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Title:

Applied Nonlinear Stochastic Dynamics

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Los Alamos
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Applications of Nonlinear Stochastic Dynamics

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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). This is a fundamental research project whose aim is exploiting the last decades' progress in understanding the dynamics of nonlinear and/or noisy systems in applications to a variety of problems in theoretical physics, chemistry and biology. The common denominator here is the fundamental role played by the ***combination*** of nonlinearity, noise and/or disorder in the dynamics of both simple and complex systems, and the underlying theoretical problems have much in common within the paradigms of nonlinear science. This project extends a technology base relevant to a variety of problems arising in applications of nonlinearity in science, and applies this technology to those problems. Thus, numerical simulations and experiments focused on nonlinear and stochastic processes provide important insights into nonlinear science, while nonlinear techniques help advance our understanding of the scientific principles underlying the control of complex behavior in systems with strong spatial and temporal internal variability.

Background and Research Objectives

During the last 15 years nonlinear, nonequilibrium science has flourished, driven by a number of new concepts and techniques, including: (i) coherent space-time structures in strongly nonlinear systems; (ii) deterministic chaos, even in low-dimensional nonlinear dynamical systems; and (iii) the coexistence of (i) and (ii), leading to a variety of "complex" phenomena with strong spatial and temporal internal

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variability. The importance of "noise" and "disorder" has long been known in *linear* systems. However, we have only recently gained enough insight into strongly nonlinear systems to appreciate that noise, disorder, and nonlinearity must often be incorporated *simultaneously*, leading to qualitatively new phenomena. Such phenomena often have extreme statistics, or "outbreaks" -- intermittent events with large deviations from the mean. Often these events, e.g., earthquakes, hurricanes, floods, sudden climate changes, or forest fires have significant effects, and consequently better understanding of them is urgently needed.

Our objective is to strengthen our understanding of these concepts and apply them to create a framework for dealing with a variety of significant problems in nonlinear science. In this endeavor, advances in stochastic and nonlinear analysis can contribute directly to nonlinear science, while development of nonlinear techniques can advance our understanding of the statistical and stochastic processes underlying the structure and dynamics of complex behavior. A key element in this understanding is establishing mesoscopic "bridges" between microscopic and macroscopic modeling and providing statistically predictive scientific principles underlying the nonlinear, nonequilibrium dynamics of mesoscale complexity.

There is a growing need to understand strong spatial and temporal internal variability, which typically appears at mesoscopic scales, a need shared by many other disciplines, including biology, fluids, and geophysics. Experimental advances, say in remote sensing for geophysics, may enable us to image increasingly detailed structures and even begin following their dynamics in some cases – such as in the TOPEX-POSEIDON satellite imaging of the ocean's variable surface height on Earth. However, the majority of these problems are characterized by measurements producing only sparse data sets. Consequently, interpretative frameworks are urgently needed for statistical predictions of phenomena that we may observe only on sparse data sets.

The scientific needs that will dictate technology in the next decade are:

1. Understanding the roles of nonlinearity and stochastic processes in controlling internal variability of nonequilibrium physical phenomena — i.e., the nonlinear***interrelation*** of system and environmental degrees of freedom and their

effects on the statistical properties of internal variability. Ultimately, this must determine the limits of predictability in nonlinear systems.

2. Assessing predictability — learning how to quantify sparse measurements in ways that are relevant to specific macroscopic properties.
3. Understanding "upscaling", how specific types of sparse measurements of complex systems can be used to predict statistical macroscopic properties, an understanding that will then provide constructive schemes for including microstructure in, e.g., effective media constitutive relations such as permeability calculations for transport of bio-agents and contaminants through random media.

Importance to LANL's Science and Technology Base and National R&D Needs

The Nation's and Laboratory's science programs are rapidly recognizing the need for the capability of statistical prediction of nonlinear nonequilibrium processes observed on sparse data sets. Nonlinear and nonequilibrium issues dominate many of the phenomena at all scales — microscopic, mesoscopic, and macroscopic. These phenomena include coherent, self-organizing and hierarchical structures, complexity, multi-scale dynamics, and chaos. The role for theory and simulation, coupled as closely as possible to experimental validation, as a means of systematically describing these phenomena is now widely appreciated by the DOE-BES and the industrial-laboratory program development efforts.

