Simulation of a Particle Domain in a Continuum, Fluctuating Hydrodynamics Reservoir

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In molecular simulation and fluid mechanics, the coupling of a particle domain with a continuum representation of its embedding environment is an ongoing challenge. In this Letter, we show a novel approach where the latest version of the adaptive resolution scheme (AdResS), with noninteracting tracers as particles' reservoir, is combined with a fluctuating hydrodynamics (FHD) solver. The resulting algorithm, supported by a solid mathematical model, allows for a physically consistent exchange of matter and energy between the particle domain and its fluctuating continuum reservoir. Numerical tests are performed to show the validity of the algorithm. Differently from previous algorithms of the same kind, the current approach allows for simulations where, in addition to density fluctuations, also thermal fluctuations can be accounted for, thus large complex molecular systems, as, for example, hydrated biological membranes in a thermal field, can now be efficiently treated.

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Introduction.—Molecular dynamics (MD) [1] is considered a valuable tool for studying molecular systems at the microscopic level. Its contribution in condensed matter and molecular science covers many subjects of high interest in current research, such as molecular docking [2] or the design of materials for advanced technologies [3].

An MD model simulates the motion of molecules according to Newton's equations of motion. Molecules, in the most popular approach, have atomistic resolution according to their chemical structure. That is, they are represented by spherical atoms kept together by rigid bond constraints or intramolecular potentials [4]. The interaction between molecules is governed by potentials acting between their respective atoms, also called force fields. The latter are derived from experimental data or from elaborate electronic structure calculations (see, e.g., Ref. [5] for the important case of liquid water).

The core of the technique is thus the time integration of a highly complex Hamiltonian system with a state space given by the collection of the positions and momenta, $(\mathbf{r},\mathbf{p})$, of all the atoms considered. Assuming ergodicity of this system, the effective value of the resulting simulations lies in their capability of potentially sampling, through long enough trajectories, classical statistical ensembles and thus allowing the user to study the system's macroscopic thermodynamic properties. More precisely, one exploits the insight that under the ergodic hypothesis and considering large time windows, the time of residence of the system in regions of the state space with given total energies of their microstates is proportional to the volume of these regions [1].

The consequence is that through the instantaneous value of a physical observable, $w(\mathbf{r},\mathbf{p})$, its average, W, can be calculated over a sufficiently large time window along the trajectory of the MD simulation; that is, $W=\langle w(\mathbf{r},\mathbf{p})\rangle_{\mathrm{time}}=\lim_{t\to\infty}\int_0^t(1/t')w(\mathbf{r}(t'),\mathbf{p}(t'),t')dt'$. Specific thermodynamics and statistical mechanics ensembles are realized in this context by isolating the system entirely from its surroundings (microcanonical), bringing it in contact with the heat source or sink of an external thermostat (canonical), or allowing for the exchange of heat and particles with a reservoir (grand canonical) [1,6]. In this fashion, the atomistic simulations allow for the microscopic or particle-based analysis of the statistical collective behavior of large molecular systems. A remarkable example is liquid water for which an atomistically resolved simulation enables detailed analyses of the statistical properties of, e.g., the hydrogen bonding network and its crucial role in determining the multifaceted behavior of water as a solvent in both nature and technological systems.

With the increase of the system size computational costs rise steeply, however, so that macroscopic simulations at atomistic resolution become prohibitively expensive. Therefore, the simulation of complex molecular systems requires efficient computational strategies that capture the essence of a physical or chemical process at reasonable computational costs. In particular, for the large class of problems with the event of interest occurring merely in a limited region of space, it is convenient to reduce the simulation to a relatively small high-resolution region represented with atomistic detail, coupled to an effective simplified environment that plays the role of a macroscopic thermodynamic bath. The challenging aspect of such a simplification is the definition of boundary conditions between the particle domain and the environment that assures the exchange of energy and matter consistently with the fully microscopically resolved system of reference.

Several approaches have been proposed during the last decade under the umbrella of the adaptive resolution technique or similar models [7–11]. In particular, the last AdResS version, developed by the authors [12–15] has been framed into a more general mathematical model of open systems which assures, in a systematic fashion, the statistical mechanics' consistency of the high-resolution region with respect to an open system embedded in a fully microscopically resolved environment [16,17]. The supporting mathematical model was also instrumental to the definition of boundary conditions for situations beyond equilibrium and was successfully tested to study open molecular systems in a stationary thermal gradient [18,19].

