

Abstract Submitted
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Application of Zwanzig-Mori projection in model coarse-graining

JIANHUA XING, ABHISHEK MUKHOPADHYAY, Virginia Tech — Reconstruction of equations of motion from incomplete or noisy data and dimension reduction are two fundamental problems in the study of dynamical systems with many degrees of freedom. We generalize the Zwanzig–Mori projection formalism, originally developed for Hamiltonian systems close to thermodynamic equilibrium, to general non-Hamiltonian systems lacking detailed balance. Then we develop a numerical algorithm to extract dynamic information for constructing the generalized Langevin equation. Numerical tests show that the formalism works remarkably.

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