For example, the scientific issues of flow through porous media are rapidly increasing in economic significance and involve intrinsically nonlinear, nonequilibrium phenomena observed only on sparse data sets. The rate and direction of oil, water or chemicals in underground flows is governed by poorly known fine-scale heterogeneities in the subsurface formation. Mathematical models, based on coupled systems of nonlinear partial differential equations (PDEs), are used to predict these flows in petroleum reservoirs and predict the extent of contamination and environmental danger posed by flows from hazardous waste sites. Even if the material properties of the subsurface formation were adequately characterized on a fine scale, because of the limitations of our computers the models must be simulated on a coarser scale.

The goal of this research must remain to develop and analyze new mathematical models that incorporate fine-scale detail into the coarse-scale computer representation of these flows by deriving new averaged equations (using, e.g., homogenization theory) and numerical methods (based on multigrid and upscaling techniques that accurately capture the average effective properties of the medium). There is a recognized national need for this research to produce significant improvements in upscaling, homogenization and mesoscale modeling of porous media flows that will provide new tools for more accurate and realistic simulations of underground aquifers and reservoirs.

Scientific Approach and Accomplishments

Our research focused principally on the five topics listed below:

1. Optical Fiber Communications, Perturbation Theory of Nonlinear Waves, and Noisy Dynamical Systems;
2. New Formulations of Ideal Continuum Dynamics;
3. New Tubulence Models;
4. Studies in Nonequilibrium Statistical Mechanics; and
5. Stochastic PDEs and dynamics.

Through workshops, seminars, and an ad-hoc LANL advisory group, we seeded nonlinear activities in many *additional* nonlinear, nonequilibrium areas. Our research focus areas complemented existing thrusts in the LANL materials community and were chosen in areas where nonlinear approaches can play clear roles and where there is good teamwork with existing efforts. Several common techniques were exploited: (i) description of coherent structures as collective, or self-confined, pulses; (ii) derivation of effective (nonlinear and/or nonlocal) equations of motion and evolution equations in terms of these (interacting) coherent structures and statistical approaches; (iii) relating time scales observed in near-equilibrium and nonequilibrium conditions to underlying stochastic processes; (iv) integrating large scale simulations with analytical approaches to study nonlinear, nonequilibrium processes.

Accomplishments included:

• Organization of a seminar series, "Stochastic Differential Equations," an International Conference, "Bioremediation and Flow through Fractured and Porous Media," in June, 1997; a weekly working group on geophysical modeling; and a year long weekly seminar on nonlinear partial differential equations during FY1998.

• Large-scale, century-long simulations of wind-driven double-gyre motion that establishes the modes of intrinsic variability underlying ocean basin circulations;

• Mathematical modeling, analysis and simulation of dispersion-managed solitons for optical communications science, which produces "power enhanced solitons" by varying the optical fiber dispersion periodically;

• Analysis and simulation of stochastic phi-fourth kink dynamics;

• Modeling and analysis of coarsening phenomena and traffic flows;

• Development and application of cycle expansion methods for nonlinear ray equations resulting from asymptotic expansions of linear partial differential equations such as the Schrödinger equation;

• Analytical and numerical studies of the interactions of strongly nonlinear coherent structures in the nonlinear Schrödinger and sine-Gordon equations with noise and disorder, with applications to condensed matter physics;

• Analytical and numerical studies of the interactions of linear and nonlinear waves with noise and disorder, with applications to fiber optics communications and large-scale ocean modeling;

• Development and mathematical analysis of new Euler-Poincaré formulations of ideal continuum dynamics with applications ranging from magnetohydrodynamics to ocean circulation and climate models;

• Development, analysis, simulation and comparison with experiment of new nonlinear equations for the dynamics of incompressible turbulence;

• Analysis and simulation of stochastic PDEs and dynamics with applications to pattern formation;

• Investigation of optical soliton interactions under resonant perturbations due to fiber losses and periodic amplification;

• Development of a scheme for stable pulse transmissions in optical fibers, and investigation of nonadiabatic dynamics of dark solitons;

