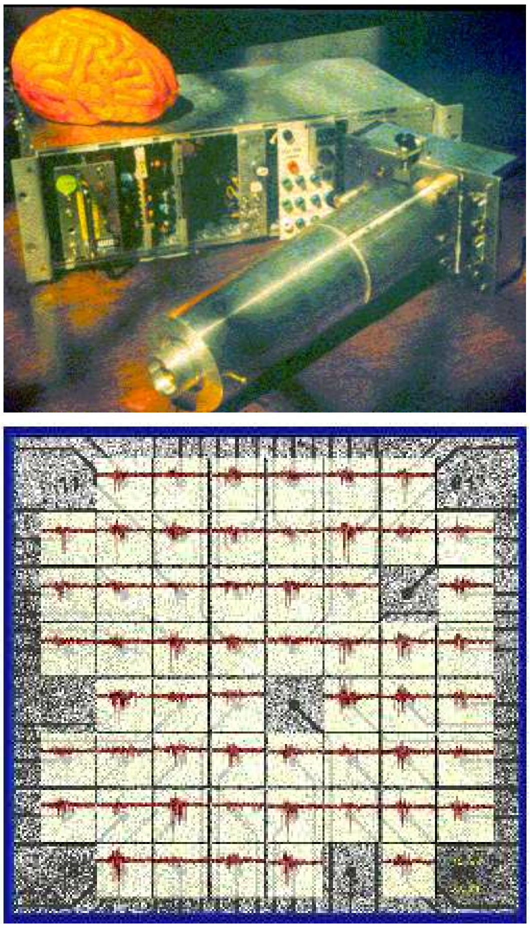

Figure 8: a) A high-speed camera for neuronal tissue recordings. b) A multielectrode array for interfacing to neuronal tissue in vitro.

To understand neural circuits at this mesoscopic scale, and to make the connection between individual cells and behavior, we will benefit from a collaborative environment where theorists, modelers, and neurobiologists work together toward a common goal. The proposed PFCNS will create just this sort of environment.

Another project, this time involving *brain scans of human subjects*, tackles the same fundamental problem: how can one recognize and usefully extract patterns from extremely *large spatiotemporal data sets*? In a new collaborative effort between EU and GT, we design, execute, and analyze experiments investigating the relationship between brain activity and cognition [85]. The central question is how to understand the large amounts of spatiotemporal data available to us in experiments that use functional Magnetic Resonance Imaging. The technique allows one to get both spatially and temporally resolved information about a subject's brain activity. We are exploring new ways to analyze the large data sets using recent ideas and techniques developed in nonlinear dynamics. In turn, we are developing experimental protocols which make the best use of these methods' strengths.

Experiments performed at EU School of Medicine monitor a subject's brain activity while the subject performs a simple motor or cognitive task. Despite ample evidence for the nonlinearity of neural activity [86], conventional neuroimaging studies take a linear, subtractive approach to experimental design and analysis. Our approach takes a different paradigm as its starting point, namely, that of bifurcation theory. Thus, we seek situations under which a continuous variation of the cognitive task results in a sudden qualitative change in a subject's behavior, an event which we then view as a bifurcation of the neural system.

In addition to direct analysis of the spatiotemporal data by modern time series methods, we will also develop a model-based approach to investigate essential (if unglamorous) issues concerning the relationship between the measured brain activity and the actual brain activity. This is needed to account for unavoidable physiological factors affecting the measurements. For instance, the relatively slow hemodynamic response smears out the measured activity in a way which could mask intrinsically interesting complex dynamics.

Focus group: Stochastic dynamics in biological systems

The interplay of stochasticity and nonlinear dynamics leads to important and often surprising results. The discovery and development of some of these effects has been the focus of intense study among physicists. More recently, attention has turned to the impact these ideas might have for biological systems. Among the most famous of these phenomena are stochastic resonance and Brownian ratchets [87].

PFCNS faculty has made primary contributions in this field, both in physical and biological contexts. A primary function of PFCNS would be to sponsor an interdisciplinary workshop and support visitors doing either collaborative or closely related work. This would complement existing projects which are funded individually. Such PFCNS sponsored interactions would create a fertile environment and foster new lines of research. Our optimism stems in part from the continuing success of the already functioning local program, the EU-GT Biomedical Technology Research Center seed grant program. A number of PFCNS faculty have entered collaborations in the life sciences with the help of this program.

Our initial emphasis will be on three current areas of interest. The areas are natural because they are important, are ripe for immediate progress, and deal with topics on which we have considerable prior expertise.

The first concerns *rectified Brownian movement.* This phenomenon potentially provides a unified mechanism for a great many basic cellular processes whereby metabolic Gibbs free energy is converted into mechanical work [88]. The fundamental idea is that in these processes ATP does not do mechanical work directly; rather, it is responsible for switching on and off asymmetric boundary conditions for thermal diffusion. In many instances, this mechanism explains what is otherwise hypothesized to be some sort of direct chemomechanical conversion of ATP into useful work. Recently, rectified Brownian movement has been used to explain several molecular and cellular processes, including ubiquinone transport across lipid membranes in electronic transport chains, allosteric conformation changes in proteins, P-type ATPase ion transporters, rotary arm enzyme complexes, the dynamics of actin-myosin cross bridges in muscle fibers, and kinesin motion along microtubules.

As a result of these recent studies, there is reason hope that rectified Brownian movement is a very general and in a sense universal mechanism in the nanobiology of intracellular processes. The challenge now is to focus on the more formidable examples, such as the interaction of myosin and actin in muscle fibers, protein and RNA transport through membrane pores, and the mechanism of bacterial flagella rotation.

