DqF Workshop *Stochastic Differential Equations: Models and Numerics*

Circumspect descent prevails in solving random constraint satisfaction problems

Erik Aurell, Royal Institute of Technology

Abstract: We study the performance of stochastic local search algorithms for random instances of the K-satisfiability (K-SAT) problem. We introduce a new stochastic local search algorithm, ChainSAT, which moves in the energy landscape of a problem instance by *never going upwards* in energy. ChainSAT is a *focused* algorithm in the sense that it considers only variables occurring in unsatisfied clauses. We show by extensive numerical investigations that ChainSAT and other focused algorithms solve large K-SAT instances almost surely in linear time, up to high clause-to-variable ratios α; for example, for K=4 we observe linear-time performance well beyond the recently postulated clustering and condensation transitions in the solution space. The performance of ChainSAT is a surprise given that by design the algorithm gets trapped into the first local energy minimum it encounters, yet no such minima are encountered. We also study the geometry of the solution space as accessed by stochastic local search algorithms.

Approximation of Functionals of SDEs and application to a recent multilevel Monte Carlo Method

Rainer Avikainen, Department of Mathematics and Statistics, University of Jyväskylä

Abstract: We consider the problem of approximating a random variable $g(X)$ by $g(\hat{X})$ for non-Lipschitz functions g using the L_p-norm as an error criterion. We find that for functions g of bounded variation, this error is

bounded from above in an optimal way by the error of approximating X by $\hat{X}$, under the assumption that X has a bounded density f_X. We apply this result to the approximation of stochastic differential equations, and show that

$$\mathbb{E}|g(X_T) - g(X_T^E)|^p \leq \text{const}(p, f_{X_T}, g)\,|\pi|^{\frac{1}{2} - \frac{\text{const}}{(-\log|\pi|)^{1/3}}},$$

where X_T is a solution of an SDE at time T, X_T^E is the Euler approximation of X_T related to a partition π with mesh size $|\pi|$, and $1 \leq p < \infty$. This inequality turns out to be of importance in discretization of BSDEs [2], and in computing expected payoffs of options by Monte Carlo methods. We explain how our result can be applied to reduce the computational complexity of a multilevel Monte Carlo method developed by M. B. Giles [3]. A particular example is the payoff function of the digital option, $\chi_{[K,\infty)}$, which falls into the class of non-Lipschitz functions with bounded variation. The talk is based on the article [1].

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Adaptive Weak Approximation of Reflected Stochastic Differential Equations

Christian Bayer, Dept. of Mathematics, Royal Institute of Technology

Abstract: Given a domain $D \subset \mathbb{R}^d$, consider the solution (X_t, Z_t), $X_t \in D$, $Z_t \geq 0$, of a stochastic differential equation in D reflected at the boundary ∂D. We present an adaptive weak algorithm in the spirit of Szepessy, Tempone and Zouraris [2001] for solutions of reflected SDEs and the corresponding parabolic Cauchy problem, where the reflection corresponds to a Neumann boundary condition. We also give the results of numerical experiments.

Stochastic Reaction Diffusion Kinetics in Bacterial Cells

Johan Elf, Dept. of Cell and Molecular Biology, Uppsala University

Abstract: I will discuss the reaction diffusion master equation (RDME) [1] as a framework for spatially resolved stochastic kinetics. I will also describe the Next Subvolume Method (NSM) [2] which is a fast algorithm for sampling exact trajectories of systems modeled by the RDME. The NSM has for instance been implemented in our software MesoRD [3], which is freely available at sourceforge.net. I will further describe a biologically relevant system where stochastic kinetics results in phenomena that can not be modeled by conventional deterministic reaction-diffusion equations [4]. Finally, I will present some ot our experimental results from single protein tracking in living E. coli cells at a time resolution of 10ms and a spatial precision of 50nm [5]. In particular, I will show that the YFP fused lac repressor displays normal diffusion over all measured timescales (10ms-100ms), which partly justifies the simple RDME approach to in vivo kinetics.

