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Smoothed dissipative particle dynamics

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We present a fluid particle model that is both a thermodynamically consistent version of smoothed particle hydrodynamics (SPH) and a version of dissipative particle dynamics (DPD), capturing the best of both methods. The model is a discrete version of Navier-Stokes equations, like SPH, and includes thermal fluctuations, like DPD. This model solves some problems with the physical interpretation of the original DPD model.

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I. INTRODUCTION

Smoothed particle hydrodynamics (SPH) is a Lagrangian particle method introduced by Lucy [1] and Monaghan [2] in 1970s in order to solve hydrodynamic problems in astrophysical contexts. It has been extensively applied in the study of accretion disc, galaxy dynamics, and star collisions among other problems [3]. The starting equations are the inviscid Euler equations, which are assumed to be a valid model for stellar material in which dissipative effects are small. The basic idea in SPH is to use an interpolant function that allows one to compute spatial derivatives of the fields at a given particle location. In this way, the hydrodynamic equations are solved with a set of particles with prescribed interactions. The resulting algorithm is very much like molecular dynamics with additional thermodynamic variables. The large amount of algorithmic knowledge in molecular dynamics [4] can be transferred directly to the simulation of partial differential equations.

Generalizations of SPH in order to include viscosity and thermal conduction and address laboratory scale situations like viscous flow and thermal convection have been presented only quite recently [5–8]. It is actually possible to derive *different* implementations of the SPH equations for dissipative fluids and every group seems to have its favorite. However, in all the implementations we are aware of, there is no explicit consideration of the Second Law. Actually, we have not been able to prove that any of the proposed implementations actually complies with the Second Law. The only exception is that of Ref. [8] where the simplest case of heat conduction in a solid is considered. Even though the equations may represent faithfully the continuum equations, and these continuum equations do respect the second law, potential problems may not be excluded in an algorithm which does not explicitly agree with the second law.

The purpose of this paper is to formulate an SPH implementation for a dissipative fluid that explicitly acknowledges the second law. This is not a tiny nicety. Actually, there is an intimate connection (the fluctuation-dissipation theorem) between the fulfillment of the second law and the possibility of describing correctly hydrodynamic fluctuations in the fluid, as we show below. A second objective of this paper is to introduce thermal fluctuations in a consistent way in SPH. These fluctuations arise naturally if the physical scales of the problem are mesoscopic as, for example, in colloidal suspensions. In this case, the hydrodynamic scale is dictated by the physical dimensions of the suspended particles which are in the submicron range. At these scales, the fluid flow starts to feel the underlying molecular nature of the fluid that shows up as fluctuations in the hydrodynamic variables, well described by the Landau and Lifshitz theory [9]. These hydrodynamic fluctuations couple to the colloidal particles through boundary conditions and are the ultimate origin of the diffusive behavior of the colloidal particles. This is the well-known point of view of the hydrodynamic theory of Brownian motion [10] that successfully predicted the experimentally observed long-time tails in the velocity autocorrelation function of the colloidal particles [11]. Hydrodynamic fluctuations of simple fluids in equilibrium and nonequilibrium situations can also be measured directly by means of light spectroscopy [12].

On the other hand, the method of dissipative particle dynamics (DPD) [13], which is very similar in spirit to SPH, does include thermal fluctuations. However, DPD as conventionally introduced suffers from several problems: (i) The conservative forces in the model do not allow for arbitrary equations of state (but see Ref. [14] for isothermal DPD), (ii) the transport coefficients cannot be specified directly in the model and a round way through kinetic theory is required in order to relate these transport coefficients with the model parameters [15], and (iii) the physical scale probed by DPD is undefined. In this paper, we deepen the connection between SPH and DPD, extracting the best of both methods (fluctuations from DPD, connection to Navier-Stokes from SPH) [16]. The above problems of DPD disappear in the model. We have advocated the view that the particles in DPD and SPH should be regarded as portions of the fluid representing moving thermodynamic subsystems [17]. Following this idea, we have presented a finite volume discretization of the Navier-Stokes equations in a Lagrangian moving Voronoi grid [18]. The Voronoi grid is relatively easy to implement in two spatial dimensions but becomes rather involved in three dimensions. For this reason, using the idea of spherically symmetric interpolants is very appealing from the point of view of algorithmic simplicity.

II. THE MODEL

The equations of hydrodynamics in a Lagrangian description are [19]

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$$\frac{d\rho}{dt} = -\rho\boldsymbol{\nabla}\cdot\mathbf{v},$$

$$\rho\frac{d\mathbf{v}}{dt} = -\boldsymbol{\nabla}P + \eta\nabla^2\mathbf{v} + \left(\zeta + \frac{\eta}{3}\right)\boldsymbol{\nabla}\boldsymbol{\nabla}\cdot\mathbf{v},$$

$$T\rho\frac{ds}{dt} = \phi + \kappa\nabla^2 T. \tag{1}$$

The time derivative in Eq. (1) is the well-known substantial derivative describing how the quantities vary as we follow the flow field. $\rho = \rho(\mathbf{r},t)$ is the mass density field, $\mathbf{v} = \mathbf{v}(\mathbf{r},t)$ is the velocity field, $s = s(\mathbf{r},t)$ is the entropy per unit mass field, $P = P^{\mathrm{eq}}[\rho(\mathbf{r},t),s(\mathbf{r},t)]$ and $T = T^{\mathrm{eq}}[\rho(\mathbf{r},t),s(\mathbf{r},t)]$, are the pressure and temperature fields given by the local equilibrium assumption. The transport coefficients (taken to be constant for simplicity) are the shear and bulk viscosities η,ζ and the thermal conductivity κ. The *viscous heating* field ϕ is defined by

$$\phi = 2\eta\overline{\boldsymbol{\nabla}\mathbf{v}}:\overline{\boldsymbol{\nabla}\mathbf{v}} + \zeta(\boldsymbol{\nabla}\cdot\mathbf{v})^2, \tag{2}$$

where the traceless symmetric part of the velocity gradient tensor is

$$\overline{\boldsymbol{\nabla}\mathbf{v}} = \frac{1}{2}[\boldsymbol{\nabla}\cdot\mathbf{v} + \boldsymbol{\nabla}\cdot\mathbf{v}^T] - \frac{\mathbf{1}}{3}\boldsymbol{\nabla}\cdot\mathbf{v} \tag{3}$$

and the unit tensor has been denoted by $\mathbf{1}$. The field ϕ captures the physical mechanism by which the energy dissipated by the viscous forces in the fluid is transformed into the internal energy.