In a second project, we explore how thermal noise affects the mechanoelectrical transduction of hair cells in the auditory system. In vitro experiments at EU by project collaborator F. Jaramillo (now at Carleton College) showed that hair cells exhibit *stochastic resonance*, so that the detection of weak signals was enhanced by the presence of added noise [89], see Fig. 9. Stochastic resonance has been observed in a variety of neuronal systems, and has led researchers to ask whether it plays a functional role, for example in the detection of predators or the identification of food [90]. To determine whether noise plays a functional role is fraught with difficulties, of course. However, the hair cell is a particularly apt candidate to explore this question, for two reasons. First, since the transduction is mechanical the relevant source of noise is easy to identify, namely Brownian motion of the hair bundle due to the surrounding fluid. Second, the physiology of these cells, and particularly the hair bundle, is well characterized, which makes it possible to write down accurate equations of motion. Intriguingly, the hair cell shows stochastic resonance at noise levels comparable to the inherent Brownian motion of hair bundles in vivo.

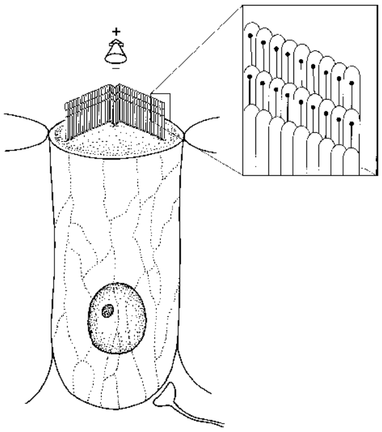

Figure 9: Illustration of a hair cell. For simplicity, only one hair bundle and one ion channel is drawn (at the top and bottom, respectively). The inset shows that the hair bundle is really an array of individual hairs, arranged in ranks.

There is room for progress on both theoretical and experimental sides. The hair bundle is made up of many hairs within each rank, which raises the interesting possibility that array enhanced effects may play a role. The study of the full model, through numerical simulations at first, will allow experiments to determine the expected *in vivo* behavior through a series of *in vitro* runs where the bundle motion is constrained to move by external manipulation, which has certain advantages over generating controlled pressure waves in the fluid.

If confirmed, the hypothesis that noise plays a functional role in hair cells could provide a neat explanation of a long-standing mystery: why are the majority of hair cells in the cochlear not free-standing, but attached to a rigid membrane? The issue is whether (as appears to be the case) noise only enhances transduction for sub-threshold stimuli. If so, the function of the free-standing population may be to detect the weakest signals, in which case being unattached is beneficial since it means much larger Brownian fluctuations.

NIH is funding ongoing experiments at Carleton, and development of a model of the hair bundle transduction process, in a collaboration between Jaramillo and Wiesenfeld. In addition to workshop activity in this focus area, PFCNS would support an extended visit of Jaramillo to GT; experimental resources would be available in the laboratory of Ditto, who has long standing expertise in the study of stochastic resonance.

The third project also involves close interactions between experiment and theory, and concerns the role of *noise in neocortical interactions*. Neocortical data obtained from experiments on rats [91] serve as a basis for a biologically relevant mesoscopic neural network model. Exact results can be obtained for noise driven binary interactions; the robustness of certain dynamical properties allow us to extrapolate to more complex types of interactions. This approach fills the gap between detailed biophysical simulations which cannot make rigorous global predictions and generalized models which allow exact statements but on a level of description remote from biology.

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M. Schatz, Assistant Professor, Physics (COS)
S. P. DeWeerth, Associate Professor, Electrical and Computer Eng. (COE)

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R. J. Butera, Jr., Assistant Professor, Electrical and Computer Eng. (COE)
W. L. Ditto, Professor, Biomedical Engineering Department (GT/EU)
R. F. Fox, Regents' Professor, Chair of School of Physics (COS)
J. Geronimo, Professor, Mathematics (COS)
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E. R. Weeks, Assistant Professor, Physics (EU)
K. Wiesenfeld, Professor, Physics (COS)

The key to the school and departmental abbreviations used throughout the proposal:

GT	Georgia Institute of Technology
EU	Emory University
EUSM	Emory University School of Medicine
GSU	Georgia State University
COS	College of Sciences
COE	College of Engineering
BME	Georgia Tech/Emory Biomedical Engineering Department
ECE	Department of Electrical & Computer Engineering
ME	Mechanical Engineering
Chem	School of Chemistry and Biochemistry
Math	School of Mathematics
Phys	School of Physics
CCMST	Center for Computational Molecular Science & Technology
CDSNS	Center for Dynamical Systems & Nonlinear Studies

8 Education, Human Resources, Diversity, and Outreach

A unique aspect of nonlinear science is that research is driven by the flux of ideas across disciplinary boundaries. Given the essential role students at all levels play in conducting research, such flux is most effectively generated through the establishment of a **cross-disciplinary training program** integrating research, education, and training with the dual goals of attracting a wide range of undergraduate, graduate, and postdoctoral students to physics and providing them with a stimulating and thoroughly modern learning environment. To ensure the success of the program, a large fraction of the PFCNS funded graduate students will be co-advised, with one advisor from student's home department and the other external, at least one of the advisors being a PFCNS member. This arrangement will greatly assist in initiating new cross-disciplinary collaborations.