Current molecular science moreover demands to go even beyond constant thermal or density fields to treat molecular systems embedded in arbitrarily fluctuating fields. For instance, cell membranes in a realistic environment are subject to a fluctuating thermal field that has a major impact on their hydration properties and morphological structure [20,21]. In technology, the possibility of externally changing or modulating in time a thermal or density field could be used to build efficient devices, e.g., for phase separation of liquids in the context of water purification [22,23].

A large-scale fluctuating environment can be described efficiently by continuum mechanics without the need for atomistic resolution. Macroscopic physical quantities in the form of space and time-dependent fields then describe the collective behavior of the particle system. The Navier-Stokes equations constitute the model of choice for liquids in this context. They describe the dynamics of a viscous fluid based on the conservation laws for mass, momentum, and energy of a Newtonian fluid [24]. Thus, the fluid mass within an arbitrary control volume can only change by exchange of mass with its environment but not by the action of sources or sinks. The same holds for the conservation of momentum with the total momentum exchange being due to the advective exchange of momentum-carrying mass elements and due to the forces acting on the surface of the volume by the pressure and viscous stress fields. Finally, energy is exchanged again by the advection of energy-carrying mass elements, by the work of the pressure and viscous forces on the element, and by thermal energy transport through heat conduction. Neglecting gravity, the Navier-Stokes equations, written in conservation form, read as

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \mathbf{u}) = 0, \tag{1a}$$

$$\frac{\partial \varrho \mathbf{u}}{\partial t} + \nabla \cdot (\varrho \mathbf{u} \circ \mathbf{u} + p \mathrm{Id} + \boldsymbol{\tau}) = 0, \tag{1b}$$

$$\frac{\partial \varrho e}{\partial t} + \nabla \cdot ([(\varrho e + p)\mathrm{Id} + \boldsymbol{\tau}]\mathbf{u} + \mathbf{j}) = 0, \tag{1c}$$

where $(\varrho, \mathbf{u}, e)$ are the density, flow velocity, and specific internal energy, respectively, and Id is the unit tensor. The thermodynamic pressure p, the viscous stress tensor $\boldsymbol{\tau}$, and the heat flux density $\mathbf{j}$ are given by the fluid's constitutive laws

$$p = \tilde{p}(\varrho, \mathbf{u}, e), \tag{2a}$$

$$\boldsymbol{\tau} = -\nabla[\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\top})] + \nabla[\lambda(\nabla.\mathbf{u})\mathbf{I}], \tag{2b}$$

$$\mathbf{j} = -k\nabla T, \tag{2c}$$

where $T = T(\varrho, p)$ is the temperature, and where we have explicitly adopted Newtonian friction in the equation of state for the stress tensor, with μ and λ being the shear and volume viscosities, respectively, and k the heat conductivity. Solving Navier-Stokes equations [Eqs. (1)] together with the equations of state [Eqs. (2)] will determine the flow behavior in the system for density, velocity, pressure, and temperature fields.

As they are formulated in Eqs. (1)–(2), the continuum equations hold in the limit of asymptotic scale separation between the atomistic and the systems scales. Of interest here, however, are large-scale flows on the mesoscale for which the continuum dynamics still involves sizable thermal fluctuations. To describe this situation, Landau and Lifshitz pioneered the formulation of a (linear) "fluctuating hydrodynamics" model [25], which essentially extends the deterministic conservation laws from Eqs. (1)–(2) by stochastically fluctuating flux densities for momentum and energy. See reports on further extensions of this theory and on computational implementations, e.g., in Refs. [26,27]. In this Letter, we describe a hybrid computational methodology that allows us to pursue molecular simulations at atomistic detail in limited regions that are embedded in mesoscale environments with general space- and time-dependent statistical evolution. That is, we describe a new variant of the AdResS technology that enables the systematic coupling of an open molecular system to a mesoscale environment governed by fluctuating hydrodynamics.

