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Rate of Convergence of a Stochastic Particle Method for 1D Viscous Scalar Conservation Law Equations

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The aim of this work is to present the rate of convergence analysis of a stochastic particle method for the 1D viscous scalar conservation law equation. The numerical method is inspired from a propagation of chaos result, which allows to associate a stochastic interacting system of particles to the PDE. The algorithm is based on the simulation of a large number N of particles with the first order Euler scheme applied to the stochastic dynamics of the interacting system. We prove a theoretical rate of convergence of order $O(\frac{1}{\sqrt{N}} + \Delta t)$. For the case of the Burgers equation, numerical experiments confirm this convergence rate.

We show that the algorithm can also be adapted to viscous scalar conservation law equation in a bounded domain. Here, the underlying stochastic interacting system of particles is reflected at the boundary to take into account the Dirichlet conditions. We show that the rate of convergence of the error is still $O(\frac{1}{\sqrt{N}} + \Delta t)$ when we use the Euler-Lépingle scheme to discretize in time the system of N particles.

‡joint work with **B. Jourdain**

Continuous methods for Stochastic Delay Differential Equations with variable delay

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We consider a stochastic version of the pantograph equation. This is an example of an Itô stochastic delay differential equation with variable delay. We discuss strong approximations to its solution obtained by a continuous extension of the Θ-Euler scheme ($\Theta \in [0,1]$). We establish $\mathcal{O}(\sqrt{h})$ mean-square convergence of approximations obtained using a mesh of uniform step h. Illustrative numerical examples are provided.

Simulating radio-wave heating of fusion plasmas

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A thermonuclear fusion reactor requires a temperature of over 100 million Kelvin and an energy confinement time of several seconds. The main reactor vessel candidates are toroidal magnetic bottles, either non-axisymmetric (stellarator) or axisymmetric (tokamak). Radio-wave heating of the ionized fuel hydrogen isotopes is modeled by the quasilinear Fokker-Planck equation. Due to the 5D phase space (stellarator) or the 3D constant-of-motion space with complicated internal boundary layers (tokamak), the Monte-Carlo method is a popular alternative to Eulerian algorithms. We will discuss why evaluating the Feynman-Kac formula, by numerically solving the naturally associated stochastic differential equation and averaging, is a superior approach. Preliminary results where, somewhat surprisingly, the Milshtein scheme leads to weak convergence of order 3/2 are also shown.

A Pure Jump Markov Process Associated
with Smoluchowski's Coagulation Equation

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The Smoluchowski coagulation equation models various phenomenon, in particular polymerisation. The aim of this work is to construct a stochastic process, whose law is the solution of the coagulation equation. This approach is a first in this direction in that we obtain a solution to the coagulation equation as the law of a stochastic process. A modified equation is introduced which deals with the evolution of the re-partition, $Q_t(dx)$, of the mass of the system. The advantage of this approach lies in our ability to apply a unified treatment to both continuous and discrete models.

The integro-partial differential equation satisfied by $\{Q_t\}_{t\geq 0}$ can be interpreted as the evolution equation of the time marginals of a Markov pure jump process. To this end, we introduce a non-linear stochastic differential equation, driven by a Poisson process, which is related to Smoluchowski's equation in the following way: if X_t satisfies the SDE, then the law of X_t is given by the modified coagulation equation. Existence, uniqueness, and pathwise behavior of solutions for this SDE are studied.

Finally, an exactly simulable stochastic particle system is derived from this SDE. We prove that the empirical measure associated with this particle system converges to the solution of the modified coagulation equation as the size of the system becomes large. We thus obtain an approximation scheme for the solution of the Smoluchowski coagulation equation. Numerical results are shown and convergence estimates obtained.

†joint work with **N. Fournier** and **E. Tanré**

Strong Convergence of Numerical Methods for
Nonlinear Stochastic Differential Equations

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Traditional finite-time convergence theory for numerical methods applied to stochastic differential equations (SDEs) requires a global Lipschitz assumption. In practice, many important SDE models satisfy only a local Lipschitz property and, since Brownian paths can make arbitarily large excursions, the global Lipschitz based theory is not directly relevant. In this work we prove a strong convergence result for the Euler-Maruyama method that requires only that the SDE coefficients are locally Lipschitz (e.g. C^1) and the pth moments of the exact and numerical solution are bounded for some $p > 2$. As an application of this general theory we show that two implicit variants of the Euler-Maruyama method converge if the drift satisfies a one-sided Lipschitz condition. This is achieved by showing that one implicit method has bounded moments and may be viewed as an Euler-Maruyama approximation to an SDE with a modified vector field. Convergence of the other implicit method is established through a perturbation argument.

