

Fundamentals of Particle Dynamics in Environmental Engineering

By

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3:00-3:30 pm Coffee Hour

3:30-4:30 pm Seminar

Please join us for the coffee hour near the seminar venue a half hour
before the seminar, 3:00 – 3:30 pm

Abstract

In environmental science and engineering, particles are generally defined as small pieces of material whose sizes range from a few nanometers to a few hundred micrometers. The recent definition of colloids embraces bio-colloids, which range from viruses (tens of nanometers) to bacteria (tens of micro-meters). Inter-particle interactions from physical, chemical, biological, and hydrodynamic origins determine spatial phases of various particles such as dispersion, aggregation, and collective transport. In this light, understanding dynamic behaviors of multi-particles in aqueous systems is a crucial component to design engineering processes such as flocculation, coagulation and (membrane) filtration and also predict natural phenomena such as marine snow settling and sediment transport.

Statistical physics provides excellent tools to mimic such complex multi-particle phenomena. Typical ensembles (such as micro-canonical, canonical, grand-canonical, and isothermal-isobaric) allow us to calculate macroscopic thermodynamic properties (in liquid states), which can be experimentally measured. Formidable mathematical complexities of the many-body dynamics often lead to approximate analytical theories at the continuum level. On the other hand, true microscopic simulation of individual particles surrounded by a swarm of interacting neighbors requires intensive computational efforts using supercomputers, allowing only a limited number of time steps. Covering above-mentioned topics, this talk will provide a holistic review of particle dynamics from fundamental physics to environmental engineering applications and will show how cutting-edge high-performance parallel computing can rigorously simulate many-body dynamics phenomena in liquid states.