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Numerical Methods for Stochastic Partial Differential Equations.

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Abstract

This is the final report of a Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The objectives of this proposal were (1) the development of methods for understanding and control of spacetime discretization errors in nonlinear stochastic partial differential equations, and (2) the development of new and improved practical numerical methods for the solutions of these equations. We have succeeded in establishing two methods for error control: the functional Fokker-Planck equation for calculating the time discretization error and the transfer integral method for calculating the spatial discretization error. In addition we have developed a new second-order stochastic algorithm for multiplicative noise applicable to the case of colored noises, and which requires only a single random sequence generation per time step. All of these results have been verified via high-resolution numerical simulations and have been successfully applied to physical test cases. We have also made substantial progress on a longstanding problem in the dynamics of unstable fluid interfaces in porous media. This work has lead to highly accurate quasi-analytic solutions of idealized versions of this problem. These may be of use in benchmarking numerical solutions of the full stochastic PDEs that govern real-world problems.

Background and Research Objectives

The laws of nature prescribe the time evolution of physical quantities. Time being continuous, they are written as differential equations. A stochastic differential equation prescribes non-deterministic evolution: from a complete specification of the values of all variables at one time follows a unique probability distribution of possible values at any later time. However, in such a description, at no later time can the values taken by all variables be predicted exactly. A stochastic description may be appropriate either because complete prediction in the sense of the last sentence is theoretically impossible (e.g., when modeling quantum-mechanical measurements), or simply because a complete specification of all variables and solution of the equations prescribing their evolution turns out to be impractical. This is almost always the case in any attempt at modeling a realistic complex system.

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Typically, a stochastic model is based on the idea that it is possible to view the problem at hand as having been divided into a “system” component and an “environment” component, where the system variables are the ones of most interest. Evolution equations are then obtained (sometimes by systematic procedures, but most often not) for a small set of variables (the system) from the complete evolution equations specified for all the variables. Interaction between the system and the rest of the variables (the environment) produces dissipative and fluctuating forces acting on the system variables, the environment acting as a sort of generalized heat bath. The environment variables are typically taken as rapidly fluctuating, justifying the use of a noise term in the evolution of the system variables. Thus, in the equations describing the system's evolution, we may find parameters that are fluctuating or fluctuating external forces. Stochastic modeling of this type is often successful even in cases where it is not obvious that a simple systematic/stochastic split exists. On the other hand, if too naive stochastic models are used, the results can be dangerously misleading. Modeling of this kind often involves a delicate balance between mathematical rigor and physical intuition. It is important to appreciate that noise is more than something which simply smears or coarse-grains a systematic evolution. The addition of even small amounts of noise can often lead to dramatic changes in the time evolution of the variables of interest. Examples of this kind of behavior include stochastic resonance, noise-driven transitions, and time evolution problems far from equilibrium.

The addition of noise to ordinary differential equations proceeds by adding increments of the Wiener process at each time step; informally we may think of this as a particle continuously subject to small impulses. If a system is described by a set of smooth functions, rather than by multiple variables, then we have to add noise to a partial differential equation (PDE), in which case one adds increments of the Brownian sheet that are random in space as well as in time. (One can imagine, for example, the motion of a flexible sheet in a sandstorm.) When this is done we have a stochastic partial differential equation (SPDE). SPDEs are ubiquitous in the study of complex phenomena such as turbulence, properties of real materials, multiphase flow, porous media, and structural biology.

The mathematical properties of stochastic ordinary differential equations are in the main well-understood [8][9]. However, despite their practical importance, and despite the fact that there exists an extended mathematical literature on these equations [10][11], SPDEs, especially of the form encountered in real-life modeling problems, remain rather poorly understood. (In passing we note that stochastic equations are often called Langevin equations in the physics literature.)

To further the state of the art in the numerical treatment of SPDEs we decided to focus on two problems: (1) general tools for the characterization of errors in space and time when SPDEs of a certain class are solved on a lattice (as is always the case in numerical simulations), and (2) the development of new methods to reduce these errors via controlled and systematic methods. Since SPDEs in general constitute a huge class of equations, we decided to concentrate on problems where a fluctuation-dissipation theorem exists, i.e., where the equations have a stationary solution at late times (in the ensemble sense). While certainly not making up a majority of SPDEs, this reduced class is of great physical interest and insights gained from the tools developed for it can be profitably applied to more general forms of SPDEs.