On the other hand, equipping students with skills that are cross-disciplinary, method based, rather than discipline specific, nonlinear science is uniquely positioned to **offer the students a broad, diverse education**, and prepare them for today's rapidly evolving professional environment. Coupled with the cross-disciplinary nature of PFCNS, such training will meet the recommendation of the NRC report [1] to physics departments "to review and revise their curricula to ensure that they are engaging and effective for a wide range of students and that they make connections to other important areas of science and technology". In order to effectively achieve these goals, the proposed research and training programs will transcend departmental boundaries, differing from the conventional training model in a number of significant ways.

The success of the training program will crucially depend on the availability of the infrastructure that can only be created by a Center such as the proposed PFCNS. The need for a strong foundation in the analysis of nonlinear dynamical systems is common to many research programs in science, engineering, and mathematics. At GT, courses on nonlinear dynamics [92] are currently taught in the mathematics and physics departments, each from a different perspective, and draw students from biomedical, chemical, aerospace, civil, electrical and mechanical engineering, materials science, and chemistry. While students would clearly benefit from a program based on a broad, coherent, and unified view of nonlinear science, college and school boundaries need to be superseded by a framework that integrates what otherwise would be isolated collaborations between individual faculty members. The program built around the PFCNS initiative will generate a new level of integration in graduate and post-graduate education by involving faculty in different departments in an effort to unify the nonlinear science curriculum across the participating schools. Equally important, combining the resources of the Center's MRCs will make it possible to offer undergraduate level cross-disciplinary courses to students from participating institutions.

The core of the cross-disciplinary training program will consist of an **Introductory Nonlinear Science** course on the mathematical and computational techniques of nonlinear science followed by a rotating sequence of **Applications of Nonlinear Dynamics** courses based on the research interests of individual Center members and rounded out by a semester of **Special Topics in Nonlinear Science** featuring research on specific projects carried out by small teams supervised by faculty members with complementary expertise and perspectives. The level of courses will vary from advanced undergraduate to second year graduate, targeting the range of students that can be most effectively recruited into research programs. As one of the new initiatives, PFCNS will offer an advanced web-based year-long gradute nonlinear course [6], which will play an important role in reaching and educating students at remote locations and attracting them to the program. The courses will gather all nonlinear science students in an activity that stresses commonalities among various fields, and it will provide a sense of intellectual community fundamental to the success of the program. The course work will require coordinated collaboration with peers and teachers from different backgrounds, helping students develop communication skills that will prove invaluable in future careers in industry or academia.

This training will equip young researchers with the tools and intuition needed to tackle complex nonlinear problems arising in many guises and various technical fields. In order to offer students a deep learning experience outside the Ph.D. thesis research, the educational core of the training program will be supplemented by the following important components. A **welcoming workshop/retreat**, before the start of each fall semester, will introduce the incoming young researchers to the PFCNS. New students will pair up with a nonlinear science advisor, preferrably from outside their own department, who will oversee the student's progress during the first two years in tandem with the departmental advisor. An **Interdisciplinary Nonlinear Science Seminar** series [92], initiated in January 2001, has drawn a wide attendance from the participating departments and institutions. PFCNS would enable us to run the seminar on an ongoing basis and to broaden its scope to engineering and biological applications. **Graduate Student Seminars** organized for and by the students will give them opportunity for public presentation of their own research in a supportive setting, engage them in mutually beneficial exchange of ideas, and generally enhance their communication skills; it will also provide a forum for directed discussions on ethics and conflict of interests in research. An active **visitor program** will help promote and maintain national, international, and industrial collaborations. Priority will be given to visitors whose research relates to that of participating PFCNS faculty, and who demonstrate potential as external mentors to our graduate students and junior researchers. A **Regional Nonlinear Workshop**, a yearly cross-disciplinary meeting organized jointly with other Southeastern universities such as Duke, U. of Alabama, and U. of Florida, will expose students from regional universities to the forefront of research, and give them an opportunity to present their own work in poster sessions. **Joe Ford Fellowships**, named in honor of late GT Professor Joseph Ford, one of the pioneers of classical and quantum chaos, will sponsor several outstanding postdoctoral fellows each year. These Fellows, associated with the Center, rather than its individual members, will have complete freedom in choosing their research directions and serve as a glue between different research projects. In addition, by combining the resources of the Center, the Departments, and the Institute, the PFCNS will be able to make competitive **graduate fellowship** offers to incoming graduates, making the program more attractive to a wider range of students. These fellowships will be primarily used to support co-advised students, covering the first two years during which students are normally supported as teaching assistants, allowing them to concentrate on the study and research in nonlinear science.

Joining the forces of the affiliated faculty and students is instrumental in making a coherent contribution to a number of outreach programs organized under the umbrella of the GT Center for Education Intergrating Science, Mathematics, and Computing (CEISMC) [93] and targeted at the middle and high school students and teachers. For instance, participation in such programs as **FutureScape** and the NSF-sponsored **Integrating Gender Equity And Reform** (InGEAR) will help educate girls and young women about careers in nonlinear science, broaden their horizons and raise their aspirations by exposing them to careers they may not have contemplated otherwise. The Center will also actively participate in the new **Post-secondary Readiness Enrichment Program** (PREP) created by the University System of Georgia. This program addresses primarily the seventh grade and is designed to assist students and their parents in making timely, informed decisions that will adequately prepare young people for their higher education and career goals. The Center will also provide the foundation for continuing educating in the area of Nonlinear Science of those high school and middle school science and mathematics teachers enrolled in the year-round **Georgia Industrial Fellowships for Teachers** (GIFT) program, whose primary goal is to provide the exposure to the cutting edge research in the academic and industrial settings.