Our aim is to discretize the above equations in the spatial domain of the fluid. A large set of M points is seeded in this spatial domain. Every point is regarded as a moving thermodynamic subsystem. It has associated a position $\mathbf{r}_i$, velocity $\mathbf{v}_i$, constant mass m, and entropy S_i. The mass is a fraction $m = M_T/M$ of the total mass M_T of the system. Two more extensive variables must be associated to every particle in order to describe a thermodynamic system, which are the volume $\mathcal{V}_i$ and the internal energy E_i. The internal energy is a given prescribed function of $m,S_i,\mathcal{V}_i$,

$$E_i = E^{eq}(m,S_i,\mathcal{V}_i), \tag{4}$$

where, by the local equilibrium assumption $E^{eq}(m,S,\mathcal{V})$ is the same function that describes the equilibrium thermodynamics of the whole fluid. Every particle has also a pressure P_i and a temperature T_i given by the equations of state

$$T_i = \frac{\partial E^{\mathrm{eq}}}{\partial S_i},$$

$$P_i = -\frac{\partial E^{\mathrm{eq}}}{\partial \mathcal{V}_i}. \tag{5}$$

In Ref. [17] we considered the volume as an independent variable. It proves much more convenient and intuitive to define the volume associated to a particle in terms of the positions of the particle and its neighbors. Consider a bell-shaped interpolant function $W(r/h)$ with a finite support h and which is normalized to unity

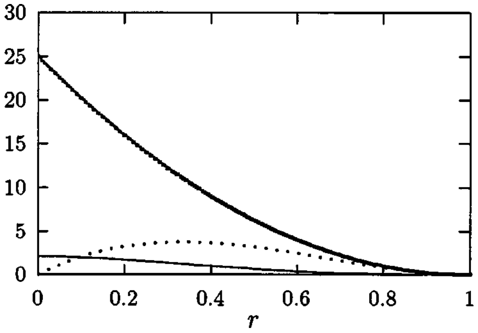

FIG. 1. The functions $W(r)$ (solid line), $F(r)$ (bold line), and $rF(r)$ (dotted line).

$$\int d\mathbf{r}\, W(r) = 1. \tag{6}$$

In the limit $h \to 0$ $W(r)$ tends to the Dirac δ function. The volume $\mathcal{V}_i$ of particle i is defined as the inverse of the density d_i which, in turn, is defined by

$$\frac{1}{\mathcal{V}_i} = d_i = \sum_j W(|\mathbf{r}_i - \mathbf{r}_j|). \tag{7}$$

Note that if there are many neighboring particles around a given one, the contribution to the sum in Eq. (7) will be large and so will be the density of the particle. Its associated volume will be thus smaller. We regard $\mathcal{V}_i$ as the thermodynamic volume to be associated to the particle. One should note that, in general, $\Sigma_i\mathcal{V}_i \neq V_T$, where V_T is the total volume of the container. We expect, however, that the thermodynamic volume and the geometrical volume will be very close to each other in the case that there are many particles in the system, due to the normalization (6).

For future reference, we introduce also the positive function $F(r)$ through

$$\boldsymbol{\nabla}W(r) = -\mathbf{r}F(r), \quad F(r) \geq 0. \tag{8}$$

A usual selection in SPH is the Lucy function for $W(r)$,

$$W(r) = \frac{105}{16\pi h^3}\left(1 + 3\frac{r}{h}\right)\left(1 - \frac{r}{h}\right)^3 \tag{9}$$

from which the function $F(r)$ follows

$$F(r) = \frac{315}{4\pi h^5}\left(1 - \frac{r}{h}\right)^2. \tag{10}$$

In Fig. 1 we plot the functions $W(r),F(r),rF(r)$.

Our aim is to propose a discrete model that approximates Eqs. (1). More precisely, we want to formulate a set of equations for the discrete variables $\rho_i,\mathbf{v}_i,S_i$ which have as solutions very approximately the solutions of Eqs. (1) when evaluated at the points $\mathbf{r}_i$.

As a first step, in accordance with the Lagrangian description implicit in Eqs. (1), we assume that the evolution of the positions of the particles is given by its velocity,

$$\dot{\mathbf{r}}_i=\mathbf{v}_i . \tag{11}$$

If $\mathbf{v}_i$ is a discrete representation of the velocity field, then the particles form an irregular grid that moves following the flow field. We expect that this evolution captures the full Lagrangian nature of Eqs. (1) and no additional convective terms are required.

A simple discrete model for Eqs. (1) would be

$$\begin{aligned}\dot{d}_i&=-d_i(\boldsymbol{\nabla}\cdot\mathbf{v})_i ,\\ \dot{\mathbf{v}}_i&=-\frac{(\boldsymbol{\nabla}P)_i}{md_i}+\frac{\eta}{md_i}(\nabla^2\mathbf{v})_i+\frac{1}{md_i}\left(\zeta+\frac{\eta}{3}\right)(\boldsymbol{\nabla}\boldsymbol{\nabla}\cdot\mathbf{v})_i ,\\ T_i\dot{S}_i&=\frac{(\phi)_i}{d_i}+\frac{\kappa}{d_i}(\nabla^2T)_i .\end{aligned}\tag{12}$$

We have introduced md_i as a discrete version of the density field ρ at $\mathbf{r}_i$. Of course, Eqs. (12) is still a meaningless collection of symbols until we specify how the spatial derivatives of the fields are represented at each particle location.