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Parallel Solution of Multiscale Stochastic Chemical Kinetics

Stefan Engblom, Div. of Scientific Computing, Dept. of Information Technology, Uppsala University

Abstract: The time-parallel algorithm parareal is proposed as a solver for stochastic models in chemical kinetics. A fast solver at the coarse scale (evaluated in serial) is available in the form of the usual macroscopic rate

equations. A stochastic simulation is then used to obtain an exact realization of the process at the mesoscopic scale (in parallel).

The underlying stochastic description is a jump process over the positive integer lattice driven nonlinearly by the Poisson random measure. We state a convergence result which suggests that a homogenization of the solution is advantageous. A simple but highly general such technique is devised.

Numerical experiments on models representative to the field of computational systems biology illustrate the method. For non-stiff problems, it is shown that the method is able to quickly converge even when stochastic effects are present. For stiff problems we are instead able to obtain fast convergence to a homogenized solution. Overall, the method builds an attractive bridge between on the one hand, macroscopic deterministic scales and, on the other hand, mesoscopic stochastic ones. This construction is clearly possible to apply also to the solution of stochastic problems within other fields.

Multilevel Monte Carlo path simulation

Mike Giles, Mathematical Institute, Oxford University

Abstract: In this talk I will explain the key ideas behind multilevel Monte Carlo path simulation, and current progress in its further development including: use of Milstein discretisation, QMC extension, "vibrato" MC for digital options, and the extension to SPDEs, if time permits.

Stochastic Modelling and Simulation Issues in Gene Regulation

Des Higham, Department of Mathematics á University of Strathclyde

Abstract: Many interactions inside the cell involve species that are present in relatively small quantities. In these cases, stochastic modelling and simulation is relevant and noise is typically summarized through means, correlations and variances. In gene regulation, the modelling framework of chemical kinetics has proved successful, see, for example, Thattai and van Oudenaarden, PNAS, 2001 and Raser and O'Shea, Science, 2004. A fully discrete Markov jump processes can be used to model such systems, and Gillespie's algorithm allows for pathwise simulations. However, for large systems and/or fast reactions, these simulations can be prohibitatively expensive. Under appropriate modelling assumptions (Kurtz, SIAM, 1981) we

can approximate the discrete-valued model by a stochastic differential equation, known as the Langevin equation, that is cheaper to simulate and more amenable to analysis, using the tools of stochastic calculus. However, other than other than the fact that they agree in the appropriate, thermodynamic, limit, little is known about how well the Langevin equation approximates the Markov jump version.

In this talk, we will compare the Markov jump and Langevin frameworks in order to quantify how much is lost by taking the diffusion limit. Analytical results will be given for simple gene regulation models arising in the literature, and numerical experiments will be presented for more complicated models that are outside the class of first-order networks.

It is also possible to construct hybrid models that combine elements of the discrete and continuous state spaces. These allow for multi-scale simulation tools, where components are treated differently, according to the way that they contribute to the overall system. For example, in a simple one gene setting, activator transcription factor binding/unbinding can be treated discretely, while the more abundant mRNA and protein species can be regarded as continuously-valued. In this context we arrive at stochastic differential equations driven by Markov switches, and appropriate stochastic analysis tools can be used to investigate the model properties.

Complex Networks

Petter Holme, Royal Institute of Technology

Abstract: Many systems in the world – from chemical reactions in organisms to friendships across our planet, from trade patterns between nations to magnetic materials – consist of huge numbers of interacting units. The global features of such systems might be hard to predict from the properties of the individual units. A key to understanding the such systems is the interaction between the units. In some cases the interactions can be assumed symmetric. This is the case in magnetic materials where the units are atoms organized in a crystal lattice. In other cases the interactions are to some extent random, but there are also regularities, or structure, in the couplings. One approach to investigate the global properties of such systems is to use statistical graph theory. A first step in this direction is to construct quantities to measure the regularities, or network structures. Then, one can investigate how the network structure affects the dynamic systems confined to the network. In some cases, one can address questions about the mechanisms of the network

evolution, including feedback from the dynamic system on the networks. I will discuss complex network methods with examples from biochemistry and epidemiology.