At the college level, following up on the success of the NSF Southeast Applied Analysis Center [5] outreach program, PFCNS members will be sent to deliver lectures on various topics of modern physics, biology and mathematics as **Center Ambassadors** to Southeast region non-research educational institutions and historically black colleges and universities. PFCNS will offer teaching reduction to the members who perform exceptionally as such lecturers, and implement a series of measures to aid recruitment and retention of students from under-represented groups, such as offering **Summer Internships for Minority Undergraduates**. Both GT Physics and GT Chemistry run highly successful NSF-funded **Research Experience for Undergraduates** (REU) programs, bringing some 30 gifted undergraduates to GT every summer, some of which are advised by the PFCNS faculty. In summary, the goals of the PFCNS outreach program are to bring the inspiration of cutting edge physics research to bright undergraduates, K-12 students, and teachers, to build bridges to faculty isolated at non-research institutions, and to inform talented students about the attractiveness of GT graduate programs.

The *assessment* of effectiveness of PFCNS outreach program is detailed on p. 45.

The above range of activities, while highly desirable, cannot be sustained by the individual grants. The very existence of the proposed program hinges on the availability of cross-disciplinary funding, something that only PFCNS can make possible.

9 Shared Facilities

The PFCNS will require substantial single- and parallel-processor computing resources to implement the MRCs' objectives. GT's CCMST [94], whose co-director, R. Hernandez, is a CNS member, is presently providing a limited number of compute cycles on a 72-processor IBM SP2 to CNS members. Up to one third of this machine will be available to the PFCNS with the part-time funding of a research scientist and a commitment to PFCNS to upgrade part of the facility at year 3.

10 Collaboration with Other Sectors

Cross-disciplinary workshops, internships and other training initiatives will make use of the extensive connections the PFCNS faculty has with other institutions and labs. We now provide a few examples of such cross-fertilization initiatives already in place. First, the already established **institutional cross-connections**:

- PFCNS will collaborate intensively with the *NSF IGERT* programs at Northwestern [3], Cornell and U. of Arizona, as well as with a number of other leading centers for nonlinear science (check the Center webpage [95] for a complete list). The ties are particularly close to the Northwestern IGERT, originally led by P. Cvitanović.
- GT is one of the six university partners in the team which operates the *Oak Ridge National Laboratory* (ORNL), linking the lab to academic research. Geographically close, and with common interests in complex and nonlinear systems, GT PFCNS and ORNL already plan several collaborative initiatives (detailed below).
- As a member of the External Advisory Board for Space Medicine and Life Sciences Research Center, GPN advises researchers at the *Morehouse School of Medicine* on fluid mechanics aspects of tissue growth.
- The PFCNS fluid dynamics GT Physics & ME program [MS,RG,GPN] interacts the *Institute of Paper Sciences & Technology* (C. Aidun) housed at GT, where the fundamental problem of pattern formation is relevant to increased efficiency in coating of paper.
- GSB and KW have formed a "Hyperscanning Consortium" with colleagues at Baylor College of Medicine, Princeton University and Caltech, in order to perform synchronized MR scanning of people interacting with each other, and study brain patterns of interacting groups of humans.

Every PFCNS faculty member has extensive external collaborations. Here we highlight a few examples of **cross-institutional research ties** that would be enhanced by the PFCNS visitor, internship and workshop programs:

- KW and R. York (UC Santa Barbara, Electrical Eng.), T. Heath (GT Research Inst. staff scientist) - *Fast Dynamical Control of Antenna Arrays*: Experiments at Santa Barbara are testing a new scheme for very fast manipulation of electromagnetic beams, scheme based on GT theoretical advances in understanding how synchronized nonlinear oscillators behave under variations of the element parameters.

- ERW and H. Stone, S. Koehler, and S. Hilgenfeld (Harvard) – *Drainage flow through channels in foams*: Changing the surfactant properties changes the flow from plug-like to Poiseuille-like inside the channels.
- KW and F. Jaramillo (Carleton College, Biology) - *The role of noise in the auditory system*: The "stochastic resonance" experiments are being performed at Carleton College, and a model for the hair cell is under development at GT (see p. 31).

Internships: We have contacted a number of potential hosts who have expressed their interest in participating in the internship program (see p. 41). Close contacts between the interns' advisors and hosts will contribute substantially to turning internships into full-fledged collaborations. To give a flavor of what we have in mind, we give here two examples of potential hosts and what they would offer. Others will be contacted on case by case basis, pending specific PFCNS student or host research initiatives.

- *D. del-Castillo-Negrete, Oak Ridge National Laboratory.* Theorist, expert on the application of dynamical systems methods to the study of transport problems in fluids and plasmas, dynamics of many-body Hamiltonian systems with long range interactions, and pattern formation in reaction-diffusion systems, research interests shared with the PFCNS faculty. GT and ORNL are already partners on the institutional level, with long experience of GT students working at ORNL.
- *R.E. Ecke and R. Mainieri, Los Alamos National Laboratory.* Experiments on pattern formation in fluids. Theory of nonlinear dynamics, statistical mechanics of chaotic systems.

An internship at ORNL and LANL will provide a student with a unique opportunity to explore the research environment at a National Laboratory.