Let us consider the continuity equation. According to the definition (7) and the equation of motion (11), we have

$$\dot{d}_i=-\sum_j F_{ij}\mathbf{r}_{ij}\cdot\mathbf{v}_{ij} , \tag{13}$$

where we have introduced the notation

$$\begin{aligned}F_{ij}&=F(|\mathbf{r}_i-\mathbf{r}_j|),\\ \mathbf{r}_{ij}&=\mathbf{r}_i-\mathbf{r}_j ,\\ \mathbf{v}_{ij}&=\mathbf{v}_i-\mathbf{v}_j .\end{aligned}\tag{14}$$

Comparison of Eq. (13) with the continuity equation in Eq. (12) suggests the following representation of the divergence of the velocity

$$(\boldsymbol{\nabla}\cdot\mathbf{v})_i=\frac{1}{d_i}\sum_j F_{ij}\mathbf{r}_{ij}\cdot\mathbf{v}_{ij}=\frac{\dot{\mathcal{V}}_i}{\mathcal{V}_i}. \tag{15}$$

This is compatible with the intuitive idea that the divergence of a velocity field is closely related to the relative rate of change of the volume.

A further argument to show that Eq. (15) is a faithful representation of the divergence can be given by considering the following interpolant of the velocity field

$$\mathbf{v}(\mathbf{r})=\frac{\sum_j W(|\mathbf{r}-\mathbf{r}_j|)\mathbf{v}_j}{\sum_j W(|\mathbf{r}-\mathbf{r}_j|)}. \tag{16}$$

By taking the divergence of Eq. (16) leads to

$$\begin{aligned}\boldsymbol{\nabla}\cdot\mathbf{v}(\mathbf{r})=&-\frac{\sum_j (\mathbf{r}-\mathbf{r}_j)\cdot\mathbf{v}_jF(|\mathbf{r}-\mathbf{r}_j|)}{\sum_j W(|\mathbf{r}-\mathbf{r}_j|)}\\ &+\mathbf{v}(\mathbf{r})\cdot\frac{\sum_j (\mathbf{r}-\mathbf{r}_j)F(|\mathbf{r}-\mathbf{r}_j|)}{\sum_j W(|\mathbf{r}-\mathbf{r}_j|)}.\end{aligned}\tag{17}$$

By evaluating this expression at $\mathbf{r}=\mathbf{r}_i$, we obtain the approximation for the divergence in the form of Eq. (15).

We have seen, therefore, that the definition of the density (7) and the equation of motion (11) already account for the continuity equation, which is therefore redundant. However, in some situations it might represent an advantage to actually solve the continuity equation [2].

The argument leading to Eq. (17) is unsatisfactory for the case of the pressure gradient $(\boldsymbol{\nabla}P)_i$ because total momentum would not be conserved. We follow instead a different procedure, which is based on energy considerations. We note that if we set the transport coefficients to zero in Eqs. (12) we obtain a discrete model for an inviscid fluid. Of course this fluid conserves energy. The total energy of the system is given in the particle model by

$$E=\sum_i\left[\frac{m}{2}\mathbf{v}_i^2+E_i\right]. \tag{18}$$

Its time derivative is given by

$$\dot{E}=\sum_i [m\dot{\mathbf{v}}_i\cdot\mathbf{v}_i-P_i\dot{\mathcal{V}}_i] \tag{19}$$

because, in absence of dissipation $\dot{S}_i=0$. By substituting the equations of motion (12) with η,ζ,κ set to zero we obtain

$$\dot{E}=\sum_i\left[-\frac{(\boldsymbol{\nabla}P)_i}{d_i}\cdot\mathbf{v}_i-\frac{P_i}{d_i}(\boldsymbol{\nabla}\cdot\mathbf{v})_i\right]. \tag{20}$$

By using the form (15) for the divergence of the velocity and after simple rearrangements we end up with

$$\dot{E}=-\sum_i\frac{(\boldsymbol{\nabla}P)_i}{d_i}\cdot\mathbf{v}_i-\sum_{ij}\left[\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right]F_{ij}\mathbf{r}_{ij}\cdot\mathbf{v}_i , \tag{21}$$

which suggest that a suitable expression for the pressure gradient is given by

$$\frac{(\boldsymbol{\nabla}P)_i}{d_i}=-\sum_j\left[\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right]F_{ij}\mathbf{r}_{ij} . \tag{22}$$

This is the form for the pressure gradient preferred by Monaghan [2].

The final form for the *reversible* part of the dynamics is, therefore,

$$\dot{\mathbf{r}}_i=\mathbf{v}_i,$$
$$m\dot{\mathbf{v}}_i=\sum_j\left[\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right]F_{ij}\mathbf{r}_{ij},$$
$$\dot{S}_i=0. \tag{23}$$

Note that these equations also conserve total momentum $\mathbf{P}=\Sigma_i m\mathbf{v}_i$ due to the symmetries under exchange of the indices i,j. It is obvious that the rate of change of the entropy of the total system, defined as

$$S=\sum_i S_i \tag{24}$$

is zero, $\dot{S}=0$. This is consistent with the fact that the reversible part of the dynamics should not produce any entropy increase.