The examples discussed above lead to the simulation and modeling questions of how to define boundary conditions that couple the particle domain to a fluctuating environment described by a much less detailed mathematical model. Such boundary conditions need to be designed so that the statistical and thermodynamic conditions of the particle domain adapt to the instantaneous information coming from the fluctuating environment and, vice versa, the fluctuating environment adapts to the instantaneous response of the particle domain.

In this Letter, we realize such an algorithm by coupling the AdResS scheme (for the open molecular system) to a continuum fluctuating hydrodynamics scheme based on the Navier-Stokes model (for a fluctuating thermodynamic environment) via boundary conditions inspired by the mathematical model of the open system. The method is tested for fluid argon under different initial conditions, following its relaxation to equilibrium. The relaxation is specifically analyzed in the particle domain of AdResS and shows that it leads to the expected behavior from a continuum as well as from the corresponding fully resolved particle point of view. It must be reported that previous attempts of coupling particle domains to the continuum and in particular with other versions of AdResS have been technically satisfactory for the description of density fluctuations [27–32]. However, the current work with a systematic one-to-one correspondence between the technical implementation and the mathematical and physical formulation of boundary conditions at the microscopic level produced an algorithm with a major improvement, i.e., it allows, in addition to density fluctuations, for thermal fluctuations whose description is not possible in previous algorithms.

AdResS vs the mathematical open system model.—The latest version of the AdResS method directly couples a high resolution (atomistic) region of physical interest, AT, to a region of noninteracting point particles (tracers, TR) through an interface region Δ at atomistic resolution. In the AT and Δ regions particles undergo standard atomistic interactions as in a full atomistic simulation. In the Δ region they are, in addition, subjected to a thermostat and an external and purely space-dependent one-particle force called the "thermodynamic force," $F_{\mathrm{th}}(x)$. Such force assures, together with the action of the thermostat, the thermodynamic consistency of the Δ and AT regions. Specifically, the thermodynamic force is calculated self-consistently during an equilibration run of AdResS: Starting from a first guess $F_{\mathrm{th}}^{(0)}(x) = 0$, the update at step k is $F_{\mathrm{th}}^{(k+1)}(x) = F_{\mathrm{th}}^{(k)}(x) - c\nabla\varrho_k(x)$, with the density profile $\varrho_k(x)$ calculated from an AdResS simulation using $F_{\mathrm{th}}^{(k)}(x)$; $c > 0$ is a coefficient that controls the speed of convergence. The iteration stops when the deviation of $\varrho_k(x)$ from a reference density profile is within a prescribed tolerance. Once $F_{\mathrm{th}}(x)$ has been determined, it remains unchanged without any need for recalibration in subsequent applications [33]. A statistical mechanics analysis of this setup allows one to identify $F_{\mathrm{th}}(x)$ with the correction needed to balance the chemical potential of the TR + Δ region to the chemical potential of reference the AT region [14,34,35]. In addition, the thermostat assures the thermal consistency of the Δ and AT regions at the target temperature. The tracer region, TR, acts as an artificial reservoir of particles; the entrance or exit of particles into or from the Δ region is regulated by the thermodynamic force and assures the proper balance (see Fig. 1).

This scheme has been proved to reproduce the features of a grand canonical ensemble [15,35]. The numerical setup, in turn, inspired the development of a physico-mathematical model of the open system that provided further conceptual support to the definition of AdResS as a numerical method to simulate open systems [16,17]. Specifically, the mathematical model concludes that to properly simulate an open system, it is sufficient to define the boundary conditions in Δ without the need of requiring a physically meaningful behavior of the particles in the TR region. The analytic details of the physico-mathematical model can be found in Refs. [16,17], here we provide just a short, albeit essential, summary:

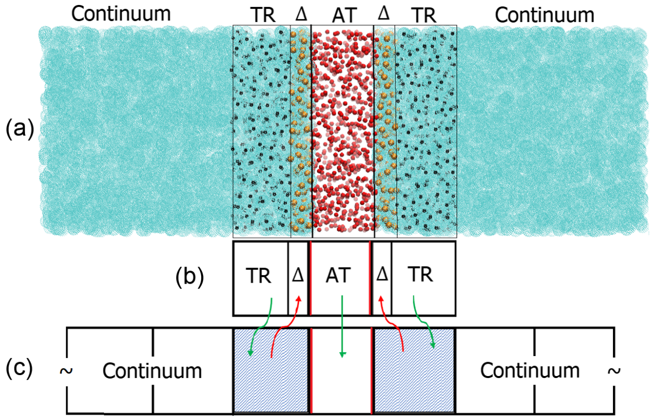

FIG. 1. Illustration of the AdResS (or open system model) and its coupling to the continuum (a), the technical setup of AdResS only (b), and its inclusion into a continuum solver as particle domain (c). The particles of the Δ region and the tracers of the TR region of AdResS overlap with the continuum description and exchange information (green and red arrows) in a way that boundary conditions from the continuum to the AT region and vice versa are defined.

We consider a large, closed, system with N interacting particles named "Universe" and the corresponding Liouville equation for its phase-space probability distribution $F_N(\mathbf{X}, t)$; $\mathbf{X} \equiv \{\mathbf{X}_1, \ldots. \mathbf{X}_N\}$; $\mathbf{X}_i \equiv (\mathbf{q}_i, \mathbf{p}_i)$; $(i = 1, \ldots, N)$, where $\mathbf{q}_i$ and $\mathbf{p}_i$ are the position and momentum of the ith particle and t is the time. Let us now assume our main interest is in some open subsystem, Ω, of the Universe that contains a time-dependent instantaneous number of particles n. The equivalent of the Liouville equation for Ω results in a hierarchy of equations for the probability distribution functions in the phase spaces of $0 \leqslant n \leqslant N$ particles in Ω, labeled $f_n(\mathbf{X}_\Omega, t)$. The equation for the evolution of $f_n(\mathbf{X}_\Omega, t)$ is derived by integrating all the particles' degrees of freedom outside Ω in the Liouville equation of the Universe. Differently from the Liouville equation of the Universe, the equation for $f_n(\mathbf{X}_\Omega, t)$ is characterized by a term describing the coupling of Ω to the external reservoir. Such a term implies that to have a physically consistent exchange of energy and particles between Ω and the reservoir, particles at the boundary, exiting from or entering in Ω, should be distributed according to the one- and two-particle distribution function of reference (i.e., as in the fully resolved Universe) at the given temperature. Under conditions of equilibrium, such a setup is shown to be consistent with a grand canonical representation of Ω.

The close similarity of this model to the computational setup of AdResS lies in the fact that the above-mentioned conditions regarding the information exchange between the open system and the surrounding reservoir(s) are effectively implemented in AdResS through the action of the thermodynamic force and the thermostat in Δ. In fact, at the boundary of the AT region the targeted temperature and density or one-particle distribution function are imposed while the radial (two-particle) distribution function is automatically recovered and used as a criterion of validation of AdResS (see also Refs. [13,17]). Furthermore, when an open system is in contact with two distinct reservoirs, the mathematical model suggests that the coupling at each system-reservoir boundary should be done as if the system was in equilibrium with the single reservoir, independently from the other. In AdResS, the corresponding effective numerical condition consists in applying at each boundary of AT the thermodynamic force and the thermostat corresponding to the thermodynamic state of each reservoir [17,19].

This framework, considering explicitly the time dependence of the whole system, allows for a further relevant step forward, which is to account for reservoirs with fluctuating temperature and density. According to our mathematical model, the corresponding boundary condition must allow for the instantaneous exchange of particles and energy according to the time-dependent thermodynamic conditions at the system-reservoir interface. Accordingly, in AdResS, the effective realization of the idea above consists of applying at time t a thermodynamic force in Δ that corresponds to the instantaneous thermodynamic condition of the reservoir. The technical essence of the present Letter is the numerical implementation of this concept, with the thermodynamically fluctuating reservoir implemented via fluctuating hydrodynamics (FHD) and synchronized with the particle system through a varying thermodynamic force tabulated in a predefined dictionary of thermodynamic forces. Below the scheme is explained in detail; instead, the explicit connection to the mathematical model is reviewed in the Supplemental Material [36], which is complemented by Refs. [14,16–18,34].