Workshops: PFCNS plans a series of workshops. On the national level, PFCNS will propose to host the *Dynamics Days 2005*, the main US annual meeting in nonlinear science, possibly in collaboration with the Oak Ridge National Lab. The *Regional Nonlinear Workshop* (see p. 41) currently under preparation is

- **ORNL-PFCNS Interdisciplinary Workshop on Transport**
  DATE: June 2003
  LOCATION: Oak Ridge National Laboratory
  ORGANIZERS: D. del-Castillo-Negrete (ORNL) and P. Cvitanović (PFCNS)
  FUNDING: Shared ORNL/PFCNS, with emphasis on graduate student stipends. 40 participants
  PROCEEDINGS: A focus issue of the CHAOS journal
  SPEAKERS: *(preliminary list) C. Jones (Brown, transport in oceanographic flows), R. Pierrehumbert (U. Chicago, transport in atmospheric flows), T. Tel (Eotvos U., Hungary, transport in chemical active flows), D. Astumian (U. of Maine, transport in biological systems), S. Wiggins (Bristol U., UK, transport in dynamical systems),*

R. Behringer (Duke, transport in granular flows), J. Gollub (Haveford College, experiments on transport), G. Zaslavsky (Courant Institute, NYU, transport in plasmas).
ABSTRACT: The study of transport is an important problem of common interest to many areas of science and technology including plasma physics, biology, chemistry, oceanography, atmospheric sciences, engineering, and dynamical systems. The goal of this cross-disciplinary workshop is to bring together experts from these areas for a discussion of nonlinear dynamics and complex systems techniques in the study of transport.

PFCNS academic environment: No less important than ties to other institutions is the immediate context in which PFCNS will operate. The overriding concern in setting up the Center structure (see sect. 13) is ensuring sufficient fluidity in faculty composition to enable us to recruit new talent into PFCNS as new cross-disciplinary research directions open up. GT and EU provide rich intellectual environment which will greatly enhance PFCNS effectiveness as a platform for cross-disciplinary interactions. GT School of Mathematics CDSNS [96] contributes excellent visiting researchers, seminars, and training opportunities in mathematical methods for nonlinear science. To name but a few, preeminent scientists such as E. Carlen, M. Loss, L. Erdos, E. Harrell (GT mathematical physics group), K. Mischaikow (GT Mathematics / director CDSNS), W. Gangbo (GT Mathematics / CDSNS), M. Borodovsky (GT Biomathematics), D. Dusenbery, R. Wartel (GT Biology), G. Hentschel and F. Family (EU Physics), and N. Chernov and N. Simanyi (U. Alabama Mathematics, Birmingham) will interact with PFCNS faculty and visitors. These excellent researchers could have equally well already been listed as PFCNS faculty, and they and others in Atlanta area will be inducted if new research directions merit their joining PFCNS.

11 International Collaboration

PFCNS plans to co-organize a number of international workshops. P. Cvitanović is the *Secretary of the European Dynamics Days Governing Board*, a *Honorary Chair of the Let's Face Chaos* conference (Maribor, Slovenia May 2002), and a member of other international conference committees. Since 1981 he has organized or co-organized more than 25 conferences, workshops and schools in Europe and US, and has a well established international partner network. Internationally, some fifteen *"Sister Nonlinear Science Centers"* located in Mexico, Germany, Denmark, United Kingdom, Italy, Israel, Argentina, Hungary, Chile and Austria are PFCNS's potential partners in organizing workshops, exchanging researchers, and hosting interns (for a complete list, please check the Center webpage [97]). A few examples:

- *Center for Chaos and Turbulence Studies* [4] - M.H. Jensen, director. A leading European center in physics of complex systems ranging from neuronal activity to quantum chaos, housed at the Niels Bohr Institute, Danish Technical University, and Nordita, Copenhagen. CATS will host PFCNS researchers and interns. PFCNS will host the Danish Research Academy *Danish Ph.D. School in Nonlinear Science* supported students and visitors. As many European Ph.D. programs require research training abroad, these and other similar exchanges will be very beneficial to the overall PFCNS recruiting effort.

- *Centro Internacional de Ciencias*, Cuernavaca, Mexico - T.H. Seligman, director. Promotes scientific exchange, with particularly strong Latin American visitor and conference program. PFCNS and CIC have a tentative agreement to co-organize two "pan-American" workshops, the first one on "Classical and quantum chaos in few- and many-body systems" in winter 2004 and the the second one in winter of 2006.
- *Max Planck Institute for the Physics of Complex Systems*, Dresden - H. Kantz, Head, Nonlinear dynamics and time series analysis group. The main European meeting ground for young researchers and leading international scientists in physics of complex systems, with intensive workshop, visitor, postdoctoral and exchange program. Collaboration with PFCNS desired in order to strengthen ties to US.

In addition - the space allotted does not allow a detailed listing - each individual PFCNS faculty member maintains **international research ties** that will enhance and be enhanced by the PFCNS visitor, internship and workshop programs.

12 Seed Funding and Emerging Areas

The unique position of nonlinear science lying on the interface of two or three different disciplines is reflected in the funding patterns specific to cross-disciplinary research: although established research programs have somewhat broader funding opportunities, it is substantially more difficult to find individual funding opportunitities for new research directions, since typically they will not be given priority by either of the core disciplines. This puts special emphasis on the availability of **seed funding in emerging areas**, especially high-risk ones.