We consider now the dissipative terms in Eqs. (12) involving second spatial derivatives. We present now a novel argument for obtaining approximate expressions for the second derivatives at the particles which is based on the following identity for an arbitrary function $A(\mathbf{r})$,

$$\int d\mathbf{r}'[A(\mathbf{r}')-A(\mathbf{r})]F(|\mathbf{r}'-\mathbf{r}|)\left[5\frac{(\mathbf{r}'-\mathbf{r})^\alpha(\mathbf{r}'-\mathbf{r})^\beta}{(\mathbf{r}'-\mathbf{r})^2}-\delta^{\alpha\beta}\right]$$
$$=\nabla^\alpha\nabla^\beta A(\mathbf{r})+\mathcal{O}(\nabla^4Ah^2). \tag{25}$$

This identity is demonstrated in the Appendix by expanding $A(\mathbf{r}')$ around $\mathbf{r}$ and making use of the isotropic nature of $F(r)$. The high order terms are negligible if the function $A(\mathbf{r})$ is sufficiently smooth on the scale of h. The form of the interpolant (25) is suggested after a similar expression given in Ref. [8] for the Laplacian. Actually, taking the trace of Eq. (25) leads to

$$2\int d\mathbf{r}'[A(\mathbf{r}')-A(\mathbf{r})]F(|\mathbf{r}'-\mathbf{r}|)=\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}A(\mathbf{r})+\mathcal{O}(\boldsymbol{\nabla}^4Ah^2), \tag{26}$$

which is the form used in Ref. [8]. Of course, we had to generalize the expression of the Laplacian in Ref. [8] in order to deal with the vector nature of the velocity field, as opposed to the simpler scalar nature of the temperature in the case of heat conduction in solids.

The next step consists on discretizing the integrals according to

$$\int d\mathbf{r}'\to\sum_j\mathcal{V}_j=\sum_j\frac{1}{d_j}. \tag{27}$$

Again, this approximation will be valid if the scale of variation of the field $A(\mathbf{r})$ is large in front of h.

In this way, we discretize the dissipative terms involving second derivatives in Eq. (12) as

$$\frac{1}{d_i}(\nabla^2\mathbf{v})_i=-2\sum_j\frac{F_{ij}}{d_id_j}\mathbf{v}_{ij},$$
$$\frac{1}{d_i}(\boldsymbol{\nabla}\boldsymbol{\nabla}\cdot\mathbf{v})_i=-\sum_j\frac{F_{ij}}{d_id_j}[5\mathbf{e}_{ij}\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}-\mathbf{v}_{ij}],$$
$$\frac{1}{d_i}(\nabla^2T)_i=-2\sum_j\frac{F_{ij}}{d_id_j}T_{ij}, \tag{28}$$

where we have introduced the notation

$$T_{ij}=T_i-T_j,$$
$$\mathbf{e}_{ij}=\frac{\mathbf{r}_i-\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|}. \tag{29}$$

Upon substitution of Eq. (28) into Eq. (12) we obtain the following equations for the variables $\mathbf{r}_i,\mathbf{v}_i,S_i$,

$$\dot{\mathbf{r}}_i=\mathbf{v}_i,$$
$$m\dot{\mathbf{v}}_i=\sum_j\left[\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right]F_{ij}\mathbf{r}_{ij}-\left(\frac{5\eta}{3}-\zeta\right)\sum_j\frac{F_{ij}}{d_id_j}\mathbf{v}_{ij}$$
$$-5\left(\zeta+\frac{\eta}{3}\right)\sum_j\frac{F_{ij}}{d_id_j}\mathbf{e}_{ij}\mathbf{e}_{ij}\cdot\mathbf{v}_{ij},$$
$$T_i\dot{S}_i=(\phi)_i-2\kappa\sum_j\frac{F_{ij}}{d_id_j}T_{ij}. \tag{30}$$

We still need a discrete version for the viscous heating term $(\phi)_i$. Rather than trying to invent discrete versions for the velocity gradient in order to compute $(\phi)_i$, we resort to the physical meaning of this term, that friction forces should produce an increase of internal energy in order to conserve total energy. Actually, by using Eq. (30) in Eq. (19) and requiring $\dot{E}=0$ readily suggest the appropriate form for $(\phi)_i$,

$$(\phi)_i=\left(\frac{5\eta}{6}-\frac{\zeta}{2}\right)\sum_j\frac{F_{ij}}{d_id_j}\mathbf{v}_{ij}^2+\frac{5}{2}\left(\zeta+\frac{\eta}{3}\right)\sum_j\frac{F_{ij}}{d_id_j}(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})^2. \tag{31}$$

The set of Eqs. (30) with (31) and the equations of state (5) are a closed system of ordinary differential equations for the independent variables $\mathbf{r}_i,\mathbf{v}_i,S_i$.

We discuss now the physical meaning of the different terms in the model given in Eqs. (30). The particles move according to their velocities and exert forces of a range h among each other of different nature. First, a repulsive force directed along the line joining the particles that has a magnitude given by the pressure and densities of the particles. Roughly speaking, the larger is the pressure in a given region, the higher the repulsion between them. The fluid particles are also subject to friction forces that depend on the relative velocities of the particles. There is a component of these forces, directly proportional to $\mathbf{v}_{ij}$ that breaks the conservation of total angular momentum. If one wishes to respect this conservation law, then it is necessary to introduce in the model a spin variable associated to every particle [20]. This spin variable represents the intrinsic angular momentum of the finite sized particles. In a molecular view, this spin is directly related to the angular momentum of the system of molecules that form the fluid particle with respect to the center of mass of the particle. We showed that this spin variable is a very rapid variable when the fluid particles are small, and decay towards the vorticity field in a short time scale [19]. For simplicity, we do not consider this issue in this paper and simply expect that for sufficiently well resolved flows, angular momentum conservation is sufficiently well satisfied. A word is in order about the artificial viscosity introduced in SPH in order to deal with shocks [21]. The artificial viscosity depends on $\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}$ and on $(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})^2$. The linear term should be interpreted as a physical viscosity as it is apparent from the above derivation. The quadratic part, which is needed to prevent penetration in high Mach shocks, is a Von Neumann-Richtmeyer artificial viscosity which becomes operative only for particles that are approaching each other very fast and almost directly head on [7].

