

Seminar

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Topic

On the Kinetic Description of Objective Molecular Dynamics (OMD): multiscale modeling, numerics, data-driven applications

Date | Time

2 January 2025 (Thursday) | 15:00 – 16:00 (HK Time)

Venue

TU817

Abstract:

In the first part of this talk, a multiscale modeling framework for objective molecular dynamics (OMD), a reduced molecular dynamics approach with inherent symmetries, will be presented. This hierarchical framework bridges OMD with statistical kinetic equations and macroscopic hydrodynamic models. In the kinetic regime, we identify two distinct interaction scalings, leading to either a mean-field-type or Boltzmann-type equation. At the macroscopic level, we derive reduced Euler and Navier-Stokes systems through a detailed asymptotic analysis. The second part of the talk introduces a fast spectral method for numerically solving the derived kinetic equations, supported by convergence analysis and numerical simulations to confirm its effectiveness. If time permits, I will discuss our recent progress in applying data-driven methodologies to kinetic theory.