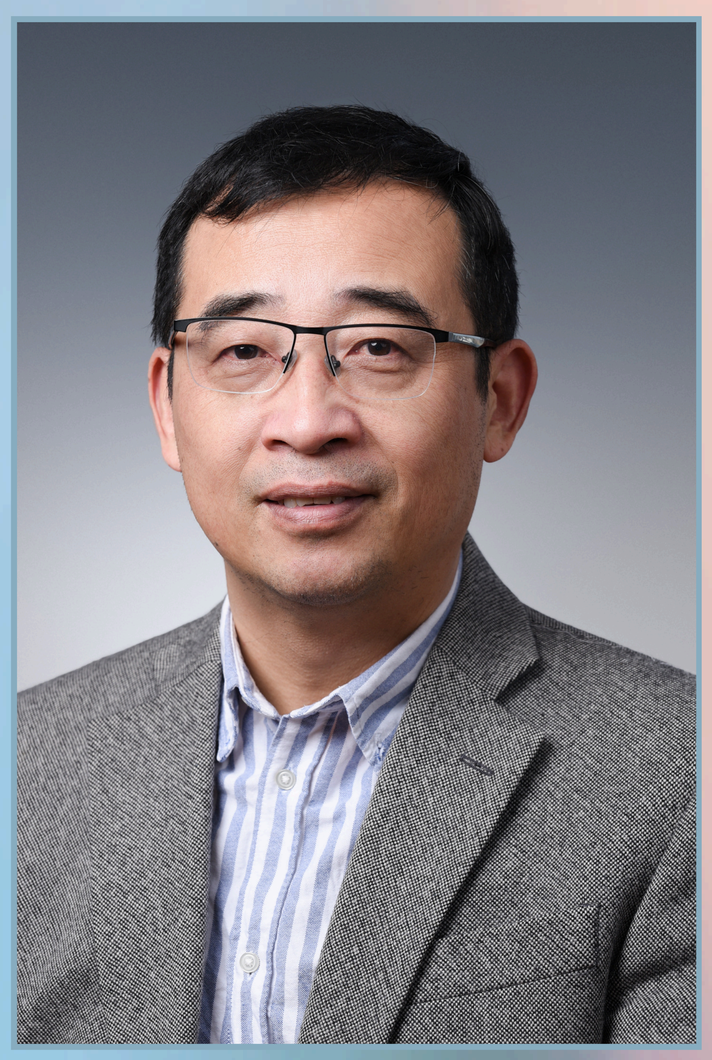
Friedrich-Alexander-Universität
Research Center for
Mathematics of Data | MoD

FAU MoD Lecture Series



#FAUMoDLecture

WWW.MOD.FAU.EU

Shi Jin

SHANGHAI JIAO TONG UNIVERSITY

Random Batch Methods for classical and quantum molecular dynamics

Random batch methods were introduced for general interacting particle systems with large number (N>>1) of particles, with a linear complexity of O(N).

We extend this method to molecular dynamics with Coulomb interactions, in the framework of Ewald summation. We will show its superior performance compared to the current state-of-the-art methods (for example PPPM) for the corresponding problems, in both computational efficiency and parallelizability.

We use it not only to reduce the cost of long range interactions but also the short-range ones, and as a result we are able to simulate 10 million molecules with just one GPU.

We also extend it to quantum Monte-Carlo simulation.

WHEN

Fri. **May 2, 2025**

10:00H
(Berlin time)

WHERE

On-site / Online

FAU. Friedrich-Alexander-Universität Erlangen-Nürnberg
Room H12
Felix-Klein building
Cauerstraße 11
91058 Erlangen
Bavaria, Germany

Live streaming:
www.fau.tv/fau-mod-livestream-2025

Nana Liu

SHANGHAI JIAO TONG UNIVERSITY

Quantum simulation for partial differential equations

Quantum simulators were originally proposed to be helpful for simulating one partial differential equation (PDE) in particular – Schrödinger's equation. If quantum simulators can be useful for simulating Schrödinger's equation, it is hoped that they may also be helpful for simulating other PDEs. (...)
In this talk, I will introduce the notion of Schrodingerisation: a procedure for transforming non-Schrödinger PDEs into a Schrödinger-form. This simple methodology can be used directly on analog or continuous quantum degrees of freedom – called qumodes, and not only on qubits. This continuous representation can be more natural for PDEs since, unlike most computational methods, one does not need to discretise the PDE first. (...) I show how this method can also be applied to both autonomous and non-autonomous linear PDEs, certain nonlinear PDEs, nonlinear ODEs and also linear PDEs with random coefficients, which is important in uncertainty quantification.