• Demonstration of a method for controlling front dynamics in reaction-diffusion systems with nonuniform external fields;

• Analysis and simulation of "pulsons," a new type of weak solution of nonlinear Lie-Poisson wave Hamiltonian equations;

• Sponsored workshops "Bioremediation and Flow through Fractured and Porous Media" and "New Developments and Applications in Stochastic PDEs;"

• Sponsored workshops " Singularities in Nonlinear Physics, Mathematics and Engineering," January 1998, and "Nonequilibrium Dynamics," April 1998; and

• Organized seminar series, "Statistical Solutions of the Navier-Stokes Equations."

We briefly summarize *selected* aspects of this activity.

Optical Fiber Communications, Perturbation Theory of Nonlinear Waves, and Noisy Dynamical Systems

[I. Gabitov, T-7; Ben Luce, CNLS/T-7; Sergey Burtsev, CNLS (with Darryl Holm, T-7); David Sigeti, X-CM; and external collaborators]

A. Fiber Optical Communications (I. Gabitov, D. D. Holm and B. P. Luce) There is now a general research program on optical fibers involving CNLS postdoctoral fellows and T-7 staff members. The motivation for this project stems from the fact that optical fibers, due to their low dispersion, are capable of supporting much higher information bit-rates than are conventional copper wire. The CNLS and T-7 fiber optic researchers have had extensive contacts with external researchers and industry during the past year. Two world-renowned researchers, Linn F. Mollenauer (Lucent Technologies) and Akira Hasegawa (Osaka University), gave invited talks in the field of nonlinear fiber optics at the 1997 CNLS Conference, along with several other well-known fiber optic researchers. Other visitors in relation to optical fibers have been Ildar Gabitov (Landau Institute of Theoretical Physics, Moscow, now a staff member at LANL in Group T-7), Vladimir Karpmen (Tel Aviv), Arthur Yang and Bill Kath (Northwestern), and Pavel Mamyshev (Lucent Technologies).

Spurred by discussions with some of the researchers listed above, Gabitov (T-7) Holm (T-7), Luce (CNLS/T-7), Camassa (T-7), and Burtsev (CNLS/T-7) intensively investigated a technique called dispersion-managed solitons, which produces "power enhanced solitons" by varying the optical fiber dispersion periodically. This power enhancement results from a decrease in the nonlinear wave mixing due to the rapidly varying dispersion, thereby requiring an increased intensity to compensate. Burtsev, Gabitov and Luce investigated the dispersion maps (which determine the form of the periodic variation in dispersion) using both the Lie transform technique and numerically. Much was learned from this study about the behavior of dispersion managed pulses.

Having become familiar with the power enhancement effect of dispersion managed solitons, Holm and Luce discovered that a different technique called sliding frequency guiding filter soliton transmission, which employs filters that shift the carrier frequency of solitons to reduce noise, is also capable of power enhancement if higher order filters are used. Camasa and Burtsev also investigated sliding frequency guiding filters with collaborators L. F. Mollenauer and P. V. Mamyshev of Lucent technology. In this collaboration, it was shown that sliding filters can be used to convert chirped non-return-to-zero pulses into solitons. Burtsev, Camassa, and I. Timofeyev (a student from RPI) developed and tested algorithms to solve the inverse scattering problem for the nonlinear Schrodinger equation, which governs to leading order the propagation of fiber optical pulses. Victor Ruban and Alexander Zenchuk, T-7 graduate research assistants from Landau Institute for Theoretical Physics in Russia, began the development under the guidance of Burtsev of parallel codes for solving fiber optical transmission problems. Two separate codes are now under development: one code is based on MPI (Message Passing Interface) and the other on shared memory (for example, CNLS's Origin 200 machine).

B. Perturbation Theory of Nonlinear Waves (I. Gabitov, T-7, B. P. Luce CNLS/T-7 and external collaborators)

During Fall/Winter of 1996/1997, Luce completed a three-year project begun with G. Cruz-Pacheco, D. Levermore of the University of Arizona at Tucson on the perturbation theory of nonlinear Schrodinger (NLS) type equations under complex Ginzburg-Landau (CGL) type perturbations. This class of equations describe, for example, the evolution of pulses in nonlinear fiber optical systems. A very clear picture of the persistence of NLS homoclinic and traveling wave solutions under CGL perturbation was obtained.

