Contribution ID: **8** Type: **Oral talk**

Multiscale hybrid model of liquids: modified equations of motion

Wednesday, 21 December 2022 16:20 (20 minutes)

Classical Molecular Dynamics (MD) methods are the most accurate simulation methods. Solving Newtonian equations of motion by computing the inter-particle forces provides detailed information about the system at the atomistic scale. Nowadays these methods could be used for obtaining a representation of some macroscopic (thermodynamic) and some microscopic (as radial distribution functions and autocorrelation functions) properties of some liquids, qualitative or quantitative descriptions of complex biomolecular structures and their functionality.
Modern specialized computers can simulate liquid molecular systems of several hundred million atoms in size (tens of nanometers across) using classical molecular dynamics (MD) methodology. However, modelling of processes at biologically relevant times (microseconds to milliseconds) is likely to remain infeasible in the framework of existing computational molecular dynamics concepts (at most hundreds of picoseconds - few nanoseconds can be achieved now. One of the approaches that make it possible to implement modelling on a larger scale - is MD-continuum coupling, in which the modelling of part of the MD-region is replaced by continuum representation. But the coupling of MD and HD models is a challenging task.
Different techniques are applied to match MD behaviour to continuum evolution and a range of constraint algorithms has been developed for coupling. Our Multiscale hybrid model of liquids is based on the method, proposed by Smith ER [1], where he used the Gaussian principle of least action to obtain the equations of motion of particles in the extreme case when the correspondence of the pulse MD and HD is ensured.
In order to obtain a generalized equation of motion for the MD-HD coupling scheme so as to obtain the classical equations for MD and HD in extreme cases, and to ensure a smooth transition from no representation to another in intermediate cases, the liquid system has been described as "two-phased" mixture. The two phases are a Lagrangian and an Eulerian representation of the same chemical substance, which correspond to the atomistic (MD) and the continuum (HD) model, respectively. The partial concentration of each phase is determined by parameter s. The MD phase and the HD phase concentration correspond to s and 1 – s, respectively ($0 \leq s \leq 1$). In general, s is a user-defined scale function of space and time, which controls how much atomistic information is required in a particular region of the simulation domain. Control Volume formulation can be used to build a strict link between discrete and continuous representations.
For the coupling of MD and HD, the momentum in the hybrid region is adjusted to be the same as the MD. This is done by applying a constraint force to the molecular equations of motion. The method to constrain the momentum in a control volume is derived using both the Principle of Least Action and Gauss's principle. Constrained equations of motion have been derived, using constrained Lagrangian and it has been shown, that equations of motion obtained from Gauss's principle of least constraint and Gauss's principle are identical, so the Principle of Least Action is physically sound in this case.

[1] Smith ER, Heyes DM, Dini D, Zaki TAet al., 2015, A localized momentum constraint for non-equilibrium molecular dynamics simulations, JOURNAL OF CHEMICAL PHYSICS, Vol: 142, ISSN: 0021-9606

Primary author: Ms BAKUMENKO, Maryna (Taras Shevchenko University of Kyiv, Aston University)

Co-authors: Dr NERUKH, Dmitry (Aston University); Mr BARDYK, Vitaliy (Taras Shevchenko University of Kyiv)

Presenter: Ms BAKUMENKO, Maryna (Taras Shevchenko University of Kyiv, Aston University)

Session Classification: Afternoon session

Track Classification: Condensed Matter Physics