Modeling Transient Dynamics of Coarse-Grained Molecular Systems

Georgia Baxevani[1#,], **Evangelia Kalligiannaki**[24*] 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, Greece

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

[4]Department of Statistics and Actuarial-Financial Mathematics, University of the Aegean, Greece

Presenting author. georgia.mpax@gmail.com

*evangelia.kalligiannaki@gmail.com

$ harman@uoc.gr

ABSTRACT

In recent years, the development of coarse-grained models for studying large-scale processes that cannot be practically studied with atomically detailed molecular dynamics simulations is an active research field. Defining the new effective coarse-grained system, which reduces the dimensionality, accounts for finding the model best representing the reference system both in structure and dynamic properties. In the present work, we approximate the dynamics of coarse-grained systems at the transient regime.

Under the assumption that it is possible to perform molecular dynamics simulations of the atomistic system only in a short time interval corresponding to the transient regime, we propose a Langevin equation model characterized by time-depended pair potential accounting for the combined interaction forces of the system. We present the application of the path-space force matching method to retrieve the coarse space parametrized drift. At a long time limit, the time-dependent pair potential can reproduce the classical force matching potential of the mean force. In contrast, at transient -short time- regimes, we generate time-dependent drift coefficients describing the coarse-grained systems' dynamics. The model's effectiveness is examined by comparing its structural and dynamical properties with the corresponding reference system. The methodology is illustrated for the molecular water system.

REFERENCES

[1] Georgia Baxevani, Vagelis Harmandaris, Evangelia Kalligiannaki and Ivi Tsantili. 2023. *Multiscale Modeling & Simulation,* **21**:1746-1774.

[2] Georgia Baxevani, Evangelia Kalligiannaki and Vagelis Harmandaris. 2019. *Procedia Computer Science,* **156**:59-68.

[3] Vagelis Harmandaris Evangelia Kalligiannaki, Markos Katsoulakis and Petr Plecháč. 2016. *Journal of Computational Physics,* **314**:355-383.