

Two-phase flow analogy as an effective boundary condition for modelling liquids at atomistic resolution



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ABSTRACT

A hybrid Molecular Dynamics/Fluctuating Hydrodynamics framework based on the analogy with two-phase hydrodynamics has been extended to dynamically tracking the feature of interest at all-atom resolution. In the model, the hydrodynamics description is used as an effective boundary condition to close the molecular dynamics solution without resorting to standard periodic boundary conditions. The approach is implemented in a popular Molecular Dynamics package GROMACS and results for two biomolecular systems are reported. A small peptide dialanine and a complete capsid of a virus porcine circovirus 2 in water are considered and shown to reproduce the structural and dynamic properties compared to those obtained in theory, purely atomistic simulations, and experiment.

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1. Introduction

Recent advances in hydrodynamics theory make it applicable to problems of space and time scales approaching molecular level. For example, it has been demonstrated [1,2] that the statistics of the thermal fluctuations of hydrodynamic fields can be quantitatively reproduced at the scale when the elementary volume contains only a few dozens of atoms. Such results motivated a wide spectrum of research where classical molecular dynamics is consistently connected to continuum hydrodynamics. These methods are particularly promising from the technical point of view since they have a potential of significant savings in computing resources without substantial loss of accuracy in critical regions. Biomolecular systems benefit especially strongly here because biomolecules necessarily have critical regions where atomistic representation is needed, while the system overall usually functions in close connection to a large medium of water and other molecules. The latter

is critically important, but impossible to model at atomistic level because of the sheer size of the system.

In most approaches connecting particle and continuum dynamics either local hydrodynamic properties are computed with the help of molecular dynamics [3,4]; or hydrodynamic fields serve as boundary conditions to molecular dynamics part of the system [5]. This ‘mechanistic’ partitioning of the system often creates problems and even artefacts in cases where there is no clear scale separation between different parts of the multiscale system in space and time. A straightforward example is the problem of particles leaving and entering the molecular dynamics zone. Several computational tricks are suggested, for example periodic boundary conditions in the molecular dynamics zone with prescribing a required meanflow gradient, however, more consistent, physically justified approaches are needed in the case of a strong coupling between the atomistic and the fluid dynamics regions.

We have recently suggested and implemented a new approach to the problem of computing liquids at multiple scales in space and time based on the two-phase hydrodynamics analogy [6]. Instead of separating the system into parts using boundaries, we describe the liquid as a nominally two-phase system consisting of both particle and continuum at the same time. The contribution of each prop-

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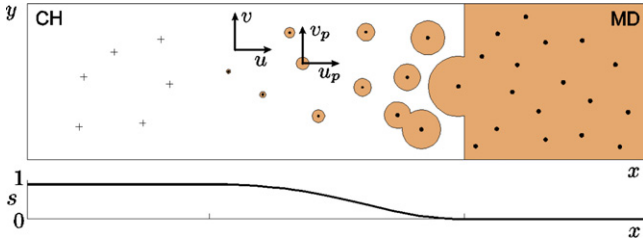


Fig. 1. A schematic representation of the hybrid simulation framework; because of the shape of the s function (bottom) purely MD particles on the right are gradually transformed into passive traces that follow the hydrodynamics flows on the left.

erty (particles or continuum), for example their ‘partial volume’, can vary depending on location and time, such as in the limiting cases only one of the descriptions remains. The governing equations are formulated as a system of the conservation laws for mass and momentum of the particle/continuum ‘mixture’. This allows to solve several problems, for example the above mentioned problem of leaving/entering particles that is solved naturally as the particles are allowed to move freely in all parts of the system while having impact on the solution only in the regions where their ‘partial volume’ is nonzero, which happens without any violation of the governing conservation laws.

In Ref. [7] a one-way coupling implementation of the same hybrid framework, which accounts for the effect of molecular dynamics on continuum hydrodynamics without the feedback, was considered and tested as an alternative open boundary treatment in the popular Molecular Dynamics (MD) package GROMACS [8]. In the current paper, the former implementation in GROMACS has been extended to dynamically tracking the atomistic-resolution features of interest. To illustrate the accuracy and efficiency of the new extended method, two simulations of two biomolecular systems from the opposite ends of the spectrum of possibilities are considered: diffusion of a small peptide, dialanine, molecule in water for long simulation times and the interaction of the capsid of a complete virus, porcine circovirus 2, with water at equilibrium conditions.