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

As science is increasingly called upon to support decision making concerning a broad range of problems having a technological component, uncertainty assessment and management is acquiring an altogether new dimension, and urgency.

There is a need for reliable prediction of the behavior of complex phenomena outside the range of controlled, repeatable experiments and direct observations. This need encompasses several time critical problems of national concern within the DOE mission. Examples include climate prediction, stewardship of our nuclear stockpile, and environmental remediation.

Knowledge of complex phenomena is limited by incomplete or inaccurate data, missing physics, and solution errors. Each of these factors is a potential source of uncertainty in the answer. Predictions of complex phenomena will be credible, and of use in decision making, only if these sources of uncertainty are quantified. At the same time, quantification of uncertainty is the first step towards corrective action to reduce, or manage, uncertainty, when this is possible.

The prediction problem divides into two components, the forward problem and the inverse problem. The forward problem is to determine the solution describing system behavior, given the governing equations and initial data. The inverse problem is to use observations of system behavior to improve the model, i.e. the governing equations and input data. For complex systems both of these prediction steps must be carried out in a probabilistic framework, to allow for incomplete knowledge of the system. [1]

Forward prediction in classical physics is usually accomplished with partial differential equations. In the probabilistic setting, these become stochastic partial differential equations. The focus of this project has been the development of effective methods for the numerical solution of SPDEs. This work is a key step in developing a

Laboratory capability for solving prediction problems of central importance to the DOE mission.

Scientific Approach and Accomplishments

One difficulty with SPDEs is that solutions are not smooth functions, thus ordinary calculus-based methods cannot be applied naively to the analysis of the convergence properties of these equations when they are put on a lattice. For example, in the case of PDEs, derivatives taken at some fiducial point are often approximated by sampling the function at a few nearby points, and given the assumption that the function is sufficiently smooth, one is allowed to improve one's estimate of the derivative by sampling the function using some more of the neighboring points (Richardson extrapolation). However, if the function is noisy such an approach must fail. This leads to the natural question of how best to characterize errors given an SPDE instead of a PDE.

It must also be appreciated that there are two sorts of errors: errors due to finite time step size as well as errors due to the finiteness of the spatial discretization. Our approach to understanding these errors was via the functional Fokker-Planck formalism to understand the temporal errors, and the transfer integral method to understand the spatial errors.

Let us first address the question of time stepping errors. Since SPDEs describe the dynamics of individual realizations over the noise ensemble, there corresponds to each SPDE an equivalent description in terms of a probability distribution functional which contains within it the information describing the ensemble considered as a whole. This is the Fokker-Planck description of the SPDE. It is clear that in the case of stochastic ODEs, the corresponding Fokker-Planck description is in terms of probability distribution functions, rather than functionals, and is therefore relatively tractable. However, the probability distribution functionals arising in the case of SPDEs are impossible to deal with as they contain enormous amounts of information, which for the foreseeable future is too large to imagine being contained in the memory of even the biggest supercomputers. Even so, the functional Fokker-Planck equations have one very important feature: they describe the evolution of a smooth functional and are in themselves not stochastic. Given an implementation of an SPDE on the lattice, there exists a constructive procedure to write down the corresponding discrete time functional Fokker-Planck equation. In this equation, even though we have no hope of actually solving it, it is straightforward to study questions of discretization error since the noise has been eliminated.

In actual computational practice, once the order of the time stepping errors has been estimated, it is not difficult to reduce the time step to a level where the remaining errors are suppressed compared to the errors from the spatial discretization. Once this is done, we

may safely ignore the discretization in time and concentrate solely on the errors due to the spatial lattice.

