The practice and theory of stochastic simulation

organized by
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Workshop Summary

Modeling stochastic effects is of increasing importance across science and technology. While purely analytic investigations are important, there scope is fairly limited. Many problems of current interest require some amount of computing. On one side, much of the careful mathematical investigations of stochastic numerical methods have concentrated on stochastic adaptations of classical numerical methods used for ordinary differential equations [PT85,Tal82]. Driven by applications, many practitioners have developed schemes which are used but supported by little theoretical justification. The aim of the workshop was to bring together people from different communities, those interested in specific, concrete applied problems with those involved in more general theoretical investigations. We were especially interested in discussing methods which include analytic understanding of specific settings to obtain faster and more effective algorithms which improve over direct, brute force approaches.

A rich source of problems which fall into this category are stochastic systems which span many spatio- and temporal-scales. Molecular dynamics and stochastic simulations in chemical kinetics are two important examples that were the main focus of the workshop. Some specific issues that we discussed were:

Long-time intergration in molecular dynamics simulatin. Traditionally, the method of choice of in molecular dynamics has been the use of Verlet integrator and/or higher order symplectic version of it (like e.g. the adaptive variational integrators, AVIs) [JL05]. Originally, such integrators were designed to sample the microcanical measure over a long-time horizon. More recently, however, symplectic integrators have be generalized to other ensembles, such as the canonical ensemble. During the workshop, we discussed these recent advances.

We also discussed alternative approaches based on stochastic differential equations. These have the advantage over deterministic systems that it is easier to prove their ergodicity. We spend some time discussing how to develop and analyze long-time integrators for stochastic differential equations which are both stable and accurate. An interesting outcome of the discussions was the realization that it is possible to generalize symplectic schemes such as AVI to the stochastic set-up.

Multiscale methods for stochastic simulation algorithms (SSA).. In kinetic Monte-Carlo, the method of choice for integration is Gillespie's SSA [Gil76] (also known as BKL after Bortz, Kalos and Lebowitz). SAA is a rejection-free method which produces an exact sample path of the process. There are, however, problems with the efficiency of SSA in situations where the rate matrix of the continuous-time Markov chain underlying the Monte-Carlo scheme contains intensities which are very different in order of magnitude. In these situation, SSA becomes inefficient because the timescale is set by the fastest reactions, whereas one often interested in computing over the much longer timescale set by the slowest reactions. To remedy this problem, a wealth of new methods based on SSA have been recently proposed:

slow-scale SSA, nested SSA, tau-leap methods, etc. [RPCG05,CGP05,CGP05]. During the workshop we made a thorough comparison of these various techniques and discussed several routes for their improvements.

Owing to the rather small number of participants, the workshop was run in a very informal fashion, typically with two talks in the morning and plenty of time for discussion in the afternoon. We feel that the workshop was a great success. People liked it a lot, many ideas were exchanged, and new collaborations were started.

Bibliography

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