THE UNIVERSITY   **OF HONG KONG**

Institute of Mathematical Research
Department of Mathematics

Numerical Analysis Seminar

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

Dr Kunlun Qi
School of Mathematics, University of Minnesota

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. As an outlook, I will discuss our recent progress in applying data-driven and machine-learning methodologies to kinetic theory.

Date:	May 22, 2025 (Thursday)
Time:	4:00 pm – 5:00 pm
Venue:	Room 210, Run Run Shaw Building, HKU

All are welcome