Coupling AdResS and FHD.—The description of the macroscopic reservoir, as anticipated above, is achieved through the FHD model, that is in essence Navier-Stokes (NavSt) equations extended by the addition of a stochastic flux term. In fact, in statistical mechanics, fluctuations are random deviations of a system from its average state as the system does not stay at the microscopic state of equilibrium but randomly samples all possible states with a Boltzmann distribution probability [37,38].

To incorporate fluctuations into macroscopic deterministic hydrodynamics, Landau and Lifshitz introduced an extended form of the NavSt equations by incorporating a stochastic flux divergence term, $\mathbf{S} = (0, \mathcal{S}, \mathcal{Q} + \mathbf{u} \cdot \mathcal{S})^{\intercal}$ [25]. The Landau-Lifshitz Navier-Stokes equations are written as $\mathbf{U}_t = -\nabla \cdot (\mathbf{F} + \mathbf{D} + \mathbf{S})$, where $\mathbf{U} = (\varrho, \mathbf{J}, E)^{\intercal}$ is a vector of conserved quantities with ϱ, $\mathbf{J} = \varrho\mathbf{u}$, and $E = \varrho e$ being the mass, momentum, and energy densities, respectively. The advective ($\mathbf{F}$) and diffusive ($\mathbf{D}$) fluxes are given by $\mathbf{F} = [\varrho\mathbf{u}, \varrho\mathbf{u} \cdot \mathbf{u}, (E + P)\mathbf{u}]^{\intercal}$ and $\mathbf{D} = (0, \tau, \tau \cdot \mathbf{u} - k\nabla T)^{\intercal}$; where $\mathbf{u}$ is the velocity, P is the pressure, T is the temperature, and $\tau = -\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\intercal} - \frac{2}{3} I \nabla \cdot \mathbf{u})$ is the stress tensor in which η and k are the coefficients of viscosity and thermal conductivity, respectively. The stochastic stress tensor ($\mathcal{S}$) and heat flux ($\mathcal{Q}$) are white in space and time and are formulated using fluctuation-dissipation relations to yield the equilibrium covariances of the fluctuations with the mean value of zero and well-specified covariances [26]. Different discretization techniques are available for solving such equations as reported in the Supplemental Material [36], which is complemented by Refs. [26,39–43].

As a technical reference for the coupling of a particle system to FHD, we utilized the state-flux hybrid scheme of Donev and co-workers [40]. In their technique, the output of the continuum solver at the neighboring cells of the particle subdomain acts as a boundary condition for the state of the particle subdomain. Particles with specific positions and velocities are inserted into the reservoir to reproduce the mass, momentum, and energy densities of the corresponding continuum cells. Conversely, the total mass, momentum, and energy of particles crossing the boundary and passing from the particle subdomain to the continuum reservoir are calculated during the particle simulation and implemented as a flux boundary condition for the continuum solver at the interface.

The fluctuating thermodynamic conditions of the FHD-simulated reservoir are accounted for in the AdResS-system by utilizing a dictionary of thermodynamic forces in the Δ region that has been precalculated as a function of density and temperature. The states obtained by the continuum solver in the grid cells immediately adjacent to the particle subdomain define the respective thermodynamic forces to be used in the next time step for the particle-based solver. In the process, parameters of the thermodynamic force functions are interpolated between dictionary entries where needed. In the other coupling direction, the calculation of the fluxes in the particle domain to be imposed to the continuum solver as a boundary condition is done as in the reference technique Ref. [40]. That is, the total mass, momentum, and energy of particles crossing the particle-continuum interface is imposed as a boundary condition to the continuum solver at the interface. The calculated flux values are consistent with the conservation laws of mass, momentum, and energy (see also the Supplemental Material [36], which includes Refs. [44–46]). The resulting scheme is summarized in Fig. 2 and its numerical validation is discussed in the Appendix. Another nontrivial further technical advancement compared to previous schemes [29,47] is that the current algorithm does not require an additional optimization step upon the insertion of particles from the continuum region. In fact, the tracer particles are noninteracting objects and their entrance in the Δ region, as well as their subsequent equilibration with the local environment, are automatically regulated by the thermodynamic force within the Δ region.