Modelling of wave particle interactions and collisions in toroidal plasmas

Josef Höök, Royal Institute of Technology,

Abstract: One of the major task in modeling heating and transport of a fusion plasma is calculating the distribution function of various plasma species. This is modeled by a nonlinear Fokker-Planck equation and is normally solved with finite difference, finite elements or Monte Carlo-methods. Since the solution often deviates weakly from a local Maxwellian δf Monte Carlo methods are popular for solving perturbed Fokker-Planck equation. Different δf-methods exists requiring modeling of the source term. To avoid an increase of the number of simulated particles commonly used scheme is to model the source term by reweighting the particles. Here a different scheme is proposed where we utilize active injection of particles together with a restart procedure, which conserves lower order momentum. By injecting particles the number of iterations is reduced.

Equilibrium polymer conformations: Large Deviations Approach

Evangelia Kalligiannaki, Applied Mathematics, University of Crete

Abstract: The equilibrium behavior of polymer systems is of great scientific interest in the last decades since the use of polymeric materials in industry and everyday use is continuously increasing.

Though (self-consistent) field theory is the basic toll for the study of static properties of complex polymer systems, is a mathematically formal procedure.

The aim of our work is two-fold: either reproduce the information obtained from filed theoretic methods, and/or give information on new quantities of interest using Large Deviation Theory, for which FT is not directly applicable.

We propose a model reduction procedure consisting of two coarse graining levels using Large Deviation techniques.

Coarse-graining, reconstruction and importance sampling methods for the simulation of many-particle stochastic systems

Markos Katsoulakis, Applied Mathematics, University of Crete

Abstract: We discuss recent work on coarse-graining methods for microscopic stochastic lattice systems. We emphasize the numerical analysis of the schemes, focusing on error quantification as well as on the construction of improved algorithms capable of operating in wider parameter regimes. We also present adaptive coarse-graining schemes which have the capacity of automatically adjusting during the simulation if substantial deviations are detected in a suitable error indicator. The methods employed in the development and the analysis of the algorithms rely on a combination of statistical mechanics methods (renormalization and cluster expansions), statistical tools (reconstruction and importance sampling) and PDE-inspired analysis (a posteriori estimates). We also discuss the connections and extensions of our work on lattice systems to the coarse-graining of polymers.

Spatial approximation of the stochastic heat and wave equations by finite elements

Stig Larsson, Department of Mathematics, Chalmers University

Abstract: We consider the linear stochastic heat and wave equations in several spatial variables driven by additive correlated space-time noise. The equations are written in the abstract form

$$du + Au\,dt = dW$$

where A is the generator of a strongly continuous semigroup of bounded linear operators on Hilbert space (analytic semigroup in the case of the heat equation) and W is a Hilbert space valued Wiener process. The equation is discretized in the spatial variable by a finite element method. We provide an abstract framework for the error analysis and we prove strong convergence estimates, i.e., error estimates in a mean square norm. In the case of the heat equation we also prove so-called weak convergence estimates and show that the rate of weak convergence is twice that of strong convergence.

This joint work with Fredrik Lindgren, Fardin Saedpanah, Ali Mesforush, Chalmers University, Mihaly Kovacs, Chalmers University and Otago University, New Zealand, and Matthias Geissert, Darmstadt.

Fokker-Planck and Stochastic differential equations with Sobolev regular coefficients

Claude Le Bris, Ecole Nationale des Ponts et Chaussees and INRIA, France

We present some recent results on the well-posedness of SDEs and the associated Fokker Planck equation when the coefficients (drift and diffusion) are typically not Lipschitz but only Sobolev regular. The talk is based upon a series of works [1,2,3] in collaboration with Pierre-Louis Lions (College de France, Paris).

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Adaptive methods for efficient sampling. Applications in molecular dynamics.