The PFCNS will be able to provide such funding quickly and in an extremely flexible way. The highest priority will be given to collaborative research lying on the interface of different disciplines and involving faculty from different departments. Second priority will be assigned to joint research by the faculty members in the same department or discipline. In both cases at least one of the investigators will come from the PFCNS faculty. In general, the goal of seed funding will be to initiate and stimulate preliminary research in the novel and promising areas of opportunity, where no existing patterns of funding exist. Once the potential of a given direction is proven at the preliminary stage, individual and/or group funding from more conventional sources will be sought.

The availability of seed funds will be especially critical for the success of **junior faculty members** who typically do not have other sources of funding which can be used to initiate new research directions. The criteria and mechanisms for selecting and evaluating projects are addressed in sect. 13. Given the difficulties that even senior faculty members face in funding new research directions, this task becomes especially and unnecessarily complicated for junior faculty, who do not yet have a track record of successful research to warrant favorable consideration by the granting agencies. Providing junior faculty with such flexible funding will save a lot of time required otherwise to prepare, submit, and undergo a review of several full-scale exploratory proposals, enabling the junior faculty to concentrate instead on the proposed research. All of this is especially true where nonlinear science with its cross-disciplinary focus is concerned.

As was repeatedly stressed throughout this proposal, a distinguished feature of nonlinear science is that it is driven by cross-pollination of ideas between different disciplines as well as between different fields within natural sciences, engineering and medicine. As a means to promote such cross-pollination, PFCNS will organize and host a series of bi-annual **Applied Nonlinear Science Workshops**, bringing together PFCNS faculty and students and researchers from regional universities, national laboratories, and industrial research centers. Each year the workshops will target a different application area (e.g., neural dynamics, control of extended systems, plasma physics, biological excitable systems, etc.), fostering collaborations and transfer of ideas, creating new approaches, and stimulating new research directions by bringing together specialists with complementary research expertise.

Organization of such workshops depends crucially on the availability of centralized funding and infrastructure. On the other hand, by limiting the scope of the meeting and bringing together a sharply focused group of researchers, such meetings will play a role that neither the individual contacts nor the very broad international conferences such as the SIAM Snowbird meeting play. The workshops will serve the dual purposes of disseminating the methodology developed by the nonlinear community to other fields with the latter providing the focus for the research directions in the nonlinear science and, at the same time, establishing new collaborations between members of different institutions.

Complementing the above research-oriented activities will be a range of education-oriented activities, such as a Regional Nonlinear Workshop, internship support for outstanding students, and the development of a web-based nonlinear courses, all of which are expected to have a strong impact on the research component.

The **Regional Nonlinear Workshop** will differ significantly from the Applied Nonlinear Science Workshop in that it will be oriented primarily towards students of all levels. Scheduled yearly, this cross-disciplinary meeting will be organized jointly with other Southeastern universities such as Duke, U. of Alabama, and U. of Florida, it will be hosted on an alternating basis by the PFCNS and the fellow institutions. The main goal of the workshop will be to expose students from regional universities to the forefront of research, and give them an opportunity to present their own work in poster sessions. This workshop will have a broader scope, encompassing the whole field of nonlinear science. This broad scope will give the students the sense of diversity and at the same time closeness of the nonlinear science community, highlighting the many existing and prospective links between different directions pursued by different research groups.

PFCNS will offer to students and post-doctoral fellows of exceptional promise (either from PFCNS, or from outside) **internship support**, the goal of which is to significantly broaden and strengthen their education and provide young researchers with additional cross-disciplinary perspectives by exposing them to different experimental, computational, and theoretical approaches, using the expertise not available at GT/EU. For example, a trainee working on theoretical projects in the home institution might intern in an experimental lab in a host institute, or *vice versa*. In other cases the internship would provide a specific experimental technique or theoretical approach not readily available at the home institution, but important for the trainee's thesis research. In addition to this, the internship program will play an instrumental role in forging new collaborations and finding new areas of opportunity.

The trainee, aided by the home institution advisor, will make the initial contact with the internship advisor. A brief proposal will then be written that clearly states the goals of the internship, which is expected to last 3-6 months and possibly form the basis for a publication. The internships will be reviewed after the first three months by the PFCNS and home institution advisors to determine whether progress is sufficient to warrant an extension. The trainee will present his/her results in the Graduate Seminar Series, and, upon returning to the home institution, in the form of a written report.

Yet another component of the educational activity of the center, and an integral part of its outreach program, a **web-based nonlinear course** will play an important role in reaching and attracting students from remote locations, providing them with the inside look at the current research topics in classical and quantum chaos. Such course could be based on the ChaosBook [6], a hyperlinked web-based course currently under design by P. Cvitanović and coauthors, a novel and unique approach to teaching an advanced graduate level nonliner physics course. In addition to the extremely valuable potential of accessing the broadest possible audience, the major advantage of a web-based course compared to a textbook-based course is a unique opportunity to incorporate the dynamical aspects into the presentation. Such dynamical aspects realized through animations, java applets, interactive scripts, and so on, can only be implemented with a considerable investment of time and resources. Given the scope of the material, this will require involvement of a group of advanced undergraduate and/or graduate students for an extended period of time. Although clearly innovative and beneficial for the whole nonlinear science community, such a project cannot be supported by any individual grant and requires a centralized approach.

13 Management

Due to the full cross-disciplinary integration of the three MRCs, the day-to-day training, research, assessment and other activities of the program will be supervised by the Director and the faculty-elected Executive Committee (EC), (see sect. 7.D for its composition), whose task is to ensure that fellowships, internships, visitor invitations, and other PFCNS resources are awarded in accordance with the goals of the program. Faculty status implies no automatic entitlement to any part of PFCNS resources; EC will base all of its decisions on the quality and cross-cutting impact of each proposal put forth by the PFCNS faculty. The overriding concern in setting up the organizational makeup outlined here (and in more detail on the CNS homepage [98]) is ensuring maximal faculty participation, and sufficient fluidity in the Center structure to enable us to recruit new talent into PFCNS as new cross-disciplinary research directions open up.