Conclusions.—A novel approach for simulating an open system at particle resolution embedded in a reservoir of energy and particles modeled by fluctuating hydrodynamics (FHD) has been presented. The mathematical model at the core of the AdResS algorithm prescribes coupling conditions that smoothly allow for an automatic dynamical exchange of particles and energy. The AdResS approach has already been demonstrated to be capable of representing complex molecular systems in and out of equilibrium by coupling it to several reservoirs at different thermodynamic states along the surface of the AT region. Thus, the new description of adjacent reservoirs through FHD allows for the simulation of similar systems but this time in the presence of fluctuating thermal and/or density fields. The option of coupling an AT region to several adjacent reservoirs in combination with our nonstationary FHD extension also constitutes a promising basis for multidimensional variants of AdResS-FHD systems, including situations with spatially inhomogeneous state distributions along a (flat) AdResS surface. Such situations would be covered by treating the faces of all FHD cells that bound on the AT interface in question as separate reservoirs. The linearity of the coupling to several reservoirs, demonstrated in previous work [17], will make this straightforward to implement.

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Appendix on the numerical scheme and its validation.—Figure 2 reports the schematic structure of the numerical scheme; here, we discuss the results of the numerical simulation that validates the method. Several numerical tests for a one-dimensional coupling setup are reported upon here. Thus, the FHD-to-AdResS change of resolution occurs only along one dimension. The coupling between the computational system components follows the principles outlined above. Additional technical details can be found in the Supplemental Material [36], which includes Refs. [48–53]. A one-dimensional coupling setup is simple enough to allow for simulations that clearly assess the general validity of the basic principles on which the technique is based and at the same time it is already sufficient for applications to complex molecular systems. One concrete example, previously mentioned, concerns how a temperature field (gradient) affects the geometry of biological membranes. The hypothesis is that even small temperature variations across the membrane could generate unexpected shape responses leading to the conclusion that the shape response of a membrane can be tuned by externally controlling a temperature gradient in its immediate vicinity at the two different sides of the membrane [54]. A prototype of the hydrated membrane, in absence of thermal gradient, has already been successfully treated with the AdResS technique [55], thus the current approach can now make the crucial further step forward by adding the thermal fluctuations along the direction that crosses the membrane (that is in a one-dimensional coupling setup). Another relevant example, also mentioned before, concerns water-ionic liquid mixtures. In such systems, a tunable one-dimensional thermal field can drive a phase separation in water-rich and water-poor domains. Also, in this case, the AdResS simulation has been successfully applied in absence of external gradients [23,56] and is now ready for the next step offered by the current algorithm.

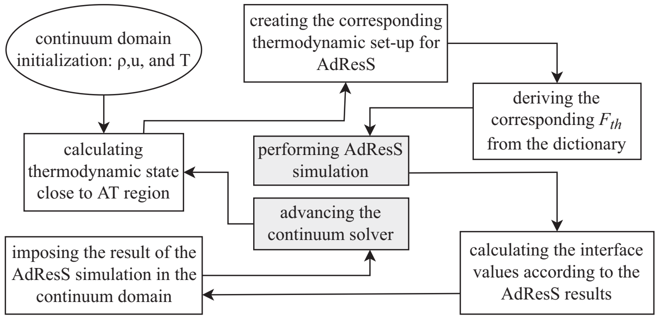

FIG. 2. The definitions of boundaries of Fig. 1 are considered. The simulation starts with an initial state of a given density, velocity, and temperature for the whole domain as if it was a pure continuum domain. Next, according to the density and temperature of the neighboring macrocells of the continuum, the thermodynamic forces for the left and right sides of the AdResS domain are calculated by interpolation from the dictionary and the particle simulation is executed. The temperature on the left and right sides of the particle domain is set according to the temperature of the neighboring macrocells. Average values of physical quantities of interest and the related interface fluxes are calculated from the particle simulation in the AT region and imposed in the continuum macrocells corresponding to the AT region and in the neighboring or interface cells to ensure that such imposing preserves the conservation laws. Finally, the fluctuating hydrodynamic solver will advance for a certain number of continuum time steps, considered as a single coupling time step, and a new state with updated density, velocities, and temperature is defined and the procedure repeated.