The terms in the entropy equation have the same meaning as those in the original equation (1), that is, viscous heating and heat conduction. The heat conduction term tries to reduce temperature differences between particles by suitable energy exchange. This heat conduction term also conserves total energy due to its symmetries. It has the form given by Cleary and Monaghan under the assumption of constant thermal conductivity [8].

It is worth considering the rate of change of the total entropy (24). A simple calculation leads to

$$\dot{S}=\sum_i \frac{(\phi)_i}{T_i}+\kappa\sum_{ij}\frac{F_{ij}}{d_i d_j T_i T_j}T_{ij}^2. \tag{32}$$

We will have that $\dot{S}\geqslant 0$ if $(\phi)_i\geqslant 0$. This will occur if $5\eta>3\zeta$. Note that the friction force in the velocity equation in Eq. (30) is unstable if $5\eta<3\zeta$, producing accelerations of the particles rather than reducing velocity differences. The model equations are valid only for fluids satisfying $5\eta>3\zeta$. Note that the bulk viscosity ζ is zero for monoatomic gases at low density and it is small for liquids [22]. Under this assumption the above model equations respect the second law. It is crucial in this discussion that the function $F(r)$ is positive. Although *the structure* of the friction force is the same as in Refs. [5,20], the interpolant method used in these works does not provide a positive definition of the kernel involved and, therefore, the second law is not guaranteed.

The restriction $5\eta>\zeta$, although not essential in practice, seems to be an undesirable limitation of the discretization procedure. One can think of another discretization procedure which, although retaining the thermodynamic consistency of the resulting algorithm, does not suffer from this limitation [17]. One should note, though, that an algorithm like that presented in Ref. [17] in order to compute second spatial derivatives involves two loops over the particles instead of the one loop needed in computing Eqs. (28), making the algorithm a factor of two slower.

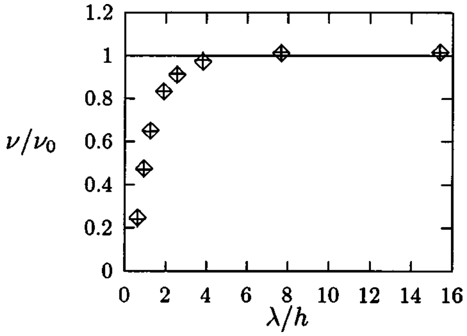

FIG. 2. The measured viscosity normalized with the input viscosity ν_0 as a function of the normalized wavelength λ. Diamonds are for $h/l_0=3$, corresponding to 30 interacting neighbors while crosses are for $h/l_0=4$, corresponding to 50 interacting neighbors.

III. SIMULATION RESULTS

We have performed a numerical simulation of Eqs. (30) in order to check in very simple situations that the model works. An ideal gas has been assumed for which the thermodynamic equation (4) is (in two spatial dimensions)

$$E(N,\mathcal{V},S)=\frac{Nh^2}{2\pi m_0}\left(\frac{N}{\mathcal{V}}\right)\exp\left\{\left(\frac{S}{Nk_B}-2\right)\right\}. \tag{33}$$

Here, N is the (fixed) number of molecules per fluid particle, m_0 is the mass of a molecule, h is the Planck constant, and k_B is the Boltzmann constant. We select units in which $Nh=1$, $Nk_B=1$, and $Nm_0=1$ and, furthermore, lengths are measured in terms of the typical distance $l_0=(M/V_T)^{1/2}$ between fluid particles, where M is the number of fluid particles and V_T is the total volume (area) of the two-dimensional (2D) simulation box. In these units, the temperature and pressure of each fluid particle are given by

$$T_i=\frac{N}{2\pi}d_i\exp\{S_i-2\},$$

$$P_i=d_iT_i. \tag{34}$$

A cubic periodic box is used. The initial state of the system is defined as follows. Particles are located in a triangular lattice with equal temperatures $T_i=1$. Two velocity profiles are assumed, a shear wave and a sound wave of wavelength λ. From the decay of this transverse and longitudinal waves it is possible to measure the viscosity and speed of sound [18]. The results are presented in Figs. 2 and 3, where the kinematic viscosity and the sound speed normalized with their respective input values are plotted as a function of the wavelength of the initial velocity profile. As the wavelength increases one observes a good agreement between the measured and input values.

A remarkable fact is that the discrepancies between measured and input values arise when the wavelength of the perturbation is of the order of 6 times the range h of the weight function. In this respect, the relevant length scale that determines whether a given hydrodynamic field will behave according to the input transport coefficients is the range h of

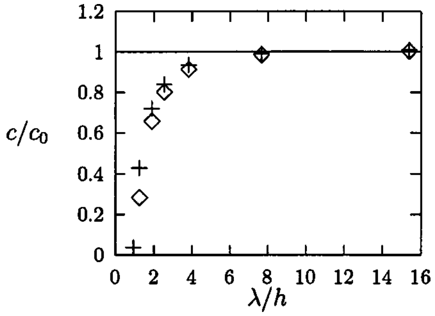

FIG. 3. The measured sound speed normalized with the sound speed of the equilibrium state $c_0=\sqrt{2T}$ as a function of the normalized wavelength λ. Diamonds are for $h/l_0=3$, corresponding to 30 interacting neighbors while crosses are for $h/l_0=4$, corresponding to 50 interacting neighbors.

the weight function and *not* the typical distance l_0 between fluid particles (which could be loosely understood as a ''lattice spacing''). Actually, in Figs. 2 and 3 we have plotted for each wavelength two different simulation results corresponding to different values of l_0, but the same value of h. Changing the ratio h/l_0 amounts to change the typical number of interacting neighbors. The discrepancies are small showing that the relevant length scale is h and not l_0. In Ref. [15] we arrived at similar qualitative conclusions for the DPD model through a kinetic theory analysis. We have also performed simulations of the model in Eqs. (30) in which only heat conduction is operative [8] and have analyzed them with a kinetic theory approach similar to that presented in Ref. [15]. The results are given elsewhere [23], but we advance that the thermal diffusivity also depends on the wavelength of the temperature profile selected and that discrepancies from the input value arise when the wavelength is of the order of the range h of the weight function.