C. Noisy Dynamical Systems (David Sigeti, X-CM, and B. P. Luce, T-7)

The effects of intrinsic noise on the exponential decay of the power spectra of deterministic dynamical systems were investigated. The intermittency characteristics of band-passed filtered signals were employed to determine the deterministic character of spectral data in various parts of the spectrum. It was found, for example, that the presence of a regime of exponential decay does not necessarily ensure that the low frequency dynamics are deterministic, contrary to common wisdom.

New Euler-Poincaré Formulations of Ideal Continuum Dynamics

(D. Holm, T-7; Jerrold E. Marsden, Caltech; and Tudor Ratiu, UC Santa Cruz)

In our previous work, we developed a useful theory of Hamiltonian reduction for semidirect products, which applies to ideal (nondissipative) fluid dynamical systems that are governed by Lie-Poisson type equations, such as compressible fluids, magnetohydrodynamics and some ocean circulation models. In this previous work, we used the Hamiltonian setting to develop a powerful method of establishing explicit nonlinear stability conditions for ideal fluid and plasma equlibria. We applied this method to obtain explicit basic nonlinear stability results for a number of fundamental theories of fluid and plasma dynamics.

We also studied the Lagrangian analogue of the reduction process and linked it with the general theory of Lagrangian reduction; that is, the reduction of variational principles with respect to their invariance groups. These group-reduced variational principles are mathematically interesting in their own right since they involve constraints on the allowed variations, analogous to what one finds in the theory of nonholonomic systems with the Lagrange d'Alembert principle. We call the resulting variational equations the ***Euler-Poincaré equations*** since Poincaré came rather close to this general picture in his work in 1901. These equations generalize the Poincaré's version of the Euler-Poincaré equations on a Lie algebra in that they depend on a parameter and this parameter in examples has the interpretation of being advected, or Lie dragged, as with the density in compressible fluid flow. In addition, we derived the basic abstract theorem about fluid circulation for these variational equations, which we call the Kelvin-Noether theorem.

We also derived a series of approximate models of ocean circulation dynamics by using asymptotic expansions of Hamilton's principle for the most accurate theory in the small dimensionless parameters that typically appear in the large-scale rapidly-rotating situations, which commonly occur, in oceanographic applications. Our approach in deriving these approximate models is particularly effective, because it preserves the invariance properties of the action principles that are responsible for the Kelvin-Noether theorem. Thus, the approximate model equations we derive each possesses its own circulation theorem and its own attendant conservation law for potential vorticity, which is an important and useful central concept in geophysical fluid dynamics at every level of approximation.

New Turbulence Models (D. D. Holm, T-7; Ciprian Foias, U Indiana; Eric Olson, U Indiana; Edriss Titi, UC Irvine; and Shannon Wynne, UC Irvine)

We used our Euler-Poincaré theory to derive a new closure model for three-dimensional (3-D) incompressible turbulence. The steady solutions of this model compared well with experimental data for mean fluid velocity profiles in pipes and channels at high Reynolds numbers. We also used the resulting equations as a Large Eddy Simulation (LES) model. We also developed a new second moment closure model for 3-D incompressible turbulence This model acts like an ***adaptive*** Large Eddy Simulation (LES) model and gives a dynamical equation for how the Taylor diffusivity tensor responds to shear forcing We used this approach in formulating a new second moment closure model for 3-D oceanic turbulence.

Studies in Nonequilibrium Statistical Mechanics (Eli Ben-Naim, CNLS)

In conjuction with the recently formed Nonequilibrium Science group, we have been studying problems that are far from equilibrium. We report progress in two problems: coarsening phenomena and traffic flows. In the former the question is how does the system approach its equilibrium steady state, while in the latter the steady state is nonequilibrium in nature because detailed balance is not satisfied. In both cases, existing theoretical tools are not applicable and analytical progress was made possible by developing new techniques.