2. The underlying two-way coupling approach and its reduction to a one-way coupling model

Two representations of liquid are combined in the same framework: 1) standard classical MD description where the matter is the collection of point masses interacting with each other through an empirically defined potential and 2) Landau-Lifshitz Fluctuating Hydrodynamics (LL-FH) continuum, that is the generalisation of Navier-Stokes hydrodynamics with stochastic sources added to statistically mimic thermal fluctuations at small scales. A nominally two-phase liquid model is considered as a representation of the same chemical substance (Fig. 1). The ‘phases’ are immersed into each other as ‘fine grains’, the surface tension effects are irrelevant, and both ‘phases’ simultaneously occupy the same control volume. The partial concentrations of the MD ‘phase’ and the LL-FH ‘phase’ are equal to s and $1 - s$, respectively, where s is a parameter of the model $0 \leq s \leq 1$. In general s is a user-defined function of space and time which controls how much atomistic information is required in a particular region of the simulation domain, Fig. 1.

The most general form of the governing equations which are suitable for the continuous and discontinuous (particle) part of the hybrid model is integral conservation laws. The integral conservation laws are formulated through a state variable coupling method so that the mass of the mixture containing the two ‘phases’ is strictly preserved as well as satisfying the second law of Newton so that the change of total momentum of the system is equal to the sum of

all forces. Notably, an alternative approach would be to formulate the same model in the framework of generalised functions where discrete particles are represented as Heaviside functions (e.g. by representing atoms as particles of a finite size corresponding to the characteristic width of the interaction potential well), their derivatives become Dirac delta functions, and so on, the model derivation is similar to obtaining the Navier-Stokes solutions with discontinuous variables [9].

Following Ref. [7], let us consider a solution domain of volume V_0 which is broken down into elementary Eulerian cubical cells of volume V . Each cell has 6 faces $\gamma = 1, \dots, 6$ and it is filled with the continuum part of the liquid and, at the same time, with the MD particles which correspond to the discrete representation of the same chemical substance. It is assumed that the continuum part of the nominally two-phase fluid has the same transport velocity as that of the mixture. At isothermal condition this nominally two-phase liquid in addition to the macroscopic equation of state satisfies the following macroscopic conservation laws. For mass:

$$\delta_t(sm) + \sum_{\gamma=1,6} (s\rho\mathbf{u}) d\mathbf{n}^\gamma \delta t = \delta_t J^{(\rho)}, \quad \text{for the LL - FH phase,} \quad (1)$$

$$\delta_t \left((1-s) \sum_{p=1, N(t)} m_p \right) + \sum_{\gamma=1,6} \left((1-s) \sum_{p=1, N_\gamma(t)} \rho_p \mathbf{u}_p \right) d\mathbf{n}^\gamma \delta t = -\delta_t J^{(\rho)}, \quad \text{for the MD phase,} \quad (2)$$

where m and $\rho = m/V$ are the mass and the density of the continuum ‘phase’ of the elementary volume V , m_p is the particle mass, \mathbf{u}_p is the MD velocity, \mathbf{u} is the average velocity of the ‘mixture’

$$\bar{u}_i = \left[s\rho u_i + (1-s) \sum_{p=1, N(t)} \rho_p u_{ip} \right] / \bar{\rho}, \quad u_i \text{ is the velocity of the continuum LL-FH ‘phase’, } \bar{\rho} = s\rho + (1-s) \sum_{p=1, N(t)} \rho_p, N(t) \text{ is the number}$$

of particles in the volume V . $N_\gamma(t)$ is the number of particles crossing the γ^{th} cell face with the normal $d\mathbf{n}^\gamma$, $\rho_p = m_p/V$ is the effective density of an MD particle p which occupies the volume V , and $\delta_t J^{(\rho)}$ is the mass source/sink term which describes the transformation of mass between the ‘phases’, δ_t describes the change of a quantity over time δt , e.g. the counters of particle mass and momentum in cell V accumulated over time δt .

For momentum this is:

$$\delta_t(sm\mathbf{u}_i) + \sum_{\gamma=1,6} (s\rho\mathbf{u}_i\mathbf{u}) d\mathbf{n}^\gamma \delta t = s \sum_{j=1,3} \sum_{\gamma=1,6} (\Pi_{ij} + \tilde{\Pi}_{ij}) d\mathbf{n}_j^\gamma \delta t + \delta_t J_i^{(\mathbf{u})}, \quad (3)$$

$$\delta_t \left((1-s) \sum_{p=1, N(t)} m_p u_{ip} \right) + \sum_{\lambda=1,6} \left((1-s) \sum_{p=1, N_\lambda(t)} \rho_p u_{ip} \mathbf{u}_p \right) d\mathbf{n}^\lambda \delta t = (1-s) \sum_{p=1, N(t)} F_{ip} \delta t - \delta_t J_i^{(\mathbf{u})}, \quad (4)$$

where Π and $\tilde{\Pi}$ are the deterministic and stochastic parts of the Reynolds stress tensor in the LL-FH model, F_{ip} is the MD force exerted on particle p due to the pair potential interactions, and $\delta_t J_i^{(\mathbf{u})}$ is the LL-FH/MD exchange term corresponding to the i^{th} momentum component.

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