We should mention that we have encountered a problem which is also typical of other SPH and DPD simulations. We observe the tendency of the system to form ordered structures (like crystals) in the equilibrium state. These implies the existence of elastic contributions that should not be present if the equations are to represent the hydrodynamics of a Newtonian fluid. Of course, under forcing boundary conditions, these crystals are destroyed and it is expected that the elastic contributions are negligible in front of the viscous forces in the system [24].

IV. SDPD IN GENERIC FORM

In this section we cast the obtained method in the form of the GENERIC framework [25]. This very general framework applies to all known dynamic equations for nonequilibrium processes in closed systems [25]. It encodes in a very elegant way the physics behind the first and second laws of thermodynamics. Given that we have shown that the proposed fluid particle model actually satisfies these laws, we expect that it is possible to write the above equations in the GENERIC form. Our main motivation for casting the previous model into the GENERIC form is that it allows to introduce systematically thermal fluctuations in a rather simple way. In GENERIC, by construction, the fluctuation-dissipation theorem is satisfied and the equilibrium fluctuations are governed by the Einstein distribution function. Another motivation for trying the GENERIC framework is that in the future we plan to introduce additional structural variables in the fluid particle model in order to model non-Newtonian fluids [26]. Such a generalization is best pursued within this framework.

The dynamic equations for the state x of a system at a given level of description are given in the GENERIC framework by

$$\frac{dx}{dt}=L\frac{\partial E}{\partial x}+M\frac{\partial S}{\partial x}. \tag{35}$$

The first term in the right hand side is named the *reversible* part of the dynamics and the second term is named the *irreversible* part. The energy $E(x)$ and the entropy $S(x)$ are functions of the state x used to represent the system. The matrices L,M satisfy a set of stringent properties. First, L is antisymmetric whereas M is symmetric and positive semidefinite. Most important, the following *degeneracy* conditions should hold

$$L\frac{\partial S}{\partial x}=0, \quad M\frac{\partial E}{\partial x}=0. \tag{36}$$

These properties ensure the first and second laws of thermodynamics, that is, $\dot{E}=0,\dot{S}\geqslant 0$. In the case that other dynamical invariants $I(x)$ exist in the system (as, for example, linear or angular momentum), then further conditions must be satisfied by L,M. In particular

$$\frac{\partial I}{\partial x}L\frac{\partial E}{\partial x}=0, \quad \frac{\partial I}{\partial x}M\frac{\partial S}{\partial x}=0, \tag{37}$$

which ensure that $\dot{I}=0$.

The deterministic equations (35) are, actually, an approximation in which thermal fluctuations are neglected. If thermal fluctuations are not neglected, the dynamics is described by the following stochastic differential equations [25]

$$dx=\left[L\frac{\partial E}{\partial x}+M\frac{\partial S}{\partial x}+k_B\frac{\partial}{\partial x}M\right]dt+d\tilde{x}, \tag{38}$$

to be compared with the deterministic equations (35). The stochastic term $d\tilde{x}$ in Eq. (38) is a linear combination of independent increments of the Wiener process. It satisfies the mnemotechnical Itô rule

$$d\tilde{x}d\tilde{x}^T=2k_BM dt, \tag{39}$$

which means that $d\tilde{x}$ is an infinitesimal of order 1/2 [27]. Equation (39) is a compact and formal statement of the fluctuation-dissipation theorem, that is, that the amplitude of the thermal fluctuations is proportional to the dissipative matrix M. Note the fact that the dissipative matrix M can be expressed in terms of the dyadic product of the noises implies automatically that M is symmetric and positive definite, which is the essential property for guaranteeing the second law. In that sense, one could say that the fluctuation-dissipation theorem is the warrant for the second law. Clearly, a model that has not a positive definite dissipative matrix M cannot be generalized in order to include thermal fluctuations.

In order to guarantee that the total energy and dynamical invariants do not change in time, a strong requirement on the form of $d\tilde{x}$ holds

$$\frac{\partial E}{\partial x} d\tilde{x} = 0, \quad \frac{\partial I}{\partial x} d\tilde{x} = 0, \tag{40}$$

implying the last equations in Eqs. (36) and (37).

The term $k_B(\partial \cdot M/\partial x)$ in Eq. (38) can be understood essentially as coming from the stochastic interpretation selected, which is Itô interpretation. In order to avoid potential misunderstandings we consider the Fokker-Planck equation governing the distribution function $\rho(x,t)$ for the stochastic variables x. The Fokker-Planck equation is mathematically equivalent to the stochastic differential equations (38) and can be obtained following a standard procedure [27]. It is given by

$$\frac{\partial}{\partial t}\rho(x,t) = -\frac{\partial}{\partial x}\left[\left(L\frac{\partial E}{\partial x} + M\frac{\partial S}{\partial x}\right)\rho(x,t)\right] + \frac{\partial}{\partial x} M \frac{\partial}{\partial x}\rho(x,t). \tag{41}$$