A. Nontrivial Relaxation properties in Coarsening

When a system is quenched from a homogeneous high-temperature disordered state to a low-temperature state it does not order instantaneously; instead, domains of equilibrium ordered phases form on larger and larger scales. It has been generally confirmed that a scale-invariant morphology is developed, i.e. the network of domains is statistically independent of time when lengths are rescaled by a single characteristic length scale. This scale typically grows algebraically with time.

Nevertheless, it was recently discovered that an additional relaxation scale is necessary to characterize more subtle properties such as persistence, i.e., the fraction of the system that is frozen in its initial state. It turns out that this behavior, which was originally found for the Ising model with nonconserving (Glauber) dynamics, is quite general and has since been predicted theoretically in systems as diverse as surface growth and interacting particles and as fundamental as the diffusion equation. These hidden relaxation laws where also confirmed experimentally in twisted nematic liquid crystals, spin-polarized noble gases, and in soap films.

We have discovered that two additional relaxation laws are characterized by two independent scaling exponents in the Ising model. We also developed and solved analytically a detailed theory that agrees qualitatively with the numerical findings and also gives good estimates for the exponents that underlie the domain statistics. The model system we investigated is long believed to be completely solvable because an exact solution for various correlation functions exists. But our findings show that current understanding of nonequilibrium relaxation is far from complete. Instead of the traditional correlators, new statistical measures are necessary to fully characterize the dynamics. It also raises an interesting question: how many nonequilibrium exponents are needed to describe the relaxation? Future work will be directed toward answering this and related questions.

B. Steady State Properties of Traffic Flows:

Traffic theory has been receiving much attention recently, both nationally and at the Laboratory. A number of approaches were suggested including fluid mechanics, cellular automata, particle hopping, and ballistic motion. We introduced a simple model to study one-lane rural traffic. This model incorporates passing and clustering and can be analyzed completely using a modified Boltzmann equation. We have solved analytically for various steady state properties such as the flux, car and cluster velocity distribution.

Our main result is that a single dimensionless parameter determines the nature of the steady state. Analogous with the Reynolds number in turbulence, this number allows writing the equations in a dimensionless form. This number is simply a dimensionless measure of the collision frequency. For small collision numbers, the flow is uninterrupted, while for large collision numbers, large clusters occur. In this strong interaction case, the flux is suppressed algebraically. Meanwhile, the velocity distribution develops a boundary layer structure, which means that cars faster than a threshold velocity are strongly affected by the presence of slower cars.

Stochastic PDEs and Dynamics (Grant Lythe, CNLS)

Stochastic partial differential equations (SPDEs) describe continuum systems with noise. Because they focus on one realization at a time, they are natural tools when noise is an active part of non-equilibrium dynamics. For example, in the real Ginzburg-Landau equation with a time-dependent bifurcation parameter, microscopic white noise produces a characteristic macroscopic domain size that is a function of the product of the rate of change of the bifurcation parameter and the amplitude of the noise. A set of three coupled PDEs, derived from a convection problem, exhibits patterns of motion of increasing complexity as a function of the product of the fourth power of the length of the spatial domain, the rate of change of the bifurcation parameter and the logarithm of the noise amplitude.

Subgrid-scale degrees of freedom of a closed system are often modeled as some kind of a "heat-bath" which drives the resolved scales. For example, consider the long-time nonlinear effects of internal waves on scales from a few meters to a few kilometers on the large-scale (>100 km) circulation of the Earth's oceans. The actual effect of these internal waves on global ocean dynamics and hence on climate is still an open question. Numerical experiments are of limited use as, even with large computers, it is not possible to model all scales from meters to thousands of kilometers. Small-scale irregular motion is separated from the large-scale mean flow by using Lagrangian coordinates: coordinates that follow the motion of fluid parcels with respect to the mean flow. Candidate models of stochastic motion in Lagrangian coordinates are being developed in collaboration with D. Holm. In any one realization of the SPDE, each fluid parcel follows an irregular path but with a well-defined velocity. Correlation functions and spectral properties of the fluctuations are calculated and simulated numerically in a self-consistent way, with a well-defined continuum limit where the size of the fluid parcels shrinks to zero.