The Director

The proposed PFCNS director is P. Cvitanović, the current director of the GT Center for Nonlinear Science (for prior experience, see sect. 6).

Director appoints PFCNS faculty and visiting faculty, and hires PFCNS post-doctoral fellows, administrative and technical personnel.

Director can appoint additional GT, EU or external faculty as one-year Associate Members of the PFCNS. After a year, such appointment lapses, unless the director deems the activity of the Associate Member to be of sufficient importance to the PFCNS to merit promotion to PFCNS faculty.

Director is responsible for PFCNS accounting.

Director presents the PFCNS yearly activity and assessment report to NSF.

Executive Committee

The day-to-day research, training, communications to participants and other PFCNS activities will be supervised by the EC. The initial EC will consist of the director and the four co-PI's on the PFCNS proposal. In order to ensure maximal faculty participation, in subsequent years the EC will be elected annually by the PFCNS faculty. A graduate student elected by PFCNS students for a one year term will serve as the EC liaison to the students.

The EC, chaired by the director, will meet prior to the start of each academic year, and then at least twice per semester during the academic year. Depending on the agenda, other faculty participants, or external experts may be invited by the director to take part as non-voting members. Points can be introduced to the meeting agenda by any PFCNS member, as well as by the graduate students' representative. The Center secretary is responsible for the minutes and their timely distribution to the PFCNS members.

The EC appoints, each year, a faculty member and a graduate student to run each of the seminar series, and another pair to organize the retreat and regional workshop. The seminar/workshop budget is set at the start of each academic year.

The EC discusses and proposes the allocation of PFCNS resources, as detailed below.

PFCNS/EU:
The PFCNS NSF grant will be administered by GT through the School of Physics accounting office. Researchers placed at EU will be supported by an NSF-approved annual subcontract to EU. At any given time PFCNS is expected to fund 1-2 post-docs co-advised by both GT and EU faculty, as well as 2-3 graduate students. However, no firm fraction of the budget is dedicated to EU vs GT, in order that the PFCNS EC retains maximal flexibility in determining the funding distribution mix which optimizes PFCNS research goals in any given year.

Allocation of Resources
The resources allocated by the EC:

- *J. Ford Fellowships.* PFCNS research associates will be recruited in a highly competitive J. Ford Fellowships search. J. Ford Fellows (hired normally for 2 years, maximally 3 years, described on on p. 35) will be free agents in the sense that they will be attached to the Center, with a small individual research grant, and not assigned to any individual faculty, and thus free to cross over research boundaries within the scope of the diverse research efforts pursued by PFCNS.
- *Seed funding, workshops.* The EC which select initiatives (detailed in sect. 12) which merit PFCNS support.
- *Visiting professors.* The EC might recommend appointment of a visiting professor (normally for an academic semester) if an exceptionally strong case is made for the PFCNS impact of such appointment.
- *Fellowships for incoming students.* One participating PFCNS program faculty member per department will be responsible for identifying potential graduate students for the program in the departmental applicant pool. The EC will review the applications, and any supplementary materials provided by the applicant's home department. Acceptance decisions will be made shortly after the decisions by the individual departments, in order that the PFCNS and departmental fellowships be effectively combined into attractive recruiting offers. Typically, the first nine months of a student's graduate study will be supported by departmental fellowships, with support through the student's second year of study guaranteed by an PFCNS fellowship.
- *Fellowships for advanced students.* After their second year students are eligible for PFCNS fellowships, contingent upon a co-advised, cross-disciplinary thesis project. The student will write a brief proposal, accompanied by his/hers advisors' letters describing the cross-disciplinary nature of the project. Decisions about the continuing fellowships, which typically begin in the Fall, will be made each Spring in order to give the students and their advisors ample planning time.
- *Internships.* Students and research associates are encouraged to apply for internships, as described in sect. 12. The student's proposal will explain his or her choice of host group, and outline the research topic to be investigated with particular emphasis on the research perspectives gained that are not available locally.
- *Visitors program.* To ensure the cross-disciplinary impact of the visitor program,

applications for visitor funding that are filed jointly by faculty members in different departments will be given preference. Graduate students will also be encouraged to nominate potential visitors through their representative on the EC.

- *Summer Internships for Minority and Women Undergraduates.*
  Applications and/or nominations for summer internships for promising women and/or minority undergraduates will be sought by advertising, through GT and EU programs, and through faculty contacts, see p. 36. Qualified students that can be paired with one of the PFCNS faculty will be offered support.
- *Travel funds for conferences.* Students and research associates may request funds to help cover the travel expenses of attending conferences and workshops. Decisions on internship, visitor, equipment and travel fund requests will be made at the quarterly EC meetings.
- *Infrastructure, operational expenditures.* As detailed on p. 47, most of the infrastructure (office space, administrative support, computing) needed for PFCNS operation is already in place, through GT funding of the pilot Nonlinear Science Center, so the proposed PFCNS can commence a full scale operation immediately. Any salary, fellowship, purchase of instrumentation, travel, computer equipment, or other expenditure or funding commitments exceeding in total $8,000 will be considered by the EC prior to director's authorization.
- *Day-to-day expenditures.* Daily operational expenditures, travel grants and short term visitor reimbursements are approved by the director.

