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# Joint Seminar
# Applied Mathematics and ICMS


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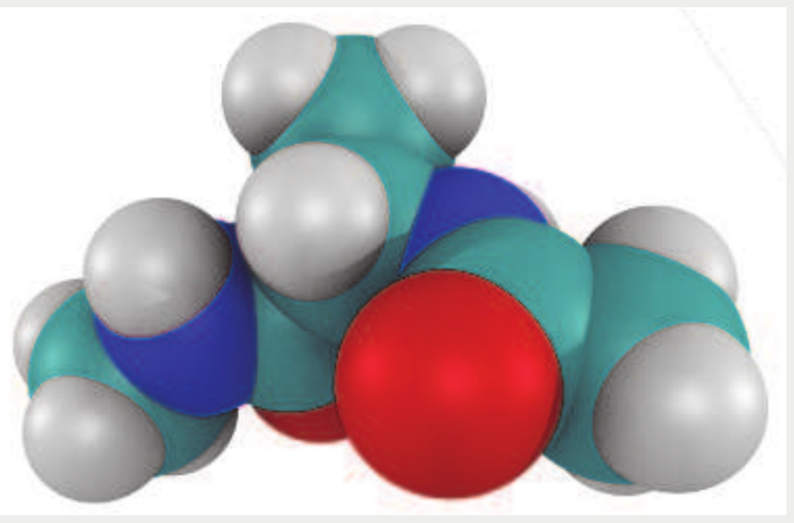
## November 6th, 2019, 4:00pm, SERC 504, Tea 3:30pm

# The Complete Set of Efficient and Precise Simulation Methods for Langevin and Molecular Dynamics


**Abstract:** One of the most basic computational struggles in computational science of dynamical systems is how to appropriately balance the desire for simulation accuracy, obtained in the small time step limit, with simulation efficiency, obtained for large time steps. Thus, understanding the influence of discrete-time on the behavior of equations of motion is crucial for the understanding and optimization of numerical simulations in physical science and engineering. We argue that for many applications the core of the problem is not that discrete-time errors are enhanced as the time step is increased, but instead that the errors are inconsistently affecting spatial and kinetic degrees of freedom. From this observation we developed a new, yet familiarly looking, complete set of Langevin simulation methods that yield exact thermodynamics for both configurational and kinetic sampling for any stable time step. In light of representative examples, we discuss the applicability and convenience of these methods, and conclude that these are the optimal methods for Langevin simulations of the thermodynamics.

## Speaker Bio

Grønbech-Jensen completed a M.Sc. in Applied Mathematical Physics (1989, Quantum Optics) and a Ph.D. in Physics (1991, Perturbation methods for nonlinear dynamics and phase-locking) from the Technical University of Denmark. After a short postdoc in Applied Physics at Stanford, he joined the Condensed Matter and Statistical Physics Group in the Theoretical Division at LANL in 1992, where he became involved with large scale molecular dynamics. In 1999 NGJ moved to UC Davis, where he has been a professor in several departments, Applied Science, Chemical Engineering and Materials Science, Mech. & Aerospace Engineering, and Mathematics. He is currently in the latter two departments. His research interests cover molecular modeling of, e.g., self-assembly and radiation damage, macroscopic quantum phenomena in superconducting Josephson systems, and algorithm development for statistical and dynamical systems.

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