In collaboration with R. Camassa and A. Findikoglu, we have initiated a study of array-enhanced stochastic resonance. Stochastic resonance (SR) is a counter-intuitive phenomenon that uses random noise to detect periodic signals so weak as to be otherwise undetectable. Recent research suggests that it is most effectively exploited by arrays with optimized coupling between elements and can be exhibited by any system whose output depends exponentially on its input. A new experimental technique is being developed that uses arrays of nonlinear elements, formed by paraelectric thin films and superconducting electrodes, and driven by microwaves. The experimental capability will allow control over the form of the nonlinearity and the strength of the coupling.

The statistical mechanics of kinks has been out of reach of numerical and analytical studies until recently. In collaboration with Salman Habib, large-scale simulations of the stochastic PDEs for phi-fourth field theory are being combined with new theoretical results to give, for the first time, quantitatively accurate results and understanding of the errors associated with space and time discretization. A proper understanding of this will allow analysis to be performed of the nonlinear stochastic dynamics of the coherent structures (kinks, solitons, vorticies) that are contained in the theories.

Workshop on Bioremediation and Porous/Fracture Flow

The first SIAM/CNLS Workshop on Bioremediation and Porous/Fracture Flow took place at the Los Alamos National Laboratory Study Center, Los Alamos, New Mexico, June 11 - 13, 1997. This workshop was organized as a satellite meeting to the SIAM Conference on Mathematical and Computational Issues in the Geosciences held the following week in Albuquerque, New Mexico. SIAM and the LANL Center for

Nonlinear Studies sponsored the workshop. The US Department of Energy and LANL provided partial support. Fifty scientists attended, with a good balance of representatives from universities, industry and national laboratories, and with a few participants from Europe, Canada and South America.

The purpose of the workshop was to bring together microbiologists, chemists, hydrologists, engineers and mathematicians to review the state of the art in mathematical analysis of in situ bioremediation and to identify major unsolved problems. Each day's proceedings included several seminar-length presentations (13 in all), followed by discussion, with a longer discussion session to wrap up each day. Workshop presentations and discussions focused on the complex interactions between bacteria and their chemical environment, the state-of-the-art in coupling biological degradation with complex chemical reactions in mathematical models, major differences between microbial degradation of organics and sequestering/mobilization of metals, bioavailability of contaminants to microbes (sorption/desorption models), optimization of field remediation procedures (neural nets, genetic algorithms), impact of heterogeneity on in situ bioremediation, stability analysis, upscaling, biofilm dynamics, and microbial community dynamics.

Major advances have occurred in the last few years in mathematical analysis of bioremediation-related processes, and just as important, much new physical data is available that can be used as a basis for further model development. In particular, the startling recent advances by experimentalists to measure biofilm structure, growth and dynamics will lead too much improved models and predictability. In addition, experimentalists are finding that our Darwinian notions of microbial competition have neglected a very important property—which microbial community dynamics also rely heavily on cooperation between members. The workshop agenda is given in an Appendix.

After 3 days of seminars and discussion, it became clear that the central problems yet to be solved center on:

1) heterogeneity/multiscale processes/upscaling—bioremediation involves complex biogeochemical interactions operating on many time scales and taking place in a stochastic medium which itself has structure over many space scales. How can upscaling to the field scale be accomplished efficiently under these conditions?

2) predictability and sensitivity—what level of predictability can we achieve, given the uncertainty in data, in characterization of the subsurface environment and even in knowledge of processes? Apart from this, how inherently predictable or unpredictable is bioremediation? How can measurements at certain scales be used to predict dynamics at other scales?
3) communication—how can we create more interaction between the applied mathematics community and the microbiologists, chemists and engineers who measure what happens in the lab and in the field? Mathematicians build models; engineers want reliable predictions. Presently models come in a great variety of types but their usefulness is doubted, or not understood, by many lab and field scientists. How can greater acceptance of models be promoted? How do we bridge the 'terminology gap' between different disciplines? Is it time to create a bioremediation community model, or at least a community library, much like the community climate model? This would provide a focus for communication and a basis for more coordinated collaborations. This could start with something as simple as a web site (perhaps at SIAM's homepage) where ideas, notes, papers, and codes related to bioremediation can be exchanged among the mathematical community. A similar site exists now for the engineering aspects of bioremediation.