Assessment

The EC will prepare an annual report for NSF that assesses the progress and success of the program. During the first two years of the PFCNS grant the focus will be on evaluating the various individual components of the program with the aim of providing the feedback necessary to modify and improve each aspect of the program. Specifically, we shall assess each of the following components separately.

- *Training.* Quantitative indicators of the success of the course are (1) the number of students enrolled, (2) the fraction of the students retained in the second semester, (3) the number of different departments represented by the graduate students and by the faculty, (4) the number of students outside the PFCNS who enroll in the course, (5) the number of faculty actively involved in the course, and (6) the number of projects that lead to publishable results. Other indicators of success are the number of group-projects that lead to longer-term investigations, and new collaborations between faculty and/or students.
- *Nonlinear Science Seminar and Visitor Program.* The seminars and the visitors should provide cutting-edge research relevant to the program participants, and also give the students a broad perspective of nonlinear science. The impact of the seminar series will be assessed through quarterly student questionnaires assessing their

interest in the presentations, as well as the extent to which they have provided the students with a general perspective of the field.

- *Regional Workshop.* A measure of success is the attendance and participation in PFCNS organized workshops by students, post-docs and senior researchers not only from GT/EU, but also from other universities in the Southeast.

After the program has been running for at least two years, it will be possible to examine some additional indicators of the effectiveness of the program:

- *Research objectives.* Have some of the target problems been solved? What is the research progress of each MRC, each focus group? Has the program led to publications that would not have been possible outside the PFCNS framework? Does the list of journals where PFCNS program publications appear reflect an impact of the PFCNS suported research on more than one field? Should a mid-course correction be undertaken?
- *Internships.* The first indicator is the number of young researchers who apply for an internship, as well as the number who submit a report applying for extension of the internship beyond the first 3 months. (Together with the assessment by the host researcher, this report aids us in determining whether the internship is meaningful and should be extended.) Students' final reports, and possibly a publication arising from the work, would provide a basis for assessment of the internship.
- *Retention.* An important indicator is the retention rate of students in the program after their first two years, *i.e.*, the number that continue with cross-disciplinary thesis research that qualifies for PFCNS fellowships.
- *Graduate training.* One of the most important indicators will be the number of cross-disciplinary Ph.D. thesis projects made possible by the PFCNS program. Evaluation of the success of these projects, compared with more traditional Ph.D. theses, will be made. An estimate of the number of thesis projects that lead to new cross-disciplinary faculty collaboration within GT/EU and with external researchers will also be made. Time-to-degree will be carefully monitored; the aim is to develop a program that does not increase this number.

14 Institutional and Other Sector Support

Georgia Tech boasts a strong faculty in nonlinear sciences, ranked 5th nationally in the 1999 U.S. News and World Report survey. Its commitment to strengthening the research effort in this field is demonstrated by recent chaired faculty appointment in physics (Cvitanović), continued recruiting efforts in mathematics (through the CDSNS) and physics (senior or junior experimental nonlinear physics faculty search for 2002), and the School of Physics strategic plan that calls for expansion in nonlinear and biosciences (possibly including chair appointments).

Georgia Tech actively encourages cross-departmental and cross-disciplinary research. The *GT Center for Nonlinear Science* (CNS) which began operation July 2001 already aims at furthering such an environment and acts as a seed program for the proposed PFCNS which will make it possible to span GT COS, GT COE, EU Medical School and Georgia State University nonlinear science efforts within the Center.

The PFCNS office and the common meeting room will be housed in Physics. The building has student computer laboratories, and an experimental computation laboratory is operational in the Math building [99]. The participating faculty laboratories are situated at GT, EU and EUSM. Shared office space and computer facilities for the PFCNS junior researchers and graduate students is already in place.

The Deans of the participating Schools and the Institute, at the level of the University's Vice-Provost for Research, strongly support the initiative, and are already funding the CNS for an initial three-year period. As a seed cost-sharing contribution, GT has committed \$147K/academic year funding for period 2001-2004, providing funding for 2-3 postdoctoral research associates, a distinguished lecturer series, visitors, workshops, the Nonlinear Science seminars, full-time secretarial support, and part-time computer/web support. In addition, GT has already committed \$30K for equipment funds to cover the equipping of research associates' offices, research infrastructure including computer network, servers, a platform for intensive computation, software, printers, and CNS office equipment.

15 Letters of Support

Appended is the GT cost-sharing commitmnent letter of support from Professor Charles L. Liotta, Vice-Provost for Research and Graduate Studies.

Summary Table of Requested NSF Support

Activity	Year One	5 Year Total
MRC 1: Chaos	\$335,636	\$1,678,183
MRC 2: Extended Systems	\$223,758	\$1,118,789
MRC 3: Dynamics and Biology	\$279,939	\$1,399,695
Shared Facilities	\$321,652	\$1,338,256
Seed Funding and Emerging Areas	\$561,375	\$2,806,875
Education and Human Resources	\$98,600	\$493,000
Outreach	\$56,250	\$281,250
Administration	\$71,152	\$355,762
Total	\$1,948,362	\$9,471,810

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[3] Northwestern U. Dynamics of Complex Systems in Science and Engineering, `www.complex-systems.northwestern.edu`.

[4] Centre for Chaos And Turbulence Studies, `www.nbi.dk/CATS/Welcome.html`.

[5] The Southeast Applied Analysis Center, `www.math.gatech.edu/saac`.

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