‡joint work with **Xuerong Mao** and **Andrew Stuart**

Approximation of stochastic differential
equations with linear functionals

Norbert Hofmann†
Johann Wolfgang Goethe–Universität Frankfurt, Frankfurt

The talk is concerned with pathwise approximation of scalar stochastic differential equations with respect to the global error in the L_2–norm. We study methods that are based on sequentially chosen linear functionals of the driving Brownian motion W. The minimal error in the class of arbitrary methods that are based on n functional evaluations on the average tends to zero like $c/\pi \cdot n^{-1/2}$, where c is the average of the diffusion coefficient in space and time. For comparison we consider the class of methods that use n discrete observations of W on the average. The minimal error in this class behaves like $c/\sqrt{6} \cdot n^{-1/2}$. Hence methods with linear functionals yield only a small improvement on the level of asymptotic constants.

†joint work with **Thomas Müller–Gronbach** and **Klaus Ritter**

Error bounds for strong numerical schemes applied
to Itô–Galerkin approximations of stochastic PDEs

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The global discretization error is estimated for strong time discretizations of finite dimensional Ito stochastic differential equations (SDEs) which are Galerkin approximations of a class of parabolic stochastic partial differential equation (SPDE) with a strongly monotone linear operator with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots$ in its drift term. If an order γ strong Taylor scheme with time-step Δ is applied to the N dimensional Ito–Galerkin SDE, the discretization error is bounded above by $K\left(\lambda_{N+1}^{-1/2} + \lambda_N^{[\gamma+\frac{1}{2}]+1}\Delta^\gamma\right)$ where $[x]$ is the integer part of the real number x and the constant K depends on the initial value, bounds on the other coefficients in the SPDE and the length of the time interval under consideration. One the other hand, if linear-implicit versions of the strong Taylor numerical schemes are used, then the discretization error is bounded above by $K\left(\lambda_{N+1}^{-1/2} + \Delta^\gamma\right)$, so the step size can be chosen independently of the dimension of the Itô-Galerkin SDE.

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Complex fluids modeled by stochastic differential equations

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In this talk we present an approach to dynamics of complex fluids such as polymers or liquid crystals. From Fokker-Planck (or Langevin) equations for the structural variables of rigid particles or a polymer backbone, we calculate material properties by using analytical and numerical methods. For example, in order to study universal features of polymer solutions considering hydrodyamic interactions, we discuss a highly efficient numerical scheme. Concerning the physics of liquid crystals, we demonstrate how to relate macrosopic (Ericksen-Leslie) coefficients to a molecular based picture.

Uniform approximation of systems of SDEs

Thomas Müller-Gronbach
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We analyze numerical methods for pathwise approximation of a system of stochastic differential equations. As a measure of performance we consider the q-th mean of the maximum distance between the solution and its approximation on the whole unit interval. We introduce an adaptive discretization that takes into account the local smoothness of every trajectory of the solution. The resulting adaptive Euler approximation performs asymptotically optimal in the class of all numerical methods that are based on a finite number of observations of the driving Brownian motion.

Some Real Challenges to Stochastic Numerics

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Starting from two orthogonal concepts of understanding, namely through basic principles or through simplicity, the crucial importance of coarse-graining from any applied scientists or engineers point of view is elaborated. Coarse-graining naturally leads to stochastic equations. A very general form of such equations in a modern formalism of nonequilibrium thermodynamics (GENERIC), understood as a theory of coarse-graining dynamics, is presented and analyzed in order to extract a variety of serious and important challenges to the theory and numerics of stochastic differential equations.

Mean-square stability of numerical schemes
for stochastic differential equations

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Stochastic differential equations (SDEs) represent physical phenomena dominated by stochastic processes. As for deterministic ordinary differential equations (ODEs), various numerical schemes have been proposed for SDEs. We have proposed *mean-square* stability of numerical schemes for a scalar SDEs, that is, the numerical stability with respect to the mean-square norm. We have previously studied *mean-square* stability analysis for only scalar SDEs, but not vector cases because of their difficulty and complexity. In this talk we will consider some types of a 2-dimensional linear test equations and try to analyze them.