This is the point where we invoked the fluctuation-dissipation relation (FDR): for a large (but by no means exhaustive) class of SPDEs there is a relation between the dissipative and noisy pieces of the equation which balances the two against each other in just such a way that at large times thermal equilibrium is approached (if the noise were to win, the system would have a runaway solution, whereas if the dissipation were to dominate the final distribution would be a delta function at a point in phase space). For SPDEs satisfying an FDR, the solution of the corresponding Fokker-Planck equation at late times is the canonical distribution at a temperature determined by the FDR. But because of the discretization errors, the equilibrium achieved is not quite the correct one: by theoretically computing certain thermodynamic quantities we can extract the dependence of the error on the spatial lattice constant.

This last step is not straightforward, however. This is because we have a probability distribution functional to deal with and to compute thermal averages we need to carry out functional integrals. It turns out that there are technical difficulties in carrying out this program in two and three dimensions due to the existence of divergences. Thus as a first step we decided to concentrate on the case of one spatial dimension where the question of the regularization of these divergences does not arise. In one dimension, the functional integrals mentioned above can be converted into the problem of obtaining the eigenspectrum of a Hilbert-Schmidt operator with a Fredholm kernel. This operator is called the transfer operator or transfer integral.

The idea now is to compute the transfer integral and from it extract the spatial error in some quantities of interest. It turns out that the transfer integral can be transformed into an infinite-order differential equation using shift operators, and this equation can then be reduced in order by employing a (formal) Campbell-Baker-Hausdorff expansion. At leading order in this expansion, the transfer integral becomes a one-dimensional time-independent Schrodinger equation, and at next-to-leading order lattice errors enter in the Schrodinger Hamiltonian. The eigenspectrum of the Schrodinger equation can be determined by approximate methods such as WKB or merely calculated numerically. It turns out that a knowledge of the first few eigenvalues is sufficient to determine quantities such as the free energy and various correlation functions. Any lattice dependences in expressions for them are lattice artifacts and can be identified immediately as numerical errors.

For a linear (free) theory the transfer integral can be computed exactly and at the same time, the SPDE on the lattice can also be solved exactly. The lattice dependences are in exact agreement (the specific SPDE implementation we used on the lattice gave us an error quadratic in the lattice spacing) providing one validation of our procedure. We then verified our result for a nonlinear theory and showed explicitly that our method predicts the order of the numerical errors correctly [2]. This error control methodology was applied to a high precision study of kink statistical mechanics [3][4].

The final question in this program is the improvement of lattice errors. As discussed above, while Richardson extrapolation cannot be used naively for SPDEs, first-order perturbation theory applied to the transfer integral formulation allows the construction of a local counter-term that cancels the quadratic part of the error. By the symmetry property of the Campbell-Baker-Hausdorff theorem that there are no odd terms in the lattice errors, we see immediately that canceling the second order error produces a fourth order method. This seemingly counter-intuitive result has also been verified by high-resolution simulations Figure 1.

The second part of our research program was to develop a new stochastic time-stepping algorithm for nonlinear (multiplicative) noise (the standard stochastic RK2/Heun integrator fails to be second order for multiplicative noise). We have succeeded in developing a new stochastic leapfrog method, which uses only one noise sequence generation per time step and is second order accurate [5]. We have tested this algorithm against exactly known test cases with excellent results, clear superiority being established over the standard RK2/Heun integrator Figure 2. The new algorithm has been applied to a study of thermal relaxation in the presence of multiplicative noise. We expect it to become an application standard for multiplicative noise SPDEs.

The Taylor-Saffman instability at interfaces between fluids having different viscosities was studied as a simple model of unstable dynamics in a porous medium. Using time-dependent conformal mapping as a solution method, we obtained a class of "fingerlike" solutions characterized by a finite number of poles. This allows a representation of the solution in terms of a finite number of parameters. We show that solutions in this class evolve to a unique stable form. This is a surprising result that may lead the way to a new understanding of the role of surface tension in selecting unique solutions to this problem. These solutions should also provide a benchmark for codes intended to solve real world versions of porous media flow problems.

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Fig. 1: The correlation length for a nonlinear field theory computed with the uncorrected potential (black dots) and with the error-compensating counterterm (diamonds). The dashed line is the exact continuum result.

Fig. 2: Results from a test problem showing the analytical solution, the stochastic leap-frog result and the result from Heun's method. Note the significant improvement due to the stochastic leap-frog algorithm.