IT Eminent Lecture Series

Multiscale Simulation of Biochemical Systems

Linda Petzold, University of California Santa Barbara

Coates Hall 145
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Abstract:
In microscopic systems formed by living cells, the small numbers of some reactant molecules can result in dynamical behavior that is discrete and stochastic rather than continuous and deterministic. An analysis tool that respects these dynamical characteristics is the stochastic simulation algorithm (SSA). Despite recent improvements, as a procedure that simulates every reaction event, the SSA is necessarily inefficient for most realistic problems. There are two main reasons for this, both arising from the multiscale nature of the underlying problem: (1) the presence of multiple timescales (both fast and slow reactions); and (2) the need to include in the simulation both chemical species that are present in relatively small quantities and should be modeled by a discrete stochastic process, and species that are present in larger quantities and are more efficiently modeled by a deterministic differential equation. We will describe several recently developed techniques for multiscale simulation of biochemical systems, and outline some of the future challenges.

Speaker's Bio:
Dr. Linda Petzold is currently Professor in the Department of Computer Science (Chair 2003-2007) and the Department of Mechanical Engineering, and Director of the Computational Science and Engineering Program at the University of California Santa Barbara. She received her Ph.D. in Computer Science in 1978 from the University of Illinois. From 1978-1985 she was a member of the Applied Mathematics Group at Sandia National Laboratories in Livermore, California, from 1985-1991 she was Group Leader of the Numerical Mathematics Group at Lawrence Livermore National Laboratory, and from 1991-1997 she was Professor in the Department of Computer Science at the University of Minnesota. Dr. Petzold is a member of the US National Academy of Engineering. She is a Fellow of the ASME and of the AAAS. She was awarded the Wilkinson Prize for Numerical Software in 1991, the Dahlquist Prize in 1999, and the AWM/SIAM Sonia Kovalevski Prize in 2003. She served as SIAM (Society for Industrial and Applied Mathematics) Vice President at Large from 2000-2001, as SIAM Vice President for Publications from 1993-1998, and as Editor in Chief of the SIAM Journal on Scientific Computing from 1989-1993.

This lecture has a reception.

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