The Geophysical Modeling Working Group

Applications in water resource management, bioremediation, and petroleum reservoir performance not only are of vital importance to society, they also offer a rich array of difficult and related mathematical modeling problems. Common to all of these applications is the need to accurately model the flow of fluids (e.g., water, gas, chemical contaminants) through heterogeneous porous media (i.e., the subsurface geology). Typical models comprise a coupled system of nonlinear partial differential equations that characterize the concentration of the biological and chemical species, and that model the transport of these species through porous media. In the deterministic case, which assumes that a fine-scale representation of the porous medium is known *a priori*, the analysis and numerical treatment is complicated by the nonlinearities and by the formidable range of interacting length scales. In addition, if the porous medium is characterized by a sparse set of field data, then a stochastic view of the model is typically adopted to account for this uncertainty.

The complexity and diversity of these problems has resulted in a number of LANL research groups developing expertise on related topics. In particular, research in these applications is ongoing in T-7 (Mathematical Modeling and Analysis), T-13 (Complex Systems), EES-5 (Geoanalysis), and the CNLS. The Geophysical Modeling Working Group provides a forum for these researchers to share their expertise and to form new collaborative relationships. Specifically, the meetings adopt one of three formats: round-table discussions on a preselected topic or paper, informal seminars given by regular members of the group, and formal seminars that are given by an invited speaker from outside the group.

CNLS Workshop on Nonequilibrium Dynamics

New theoretical and experimental results indicate that our current understanding of nonequilibrium dynamics is incomplete, and that a first-principles formulation is still missing. Slow relaxation is often the signature of such dynamics. The discovery of hidden relaxation modes in spin systems is creating a new field with over 100 publications in just three years, including several experimental confirmations. The underlying mechanism applies to a variety of problems including surface growth, coarsening kinetics, many-body systems, and even simple diffusion. Thus, these discoveries are producing a new field of science with the potential to make significant contributions to our fundamental understanding of nonequilibrium systems with a variety of applications.

In April 1998, the CNLS hosted an international workshop titled "Nonequilibrium Dynamics," focusing on coarsening kinetics and stochastic PDEs. Recent discoveries of new slow relaxation modes in coarsening systems are producing a new field with the potential to make significant contributions to our fundamental understanding of nonequilibrium systems. Further details are available on the CNLS website at http://cnls.lanl.gov/Events/Conferences/NonEquil_Dynamics/.

Appendix. Workshop agenda

SIAM/CNLS workshop on Bioremediation and Porous/Fracture Flow
June 11 - 13, 1997
Study Center
Los Alamos National Laboratory

Day 1 : The Contaminants: Biogeochemistry

8:45am Welcome and Opening remarks - Dr. Sig Hecker, Director,
Los Alamos National Laboratory, and
Dr. Hans Frauenfelder, Director,
Center for Nonlinear Studies, Los Alamos National Laboratory

9:00am Dr. Bruce Rittmann, John Evans Professor of Environmental Engineering, Dept. of Civil Engineering, Northwestern University:
Coupling the "bio" to the "geochemical" in modeling of co-contaminants;

10:00am break

10:15am Dr. Terry Beveridge, U.of Guelph:
Interaction, Concentration, and Mineralization of Environmental Metal Ions by Bacterial Surfaces

11:15am Dr. A. Francis, Brookhaven Natl. Lab.
Mechanisms of Microbial Transformations of Radionuclides and Toxic Metals in Subsurface Environments

12:15pm lunch

1:45pm Dr. Ronald Crawford, Center for Hazardous Waste Remediation Research, University of Idaho:
Anaerobic Processes for Bioremediation of Nitro-Aromatic Pollutants;

2:45pm break

3:00pm Dr. Sally Benson, Earth Sciences Dept., LBL:
Research Needs for Bioremediation of Metals and Radionuclides - Overview and Examples

4:00pm Discussion session - research directions/needs/problems

5:00pm Reception at Study Center, poster viewing

6:30pm Dinner in groups at area restaurants

Day 2: The Soil: Issues in Heterogeneity, Bioavailability & Optimization

8:45am Prof. John Cushman, Center for Applied Mathematics, Purdue U.
Flow and transport in random media: Perturbation vs Monte Carlo

