Modeling transient dynamics of coarse-grained molecular systems.

Georgia Baxevani [1#*], **Evangelia Kalligiannaki** [2] and **Vagelis Harmandaris** [123]

[1] Department of Mathematics and Applied Mathematics, University of Crete, Heraklion Crete, Greece

[2] Institute of Applied and Computational Mathematics, Foundation for Research and Technology Hellas, Heraklion Crete, Greece

[3] Computation-Based Science and Technology Research, Center, The Cyprus Institute, 2121 Nicosia, Cyprus.

Presenting author: Georgia Baxevani, email: g.baxevani@iacm.forth.gr

* Corresponding author: Georgia Baxevani, email: g.baxevani@iacm.forth.gr.

ABSTRACT

In recent years, the development of model reduction and coarse-grained methodologies for studying large-scale molecular systems that cannot be practically studied with atom detailed molecular dynamics simulations is an active research field. Defining the new effective coarse-grained system, i.e. finding the model which best represents the reference system both in structure and dynamic properties, is the main goal of mathematical, and computational, multi-scale modeling. In the present work, we approximate the dynamics of coarse-grained systems at the transient regime from non-equilibrium to equilibrium conditions.

We approximate the short time non-Markovian dynamics by Markovian dynamics with a time-dependent force field. We present the application of the path-space force matching method to retrieve the coarse space parametrized drift. We follow a data-driven approach to estimate the friction kernel, calculating correlation functions directly from the underlying all-atom Molecular Dynamics simulations. The proposed model's effectiveness is examined by comparing its structural and dynamical properties with the corresponding reference system.

In addition, we implement non-equilibrium molecular dynamics simulations at the atomistic scale. By extracting the data from the detailed atomistic simulations corresponding to a non-equilibrium steady-state of the system, we calculate transport coefficients of interest. The methodologies are illustrated for the molecular water system.

REFERENCES

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