Stability Analysis of Stochastic (Balanced) Theta-Methods

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A systematic stability analysis of stochastic variants of deterministically well-known Theta-methods for systems of stochastic differential equations is presented. We investigate the qualitative behavior of the stochastic Theta-methods with respect to linear and nonlinear stability, boundedness, contractivity and attractivity issues in the mean square and almost sure sense. It turns out that symmetric methods like that of midpoint and trapezoidal ones provide asymptotically exact methods in view of their stationary laws for linear systems. The practical implementation for nonlinear SDEs is done by their linear-implicit variants (like stochastic Rosenbrock and balanced implicit methods) or splitting methods (like partial-implicit methods) in order to reach computational efficiency, convergence and numerical stability. Finally we illustrate the applicability of our results by the nonautonomous discretization of linear, damped oscillators with one degree of freedom.

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Stochastic Macroscopic Behaviour of
Coupled Oscillators With Random Data

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The problem of deriving stochastic differential equations (SDEs) from mechanical systems with random data has a long history going back to early work of Kac, Zwanzig and their co-workers in the 1960s and 1970s. The subject has recently been re-invigorated by the possibility of using such derivations to bench-mark a variety of different algorithms used in computational molecular dynamics. This possibility stems from the fact that, in many cases, the primary objects of interest in molecular simulations are macroscopic. Having some explicitly understood model problems, where the dynamics of macroscopic quantities are completely understood, is invaluable in evaluating computational algorithms. In this talk I will review some of the history of the derivation of SDEs from ODEs with random data, and outline some recent new results which place heuristics of Kac and of Zwanzig in a rigorous setting. As a by-product I will also give an interesting construction of non-stationary Gaussian processes in terms of sums of oscillators with random frequencies.

Adaptive weak approximations of SDEs

Anders Szepessy
KTH, Stockholm

I will describe two adaptive time stepping methods based on the Euler-Monte Carlo method for weak approximation of Itô stochastic differential equations. The algorithms are based on expansions of the computational error, with computable leading order term in a posteriori form, using stochastic flows and discrete dual backward problems. The rigorous expansions leads to efficient and accurate computation of error estimates. The adaptive algorithms use either optimal stochastic time steps or optimal deterministic time steps. Stochastic time steps use Brownian bridges and require more work for given number of time steps. Deterministic time steps may yield more time steps, but require less work per step. I will include numerical examples to illustrate when adaptive stochastic and deterministic steps are better than a constant step size.

Monte-Carlo Simulations of the Infinite Dimensional HJM Model

Raúl Tempone
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We present two Monte Carlo Euler methods for a weak approximation problem of the HJM term structure model, which is based on Ito stochastic differential equations in infinite dimensional spaces, and prove error estimates useful for adaptive algorithms. These error estimates are based on stochastic flows and discrete dual backward problems, and they can be used to identify different error contributions arising from time and maturity discretization as well as the classical statistical error due to finite sampling. Explicit formulas for efficient computation of sharp error approximation are included. Due to the structure of the HJM models considered here, the computational effort devoted to the error estimates is low compared to the work to compute Monte Carlo solutions to the HJM model. Numerical examples with known exact solution are included in order to show the behavior of the estimates.

Overcoming obstacles in Monte-Carlo
simulations of statistical mechanical systems

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Stochastic methods have a long history in statistical physics since the invention of Monte Carlo methods by Metropolis et al. in 1949. Quantum systems can be tackled by mapping the partition function $\exp(-H/kT)$ to a path integral which is then sampled stochastically. Two mayor obstacles facing Monte Carlo simulations of statistical lattice models have recently been overcome. The first, critical slowing down at phase transitions, where the autocorrelation times diverge in the most interesting regime has been overcome by cluster algorithms for classical systems a decade ago, and for quantum systems in the past few years. I will review the basis ideas behind these approaches. The other problem facing large scale statistical simulations of lattice models is that an optimized high performance implementation needed a separate hand-tuned code for each model and lattice type. I will present how this obstacle can be overcome using modern generic programming techniques in C++ to obtain an algorithm which works for a wide class of models, while still being as efficient as optimized implementations for specific model.