This Fokker-Planck equation has as equilibrium solution

$$\rho^{\mathrm{eq}}(x) = g(E(x), I(x)) \exp\{S(x)/k_B\}, \tag{42}$$

which is the Einstein distribution function for equilibrium fluctuations in the presence of dynamical invariants [28]. The arbitrary function $g(E(x),I(x))$ is fixed by the initial distribution function of dynamical invariants in the system [28]. For example, if we know with absolute precision the value E_0, I_0 of these dynamical invariants, then Eq. (42) becomes

$$\rho^{\mathrm{eq}}(x) = \delta(E(x) - E_0)\,\delta(I(x) - I_0) \exp\{S(x)/k_B\}. \tag{43}$$

That Eq. (42) is the equilibrium solution of Eq. (41) is easily proved by substitution and making use of the properties of L and M. By doing so, we note that the following condition must be fulfilled

$$\frac{\partial}{\partial x} L \frac{\partial E}{\partial x} = \frac{\partial}{\partial x}\dot{x}|_{\mathrm{rev}} = 0 \tag{44}$$

which is a statement about the reversible dynamics of the system. For a system with no dissipative processes ($M = 0$), Eq. (44) is actually a version of Liouville's theorem. In graphical terms the Liouville theorem's states the incompressibility of the reversible flow in x space. In essence, Liouville's theorem guarantees that the reversible part of the dynamics has as a stationary solution, a function of dynamical invariants only. Another important property that L should satisfy is the Jacobi identity [25] that encodes the time invariance of the reversible structure of the equations.

Now we show that Eqs. (30) can be expressed in the GENERIC form. The full state of the system is characterized by the independent variables $x = \{\mathbf{r}_i, \mathbf{v}_i, S_i,\ i = 1, \ldots, M\}$. The total energy and entropy of the system expressed in terms of the state variables are given in Eqs. (18) and (24), respectively. For future reference, we compute here the derivatives of the energy and entropy functions with respect to the state variables,

$$\frac{\partial E}{\partial x} = \begin{pmatrix} \dfrac{(\boldsymbol{\nabla} P)_i}{d_i} \\ m\mathbf{v}_i \\ T_i \end{pmatrix}, \quad \frac{\partial S}{\partial x} = \begin{pmatrix} \mathbf{0} \\ 0 \\ 1 \end{pmatrix}, \tag{45}$$

where the explicit form (22) is assumed for the pressure gradient.

A. Reversible part of the dynamics

Equations (23) can be cast in the following matrix form:

$$\begin{pmatrix} \dot{\mathbf{r}}_i \\ \dot{\mathbf{v}}_i \\ \dot{S}_i \end{pmatrix} = \sum_j \mathbf{L}_{ij} \begin{pmatrix} \dfrac{(\boldsymbol{\nabla} P)_i}{d_i} \\ m\mathbf{v}_j \\ T_j \end{pmatrix}, \tag{46}$$

where the block $\mathbf{L}_{ij}$ has the simple form

$$\mathbf{L}_{ij} = \frac{1}{m}\begin{pmatrix} \mathbf{0} & \mathbf{1}\delta_{ij} & \mathbf{0} \\ -\mathbf{1}\delta_{ij} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 0 \end{pmatrix}. \tag{47}$$

Now we can form a matrix L made of the blocks $\mathbf{L}_{ij}$, in such a way that Eqs. (46) are simply $\dot{x}|_{\mathrm{rev}} = L\boldsymbol{\nabla}E$. This matrix L is antisymmetric, thus guaranteeing that total energy is conserved. It also satisfies the degeneracy $L\boldsymbol{\nabla}S = 0$ as can be easily shown, and this guarantees that the entropy is constant due to the reversible part of the dynamics. Note that the condition (44) is also satisfied by the reversible equations. Moreover, the Jacobi identity is also satisfied by L.

B. Irreversible part of the dynamics

In order to cast the irreversible part of the dynamics in the form $\dot{x}|_{\mathrm{irr}} = M\boldsymbol{\nabla}S$, we should construct the matrix M that produces the irreversible terms in Eqs. (30). Instead of trying to figure out by inspection the possible form of M as we did for L, we follow here a different route based on the fluctuation-dissipation theorem, Eq. (39)

$$M = \frac{d\tilde{x} d\tilde{x}^T}{2k_B dt}. \tag{48}$$

What forms should we postulate for the noise terms $d\tilde{x}$ in order to construct M such that $M\boldsymbol{\nabla}S$ produces the irreversible terms in Eqs. (30)? We note that the dissipative forces in the velocity equation have a shear component. We developed a model some time back in which these shear forces arise [20]. Even though we introduced a spin variable in order to have total angular momentum conservation, we take the simpler view in which this variable is not introduced. Therefore, the postulated random force in the velocity equation will be very similar to that in Ref. [20].

We postulate the following form for the thermal noises $d\tilde{x} = \{0, d\tilde{\mathbf{v}}_i, d\tilde{S}_i\}$. Note that we do not assume any fluctuation in the position because we want to respect the purely reversible equation $\dot{\mathbf{r}}_i = \mathbf{v}_i$. The velocity and entropy random terms are postulated to be

$$m d\tilde{\mathbf{v}}_i = \sum_j \left(A_{ij} d\overline{\mathbf{W}}_{ij} + B_{ij}\tfrac{1}{3}\mathrm{tr}[d\mathbf{W}_{ij}]\right)\cdot\mathbf{e}_{ij},$$

$$T_i d\tilde{S}_i = -\frac{1}{2}\sum_j \left(A_{ij} d\overline{\mathbf{W}}_{ij} + B_{ij}\tfrac{1}{3}\mathrm{tr}[d\mathbf{W}_{ij}]\right):\mathbf{e}_{ij}\mathbf{v}_{ij} + \sum_j C_{ij} dV_{ij}. \tag{49}$$

We have introduced, for each pair i,j of particles, a matrix of independent increments of the Wiener process $d\mathbf{W}_{ij}$. Its traceless symmetric part $d\overline{\mathbf{W}}_{ij}$ is given by

$$d\overline{\mathbf{W}}_{ij}^{\alpha\beta} = \frac{1}{2}[d\mathbf{W}_{ij}^{\alpha\beta} + d\mathbf{W}_{ij}^{\beta\alpha}] - \frac{\delta^{\alpha\beta}}{3}\mathrm{tr}[d\mathbf{W}_{ij}], \tag{50}$$

where the trace is defined as

$$\mathrm{tr}[d\mathbf{W}_{ij}] = \sum_\sigma d\mathbf{W}_{ij}^{\sigma\sigma}. \tag{51}$$

As a convention, superindices refer to tensorial components while subindices label different particles.