9:45am break

10:00am Dr. Andrew Tompson, Geosciences & Environmental Technologies Div.,LLNL
Bioremediation In Heterogeneous Systems: Ongoing Study

11:00am Prof. Albert Valocchi, Hydrosystems Lab, Dept. of Civil Engineering, University of Illinois

Modeling the Impact of Soil Heterogeneity on In-Situ Bioremediation
12:00pm lunch
1:30pm Dr. Leah Rogers, Geosciences & Environmental Technologies Div., LLNL
Artificial Neural Network Applications to Subsurface Modeling
2:30pm break
2:45pm Prof. Willy Lick, Dept. of Environmental Engineering, UCSB
Sorption and Bioavailability
3:45pm Discussion Session
5:30pm picnic dinner at Camp May

Day 3: The Microbes: Microbial Community Structure & Dynamics
8:45am Dr. James Bryers, Center for Biofilm Engineering, Montana State Univ.
Biofilm Engineering
9:45am Prof. Robert Dillon, Dept. of Mathematics, Tulane University,
A microscale model of bacterial processes
10:10am break
10:25am Prof. Paul Waltman, Dept. of Mathematics, Emory U.
Mathematical Models of Competition in Selective Environments
11:25am Dr. Douglas Caldwell, U. Saskatchewan:
Bacterial Self-Organization and Bioremediation
12:20pm lunch
1:30pm Wrap-up discussion
2:30pm Workshop ended

Publications:

1. Aceves, A., Holm, D. D., Kovacic, G. and I. Timofeyev, "Homoclinic orbits and chaos in a second-harmonic generating optical cavity," Phys. Lett. A 233, 203-208 (1997).

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8. Bender, Carl M. and Boettcher, Stefan, "Quasi-Exactly Solvable Quartic Potential," Journal of Physics A Mathematical and General, 31, L273-L277 (1998).

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10 Blumenfeld, Raphael, "Review of Analyses of Fracture Roughness," MRS 1995 Fall Meeting - November 27, 1995 - December 1, 1995 - Boston, MA, to appear (1998).

11. Blumenfeld, Raphael, "A Minimal Model for Crack Propagation in Amorphous Materials,"MRS 1995 Fall Meeting - November 27, 1995 - -December 1, 1995-Boston, MA, to appear (1998).

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15. Bunimovich, Leonid A. and Rehacek, Jan, "How High-Dimensional Stadia Look Like ," Communications in Mathematical Physics, 197, 277-301 (1998).

16. Cendra, H., Holm, D. D., Hoyle, M. J. W. and Marsden, J. E., "The Maxwell-Vlasov equations in Euler-Poincaré form," J. Math. Phys., 39, 3138-3157 (1998).

17. Cendra, H., Holm, D. D., Hoyle, M. J. W. and Marsden, J. E., "Lagrangian Reduction, the Euler-Poincaré equations, and semidirect products," in Arnol'd Festschrift Volume II, Am. Math. Soc. Translations Series 2, 186, (1999).

18. Chen, S., Foias, C., Holm, D. D., Olson, E.J., Titi, E.S. and Wynne, S., "The Camassa-Holm equations as a closure model for turbulent channel and pipe flows," Phys. Rev. Lett., 81, 5338-5341 (1998).

19. Chen, S., Foias, C., Holm, D. D., Olson, E.J., Titi, E.S. and Wynne, S., "A connection between the Camassa-Holm equations and turbulent flows in pipes and channels," Phys. Fluids, to appear, (1999).

20. Chen, S., Foias, C., Holm, D. D., Olson, E.J., Titi, E.S. and Wynne, S., "The Camassa-Holm equations and turbulence," Physica D, to appear, (1999).

21. Chen, S., Holm, D. D., Margolin, L. G., and Zhang, R., "Direct numerical simulations of the Navier-Stokes alpha model," Physica D, to appear, (1999).

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41. Holm, D. D. and Zeitlin, V., "Hamilton's principle for quasigeostrophic motion," Phys. Fluids A, 10, 800-806 (1998).

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