Diffusion, Coagulation, and Stochastic Numerics

Wolfgang Wagner

Weierstrass Institute, Berlin

This talk is concerned with applications of stochastic numerics to coagulation processes. The physical phenomenon of coagulation (merging of particles when they hit each other) occurs in a wide range of applications (chemistry, meteorology, astrophysics). In the first part of the talk we consider systems of diffusing particles subject to coagulation. We review some rigorous results concerning their asymptotic behaviour, and introduce the corresponding nonlinear equations. In the second part we study stochastic algorithms for the numerical treatment of the coagulation equation. We describe the direct simulation procedure, as well as an alternative algorithm leading to considerable variance reduction. Finally, some results of numerical experiments are presented.

Stochastic Differential Algebraic Equations
in Circuit Simulation

Renate Winkler

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In the development of new chips numerical circuit simulation replaces time-consuming, difficult or even impossible measurements in real experiments. State of the art are simulations based on the charge oriented modified nodal analysis (MNA), which leads to large specially structured systems of differential algebraic equations (DAEs). The increasing scale of integration, high tact frequencies and low supply voltages cause smaller signal-to-noise-ratios. In several applications linear noise analysis is no longer satisfying and the need for transient noise analysis arises.

Here we deal with the thermal noise of resistors as well as the shot noise of semiconductors modeled by additional sources of additive or multiplicative white noise currents. To assure a meaningful mathematical model we have to assume that the noise sources do not disturb the constraints of the DAE. This can be expressed in terms of the network topology.

Then the system can be described by stochastic differential algebraic equations of the form

$$A(q(x(t),t) - q(x(t_0),t_0)) + \int_{t_0}^{t} g(x(s),s)ds + \sum_{i=1}^{k} \int_{t_0}^{t} \sigma_i(x(s),s)dW^i(s) = 0 \quad ,$$

where A is a constant singular matrix which is determined by the topology of the electrical network and W is a k-dimensional Wiener process.

We use techniques from the theory of DAEs as well as of the theory of SDEs to analyze the resulting systems of stochastic differential algebraic equations and derive existence and uniqueness results for the solutions of systems with DAE-index 1 or 2.

Due to the differential algebraic structure and to stability requirements we need implicit numerical methods for the numerical simulation of such systems. Here we present convergence results for a semi implicit Euler scheme.

Polynomial Chaos Solutions of
Fluid Dynamics with Applications

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We present a Polynomial Chaos solution to differential equations to model the uncertainty in various systems. This is achieved by expanding the random processes by a complete polynomial basis, the Wiener-Hermite polynomial, then perform a Galerkin projection procedure to explicitly express the randomness as a new dimension in addition to the existing spatial-temporal domain (Ghanem & Spanos, 1991). The resulting set of coupled equations is then solved to obtain the solution for each random mode. We apply the procedure to various systems including the 1st, 2nd-order ODEs and PDEs such as the wave equation, heat equation and so on. The randomness is introduced through the uncertainty in initial/boundary conditions, physical parameters, etc. The Polynomial Chaos solution is validated by comparing with analytical solutions or solutions of Monte Carlo simulations and good agreements are obtained. We also apply the Polynomial Chaos method to fluid dynamics governed by the Navier-Stokes equations. The method is implemented in the context of unstructured spectral/hp element discretizations (Karniadakis & Sherwin, 1999) to handle the complex geometries and maintain spectral accuracy in space. The algorithm is applied to microchannel flows and to flow past a cylinder with random boundary conditions. Good agreements are achieved by comparing with analytical results or results of Monte Carlo simulations. In all the applications above, both Gaussian and non-Gaussian random inputs are considered. It is shown that the Polynomial Chaos method offers the possibility of efficient stochastic simulations of complex systems such as the fluid flows in complex geometric domain.

References

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An essentially code-free approach to the
numerical solution of SDEs

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The numerical solution of SDEs using the Finite Element Method often involves a great deal of structural preparation and analysis before the code can be generated and the numerical experiments can be undertaken. The other main solution approach, via Taylor series based time discretisation schemes can also require complex code. Both approaches need to follow the classical but laborious process of code, debug, test, change, debug... etc. In this paper l will present the use of the SIMULINK modelling and simulation package. The SIMULINK package allows the creation of simulation models via the GUI based "dragging and dropping" of components. In this way models can be created quickly and efficiently. Finally, the solution of one and two dimensional SDEs using the SIMULINK models will be compared to the solutions generated by the classical techniques.