Mori-Zwanzig Normal Mode Dynamics

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ABSTRACT

The recently introduced Normal Mode Langevin (NML) uses normal mode decomposition of the dynamics of implicitly-solvated biomolecules to propagate low frequency modes and thermalize near equilibrium fast frequencies [1,2]. Here we improve NML using the Mori-Zwanzig projection formalism in two way, both affecting properties of the propagation of low frequency modes. First, the damping tensor is computed from a molecular dynamics simulation. Second, the mean force is used instead of the instantaneous force. The computation of the mean force is done using multiple replicas and averaging. Analysis of the numerical and modelling error for a variety of systems will be presented.

[1]   C.R. Sweet, P. Petrone, V.S. Pande, J.A. Izaguirre, "Normal Mode Partitioning of Langevin Dynamics", submitted, *J. Chem. Phys*. (2007).

[2]   http://www.nd.edu/~lcls/normalmodes.html