As numerical tests, we run simulations in each of which a specific initial condition for density, velocity, temperature, and pressure is given. We then follow the evolution of

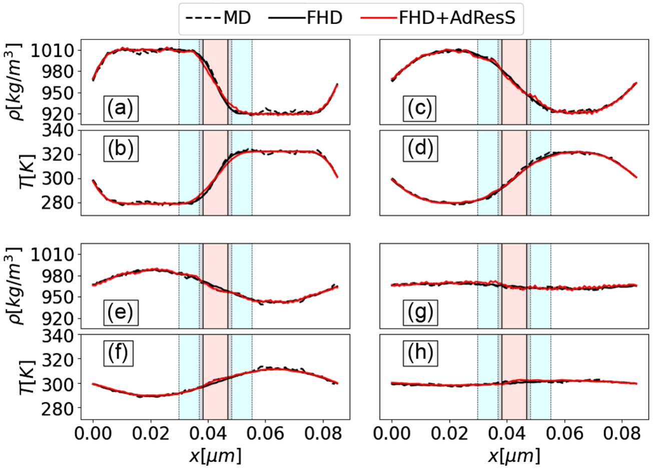

FIG. 3. Profiles of density (a),(c),(e),(g) and temperature (b),(d), (f),(h) evolved from initial step functions ($\varrho_{\mathrm{left}} = 1010$ [kg/m^3], $T_{\mathrm{left}} = 279.3$ [K], $\varrho_{\mathrm{right}} = 919.6$ [kg/m^3], and $T_{\mathrm{right}} = 322.3$ [K]) with constant pressure ($P = 100$ [MPa]) over time at $t = 0.05$ [ns] (a) and (b), $t = 0.25$ [ns] (c) and (d), $t = 1.2$ [ns] (e) and (f), and $t = 3.5$ [ns] (g) and (h). The colored regions in the middle of the box show the AdResS domain with the atomistic region (red) in contact with the TR region (blue) through a narrow transition region (gray). Results from FHD, MD, and coupled AdResS-FHD simulations are shown as black solid, dashed, and red lines, respectively.

the system and compare the result of the AdResS-FHD algorithm with the results of the full continuum and the full atomistic simulations. As a representative of all the tests, Fig. 3 reports the results obtained for a Riemann initial value problem given by zero velocity, constant pressure, and piecewise constant initial data for the density (and temperature) with the discontinuity located in the center of the domain. We follow the relaxation in time to equilibrium and show that indeed the AdResS-FHD simulation behaves as expected from the full FHD and full MD simulations. particular, in the AT region of AdResS, we find that the evolution towards equilibrium for the aforementioned test scenario occurs as in the equivalent subsystem of a full atomistic simulation of the entire domain (see Fig. 4). The results are of similar quality when instead of said initial contact discontinuity an acoustic wave with periodic initial conditions for density and temperature is imposed, but this time with a non-flat initial pressure profile according to the equation of state of the system. Such results are reported in the Supplemental Material [36].

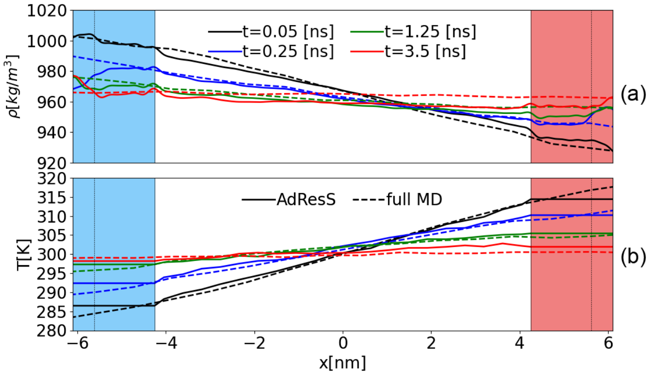

FIG. 4. The profile of density (a) and temperature (b) in the AdResS domain and in the full atomistic simulation over time, for the initial step function for the density and temperature. The red and blue regions represent the hot and cold reservoirs, respectively. The time slices are the same as for Fig. 3.

In the Supplemental Material [36] (including Refs. [57–59]), we also report the case where the system is treated in a quasi-one-dimensional setup with varying cross-section geometry. Results show that indeed the AdResS-FHD algorithm satisfactorily reproduces the behavior of reference.

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