FS1011   10 June 2025

A DCAMM seminar No. 787 will be presented by

Distinguished Professor Niels Grønbech Jensen
Departments of Mechanical and Aerospace Engineering, Mathematics
University of California; Davis, California, USA

The title of the lecture is

Linear quality analysis of stochastic Verlet-type Langevin integrators for
Molecular Dynamics and Computational Statistical Mechanics

Abstract:

One of the basic struggles in simulations of statistical and dynamical systems is how to appropriately balance the desire for simulation accuracy in the small time step limit with simulation efficiency 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 computational statistical mechanics of the Langevin equation, 1) it is not necessary to obtain accurate trajectories in order to generate accurate statistics, and 2) a numerical method should first and foremost be analyzed by its configurational properties since momentum is an unnecessary (and unphysical) quantity for discrete-time sampling of the phase-space [1]. Following the derivation of the complete set of stochastic Verlet-type integrators [2], we here provide a linear framework for analyzing the quality of the large number of stochastic integrators that have been proposed over the past five decades [3]. With some redundancy of logic we conclude that the previously identified complete set of GJ integrators is the only set that possesses the basic statistical properties, which allow for large time-step simulations that preserve statistical accuracy in the most basic measures of diffusion, drift, and sampling (Boltzmann) distribution, even if the simulated trajectories suffer from time step errors. The methods are remarkably simple and can be immediately implemented into existing codes, such as ones used for Molecular Dynamics.

[1] Grønbech-Jensen, Journal of Statistical Physics 191, 137 (2024)
[2] Grønbech-Jensen, Molecular Physics 118, e1662506 (2020)
[3] Grønbech-Jensen, arXiv:2505.04100 (2025)

DATE:	**Thursday, 19 June 2025**
TIME:	**11:00 – 11:45**
PLACE:	**Building 303B, Room 134, Matematicum** **DTU, Technical University of Denmark**

Danish pastry, coffee and tea will be served 15 minutes before the seminar starts.

All interested persons are invited.

Jan Becker Høgsberg

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