Taming and exploiting chaos in order to effectively simulate long trajectories

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Transition path sampling is unique as a practical method for sampling rare transition pathways without modifying a system's natural dynamics. Its application to biomolecular systems and complex materials has been limited, however, in part by the difficulty of applying useful displacements to Newtonian trajectory segments that are more than a few picoseconds long. We have devised a "precision shooting" method that overcomes this difficulty by controlling chaotic divergences, i.e., by accurately propagating arbitrarily small displacements in phase space. The second part of this talk will describe new simulations methods and physical perspectives from our work on self-assembly of nanometer-sized particles such as nanocrystals and protein complexes. Themes of competition between kinetics and thermodynamics, of the microscopic character of aggregation dynamics, and of cooperativity through fluctuations in nanoparticle structure will be emphasized.