Usage Report for Fiscal Year 2024

Project Title:

Testing randomness in fluctuating hydrodynamics from all-atom Molecular Dynamics modelling of liquids and nano-systems

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1. Background and purpose of the project, relationship of the project with other projects

In this work we planned to perform a series of Molecular Dynamics (MD) simulations with

- pure water (using two different water models: SPC/E and TIP3P),
- pure water next to a solid wall (a layer of mica),
- a protein molecule (trp-cage) in water,

using three different sizes of the simulation domain (7x7x7 nm, 10x10x10 nm, 15x15x15 nm) to test the influence of periodic boundary conditions. Each simulation was planned to be 10 ns long, and each case to be simulated 10 times starting from different initial states to produce 10 different ensembles, resulting in 120 simulations and 1.2 microseconds of MD data.

Our goal was to post-process the atomistic data and get the averaged properties over the pre-defined Control Volumes to eventually test the randomness in the Fluctuating Hydrodynamics model. The MD simulation should demonstrate that the averaged signal is correlated, enabling us to develop a Machine Learning (ML) model capable of predicting this signal over significantly larger time scales.

This research is valuable not only from a theoretical perspective but also in contributing to the advancement of hybrid atomistic-continuum models, which could greatly accelerate large-scale MD simulations.

2. Specific usage status of the system and calculation method

The supercomputer has not been used during Fiscal Year 2024.

3. Result

A set of Shell and Python scripts has been developed that sets up a series of MD simulations. Open-source MD software GROMACS has been modified to post-process the atomistic trajectories on the fly, during the simulation. The initial configurations of the trp-cage molecule and the solid wall were defined and set up in GROMACS.

4. Conclusion

The project has not been finished and is still in progress.

5. Schedule and prospect for the future

- Develop a script that will properly generate different atomistic ensembles
- Run the simulations
- Pre-process the output data to the format suitable for reading by the ML model
- Train the model and reproduce the averaged signal using the ML model

6. If no job was executed, specify the reason.

Unfortunately, I got access to the supercomputer only at the very end of my 2-month visit to the Center for Biosystems Dynamics Research. I didn't have a chance to start all the simulations that we were planning.

Furthermore, it turned out that the simulation output, despite spatial averaging, takes many terabytes of the disk space, so running the simulations remotely (from another country) did not look feasible.

Currently we are looking at the possibility of continuation of the project by another researcher who is either already visiting the laboratory or will be visiting in the near future.