

A course on Multiscale Computational Methods

The course will present the basics of the multiscale computational methodology, with further lectures and/or group interactions in more specific directions of interest to participants, possibly leading to future collaborations.

The multiscale computational methodology is a systematic approach, based on multigrid and renormalization-group ideas, to achieve efficient calculations of physical systems that include very many degrees of freedom (particle locations, discrete-function values, etc.). It includes fast *multigrid solvers* for discretized partial-differential equations (as well as other large systems of local equations); collective computation of *many eigenfunctions*; slowdown-free ‘*Monte Carlo (MC) simulators*’; multilevel methods of *global optimization*; and general procedures for “*systematic upscaling*”.

Systematic upscaling means the methodical derivation, scale after scale, of increasingly-larger-scale numerical “laws” (discrete equations or statistical “actions”, generally in the form of numerical tables), starting at a microscopic scale where first-principle laws are known and leading to processing rules of collective variables at much larger scales. Using a small (e.g., 2 or 3) coarse-to-fine scale ratio at each coarsening step serves to avoid severe computational slowdowns.

The multiscale computational methods are applicable to many *heavyweight nano problems*, such as: density-functional calculation of electronic structures and derivation of force fields for molecular-dynamics (MD) and molecular static (MS) simulations; acceleration and upscaling of various MC, kinetic MC, MD and MS simulations of fluids, condensed matter and macromolecules; fast summation of long-range (e.g., electrostatic) interactions; and fast solvers for steady-state and time-implicit equations of various continuum and mixed continuum-atomistic models of materials, species concentrations, moving interfaces, etc. Systematic upscaling is particularly important, since typical nano structures are complicated and lack constitutive equations, and the associated problems involve a wide range of scales.

Some of these topics, as well as multiscale algorithms in related areas such as global optimization, medical imaging and image processing, may be chosen for indepth lectures and interactions during or following the course.