Tony Lelièvre, l'Ecole Nationale des Ponts et Chaussees, France

Abstract: One aim of molecular dynamics simulations is to sample Boltzmann-Gibbs measures associated to some potentials in high dimensional spaces, to compute macroscopic quantities (such as chemical reaction constants, or diffusions constants) by statistical means in the canonical (NVT) ensemble. Numerical methods typically rely on ergodic limits for processes solution to well-chosen stochastic differential equations (SDEs). The main difficulty comes from existence of metastable states in which the stochastic processes remain for long time: this may slow down dramatically the convergence of the ergodic limit. We present a class of adaptive importance sampling methods which enable fast exploration of the configurational space, by modifying the potential seen by the particles (the associated SDE becomes

non-homogeneous and nonlinear). These methods accelerate the longtime convergence while they allow to obtain, in the longtime limit, the quantities of practical interest (the marginal law associated to the slow variables in the system). We propose a proof of convergence for some of these methods, based on entropy techniques.

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Wavelet representation of the noise in stochastic evolution equations

Fredrik Lindgren, Mathematical Sciences, Chalmers University of Technology and University of Gothenburg.

Abstract: We describe how wavelets may be used to expand Hilbert space-valued Wiener processes and how the compressibility capacity of wavelets can be used for efficient computation of these expansions. In this process the covariance matrix of the noise needs to be computed, as well as its Cholesky factorization. It turns out that wavelet expansions have advantageous properties when adaptive methods are used, especially in comparison with expansion in finite element functions. We also show how wavelet expansions can be used to simulate stochastic evolution equations with additive noise and how the properties of the wavelets are used to prove error estimates for spatial approximations based on various Galerkin methods.

This is joint work with M. Kovacs, S. Larsson and K. Urban.

Stochastic reaction-diffusion processes in systems biology

Per Lötstedt, Uppsala University

Intrinsic noise in biochemical networks can have a large impact on the macroscopic behavior of biological cells. An example is the regulation of the

transcription of genes to messenger RNA (mRNA) where genes are present in one or two copies and the copy number of mRNA is small. A discrete, stochastic description of the system is necessary since the copy number is a small nonnegative integer and there is only a probability that a certain reaction will occur when two molecules meet.

Such stochastic chemical systems with diffusion are modeled with a reaction-diffusion master equation. The state of the system is the space dependent number of molecules of each participating species. The dimension of a system discretized in space is very high ('the curse of dimensionality'), making the direct computational solution of the master equation impossible. Instead, trajectories of the system are generated and mean values of the species are computed using Monte Carlo methods.

On a macroscopic level, the governing equation is a reaction-diffusion equation for the averages of the chemical species. On a mesoscopic level in our approach, the master equation for a well stirred chemical system is combined with Brownian motion in space to obtain solutions of the reaction-diffusion master equation. The space is covered by an unstructured mesh and the diffusion coefficients on the mesoscale are obtained from a finite element discretization of the Laplace operator on the macroscale. The resulting method is a flexible hybrid algorithm in that the diffusion can be handled either on the meso- or on the macroscale level. The accuracy and the efficiency of the method are illustrated in numerical examples inspired by systems biology.

This is a collaboration with Stefan Engblom, Lars Ferm and Andreas Hellander.

Nonparametric Density Estimation for Elliptic Problems with Random Perturbations

Axel Målqvist, Division of Scientific Computing Department of Information Technology, Uppsala University

Abstract: Dealing with the effects of uncertainty in data and coefficients on the solution of a deterministic elliptic problem is an important problem in practical application. For example, such uncertainty might arise from error in experiments used to determine values or as a result of coupling to other physical systems. In such settings, the uncertainty is best described as random in nature. This leads to the problem of describing the response in a

quantity of interest computed from the solution resulting from the uncertain variations in parameters and data. This is a difficult problem for a number of reasons, e.g., computing a large number of samples is prohibitively expensive and numerical error varies as parameters and data vary.

