TRAJECTORY AVERAGED NORMAL COORDINATE ANALYSIS: POLYMER DROPLETS AND CRYSTALS

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Normal coordinate analysis (NCA) requires the diagonalization of a mass-weighted potential energy second derivative matrix (Hessian matrix). In chemical systems with thousands of atoms, the Hessian matrix can be extremely sensitive to small perturbations in structure, leading to negative eigenvalues (imaginary frequencies) and unstable modes. This problem can be eliminated by performing a molecular dynamics simulation and constructing a trajectory averaged Hessian matrix. With this method, normal coordinates and frequencies have been calculated for polymer droplets and crystals with up to 36000 atoms (in contrast to single configuration NCA, which has never succeeded for realistically modeled systems larger than a few thousand atoms). Calculations of heat capacities and other quantities that can be computed from $g(\omega)$ are described in detail for several polymer droplets and crystals. Partial diagonalization schemes and other recent algorithmic improvements in the linear algebra regime yield order of magnitude improvements in computation time while still retaining accuracy.