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Predictive Coarse-Graining

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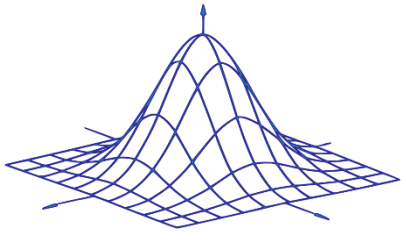
D202 Seminar room, School of Engineering, 2nd Floor

Abstract: Brute-force molecular dynamics simulations are limited by the exuberant number of degrees of freedom and the relatively small time-steps. As a result, only relatively small assemblies of molecules over small time spans are accessible with current and foreseeable computational capabilities. In order to overcome this limitation, coarse-grained models have been proposed which employ a much smaller number of degrees of freedom. These are based on the definition of a deterministic map from fine-to-coarse variables (restriction operator) and, in equilibrium settings, on approximating the exact free energy (CG or effective potential). Given a parametrization of the CG potential, the optimal parameters are subsequently determined by employing various objectives relating to matching thermodynamics properties, matching forces or information-theoretic distances. In this talk we advocate a perspective encountered in generative probabilistic models. This has the potential of quantifying uncertainties arising from information-loss that unavoidably takes place during coarse-graining as well as from the finite amount of data available (i.e. fine-scale simulations). Furthermore, it provides probabilistic predictions for the microscopic states i.e. it can reconstruct the full molecular picture. Under the same framework, model-selection issues can be simultaneously addressed not only with regards to the CG potential and its parametrization but also for the coarse-to-fine map (lifting operator). This can ultimately lead to a generalization in the definition of good CG variables which due to lack of physical insight usually have a local character, to CG variables that capture global microscopic features.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars



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