We develop and analyze an efficient numerical method for computing the response of a quantity of interest computed from the solution of an elliptic problem with randomly perturbed coefficients and data. We use a variational analysis based on the adjoint operator to deal with the perturbations in data. To deal with perturbations in the diffusion coefficient, we construct a piecewise constant approximation to the random perturbation then use domain decomposition to decompose the problem into sub-problems on which the diffusion coefficient is constant. To compute local solutions of the sub-problems, we use the infinite series for the inverse of a perturbation of an invertible matrix to devise a fast way to compute the effects of variation in the parameter. Finally, we derive a posteriori error estimates that take into account all the sources of error and derive a new adaptive algorithm that provides a quantitative way to distribute computational resources between all of the sources.

Integration by parts for Monte-Carlo simulations of sensitivity measures driven by infinite activity processes

Roger Pettersson, Växjö University

Abstract: In this talk the focus is on Monte Carlo approximation of sensitivity measures of the type $\partial E[\Phi(S_T)]/\partial S_0$ or $\partial E[\Phi(\int_0^T S_t dt)]/\partial S_0$ where $\{S_t\}_{0\leq t\leq T}$ is the exponential of a finite variation infinite activity process. Here the sum of the small jumps are approximated by a suitably scaled Wiener process. Inspired by Bally, Bavouzet and Messaoud (2007), finite-dimensional integration by parts is performed with respect to the approximating Wiener process and the large jumps.

Stochastic molecular dynamics derived from fundamental principles

Anders Szepessy, Department of Mathematics, Royal Institute of Technology

Abstract: In this talk I will show that Born-Oppenheimer, Langevin,

Ehrenfest and surface-hopping dynamics are accurate approximations of time-independent Schrödinger observables for a molecular system, in the limit of large ratio of nuclei and electron masses, without assuming that the nuclei are localized to vanishing domains. The derivation, based on characteristics for the Schrödinger equation, bypasses the usual separation of nuclei and electron wave functions and gives a different perspective on initial and boundary conditions, the Born-Oppenheimer approximation, hopping, and computation of observables in molecular dynamics modeling.

Adaptive Multi Level Monte Carlo Simulation

R. Tempone, Dahlquist Fellow, Royal Institute of Technology and Florida State University

Abstract: This work generalizes a multilevel Forward Euler Monte Carlo method introduced in [2] for the approximation of expected values depending on the solution to an Itô stochastic differential equation. The work [2] proposed and analyzed a Forward Euler Multilevel Monte Carlo method based on a hierarchy of uniform time discretizations and control variates to reduce the computational effort required by a standard, single level, Forward Euler Monte Carlo method. This work introduces and analyzes an adaptive hierarchy of non uniform time discretizations, generated by adaptive algorithms introduced and analyzed in the works [1,4]. These adaptive algorithms apply either deterministic time steps or stochastic time steps and are based on a posteriori error expansions developed first in [6] and later extended to stopped diffusions [1] and jump difussions [5]. Under sufficient regularity conditions, both our analysis and numerical results exhibit savings in the computational cost to achieve an accuracy of $\mathcal{O}\left(\mathrm{TOL}\right)$, from $\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$ to $\mathcal{O}\left(\left(\mathrm{TOL}^{-1}\log\left(\mathrm{TOL}\right)\right)^2\right)$.

This is a joint work with Håkon Hoel, Erik von Schwerin and Anders Szepessy.

References

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Multiscale Monte Carlo simulations for biological, materials, and chemical engineering applications

Dion Vlachos, Department of Chemical Engineering, University of Delaware, Newark, DE, 19716

Abstract: Multiscale simulation is emerging as a new scientific field in chemical sciences. The idea of multiscale modeling is straightforward: one computes information at a smaller (finer) scale and passes it to a model at a larger (coarser) scale by leaving out degrees of freedom as one moves from finer to coarser scales. The obvious goal of multiscale modeling is to predict macroscopic behavior of an engineering process from first principles (bottom-up approach). However, the emerging fields of nanotechnology and biotechnology impose new challenges and opportunities. For example, the ability to predict and control phenomena and nano-devices with resolution approaching molecular scale while manipulating macroscopic (engineering) scale variables can only be realized via multiscale simulation (top-down approach). As another example, the miniaturization of microchemical systems for portable and distributed power generation imposes new challenges and opportunities than the conventional scaling up chemical engineers have worked on. In this talk, various fairly new concepts of multiscale Monte Carlo (MC) methods will be discussed. Different algorithms will be illustrated with applications from systems biology (e.g., multigrid simulations to model signal transduction for cancer control), materials science (e.g., tau-leaping on microscopic

lattices for thin film deposition; optimal control strategies in heteroepitaxial growth), and chemical engineering (e.g., spatially adaptive MC methods for energy generation on catalysts; stochastic homogenization for diffusion through membranes).

Adaptive weak approximation for SDEs

Georgios Zouraris, Department of Mathematics, University of Crete, Greece.

The problem of constructing an approximation to the expected value $E[g(X(T))]$ with discretization error of the given size $TOL > 0$ is considered, where $X(T)$ is the value of the solution of an Ito SDE at the final time T and g a given real valued function. A general framework to develop an expansion of the time discretization error based on computable leading order terms in a posteriori form is presented. This general expansion can be applied to several methods for the approximation of the solution of an Ito SDE. Our previous analysis was mainly related to the Euler-Maruyama method. An application to the Drift Implicit Euler method is discussed and numerically tested. This is a joint work with E.Mordecki, A.Szepessy and R. Tempone

Monte Carlo algorithms for the Dirichlet problem for parabolic operators in the setting of time-dependent domains

Tomas Önskog, Department of Mathematics, Umeå University

Abstract:

Consider the Dirichlet problem for parabolic operators in the setting of time-dependent domains. The performance of any numerical algorithm for this problem depends on the structural assumptions on the operator, the geometry and smoothness properties of the space-time domain, the smoothness of the Dirichlet data and the smoothness of the coefficients of the operator under consideration. In this talk it is shown how the performance of various Monte Carlo methods for weak approximation of stochastic differential equations, when applied to the Dirichlet problem for parabolic operators in the setting of time-dependent domains, varies as the smoothness of the boundary, Dirichlet data and coefficients change from smooth to non-smooth. The methods evaluated and discussed include elaborations on the non-adaptive method proposed in [1] based on approximation by half spaces and exit prob-

abilities and the adaptive method proposed in [2]. Our analysis is set in the genuinely parabolic setting of time-dependent domains, which in itself adds interesting features previously only modestly discussed in the literature."

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Stochastic Differential Equations Brownian Motion ItÃ´ Calculus Numerical Solution of SDEs Types of Solutions to SDEs Examples Higher-Order Methods Some Applications. Stability Weak Solutions Higher-Order Schemes Examples Numerical Examples. Bibliography. Intro to SDEs with with Examples Stochastic Differential Equations. Stochastic Differential Equations. Stokeâ€™s law for a particle in uid. dv (t) = â^'Î³ v (t) dt.Â Some applications: Black-Scholes model for asset volatility Langevin dynamics shearing of light in inhomogeneous universes. Intro to SDEs with with Examples Stochastic Differential Equations Some Applications. Some Applications. The workshop will have two main goals. One is to bring together internationally renowned researchers working on various topics related to the theory and applications of SPDEs, to exchange the latest results and generate novel ideas for research directions and applications. This goal will be achieved through invited and contributed talks, as well as through informal discussions in smaller groups.Â Stochastic integrals and stochastic partial differential equations: an introduction (part 1). Robert Dalang, Ecole Polytechnique FÃ©dÃ©rale de Lausanne. 10:30 to 11:00. To realize the applications of stochastic differential equations with jumps, much attention has recently been paid to the construction of efficient numerical solutions of the equations.Â Ying Du, Changlin Mei, "Implicit Numerical Solutions for Solving Stochastic Differential Equations with Jumps", Abstract and Applied Analysis, vol. 2014, Article ID 159107, 11 pages, 2014. https://doi.org/10.1155/2014/159107. Show citation. Implicit Numerical Solutions for Solving Stochastic Differential Equations with Jumps.