In Eq. (49) we have also introduced an independent increment of the Wiener process for each pair of particles, dV_{ij}. This term will give rise to the heat conduction terms. Finally, the functions A_{ij}, B_{ij}, C_{ij} might depend on the state of the system through the positions and entropy of the particles. We postulate the following symmetry properties:

$$\begin{aligned} d\mathbf{W}_{ij} &= d\mathbf{W}_{ji},\\ dV_{ij} &= -dV_{ji},\\ A_{ij} &= A_{ji},\\ B_{ij} &= B_{ji},\\ C_{ij} &= C_{ji}. \end{aligned} \tag{52}$$

The independent increments of the Wiener processes satisfy the following mnemotechnical Itô rules

$$\begin{aligned} d\mathbf{W}_{ii'}^{\alpha\alpha'} d\mathbf{W}_{jj'}^{\beta\beta'} &= [\delta_{ij}\delta_{i'j'} + \delta_{ij'}\delta_{i'j}]\delta^{\alpha\beta}\delta^{\alpha'\beta'}dt,\\ dV_{ii'}dV_{jj'} &= [\delta_{ij}\delta_{i'j'} - \delta_{ij'}\delta_{i'j}]dt,\\ d\mathbf{W}_{ii'}^{\alpha\alpha'}dV_{ii'} &= 0. \end{aligned} \tag{53}$$

which respect the symmetries (52) under particle interchange. The additional dynamical invariant $I(x)$ in this model is the total linear momentum $P(x) = \Sigma_i m\mathbf{v}_i$ (no angular momentum conservation is imposed). Its derivatives with respect to the state variables are

$$\frac{\partial\mathbf{P}}{\partial x} \to \begin{pmatrix} 0 \\ m\mathbf{1} \\ 0 \end{pmatrix}. \tag{54}$$

Now, it is a trivial exercise to show that Eqs. (40), which now take the form

$$\begin{aligned} \sum_i m\mathbf{v}_i\cdot d\tilde{\mathbf{v}}_i + T_i d\tilde{S}_i &= 0,\\ \sum_i m d\tilde{\mathbf{v}}_i &= 0 \end{aligned} \tag{55}$$

are exactly satisfied, due to the symmetries (52). In this way, the postulated noises conserve exactly momentum and energy. Consequently, the irreversible part of the dynamics will also conserve momentum and energy.

According to Eq. (39), the matrix M is given by

$$M \to \mathbf{M}_{ij} = \begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0} & \dfrac{d\tilde{\mathbf{v}}_i d\tilde{\mathbf{v}}_j^T}{2k_B dt} & \dfrac{d\tilde{\mathbf{v}}_i d\tilde{S}_j}{2k_B dt} \\ 0 & \dfrac{d\tilde{S}_i d\tilde{\mathbf{v}}_j^T}{2k_B dt} & \dfrac{d\tilde{S}_i d\tilde{S}_j}{2k_B dt} \end{pmatrix}. \tag{56}$$

We compute in Appendix B the elements of this matrix.

Now we are in position to write the deterministic irreversible part of the dynamics $\dot{x}|_{\mathrm{irr}} = M\cdot(\partial S/\partial x)$, which will be given by

$$\left.\begin{pmatrix} \dot{r}_i \\ \dot{\mathbf{v}}_i \\ \dot{S}_i \end{pmatrix}\right|_{\mathrm{irr}} = \sum_j \mathbf{M}_{ij}\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ 1 \end{pmatrix}. \tag{57}$$

The matrix multiplication leads readily to the following equations:

$$\dot{\mathbf{r}}_i|_{\mathrm{irr}} = 0, \tag{58}$$

$$\begin{aligned} m\dot{\mathbf{v}}_i|_{\rm irr} &= -\sum_j \left[a_{ij}\mathbf{v}_{ij}+\left(\frac{1}{3}a_{ij}+b_{ij}\right)\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\mathbf{e}_{ij}\right],\\ T_i\dot{S}_i|_{\rm irr} &= -\sum_j c_{ij}T_{ij}+\frac{1}{2}\sum_j a_{ij}\mathbf{v}_{ij}^2+\frac{1}{2}\sum_j\left(\frac{1}{3}a_{ij}+b_{ij}\right)\\ &\quad\times(\mathbf{v}_{ij}\cdot\mathbf{e}_{ij})^2, \end{aligned} \tag{59}$$

where we have introduced the following quantities:

$$\begin{aligned} a_{ij} &= \frac{A_{ij}^2}{8k_B}\left(\frac{1}{T_i}+\frac{1}{T_j}\right),\\ b_{ij} &= \frac{B_{ij}^2}{12k_B}\left(\frac{1}{T_i}+\frac{1}{T_j}\right),\\ c_{ij} &= \frac{C_{ij}^2}{2k_BT_iT_j}. \end{aligned} \tag{60}$$

Note that Eqs. (59) are identical to Eqs. (30) if we choose

$$\begin{aligned} a_{ij} &= \left(\frac{5\eta}{3}-\zeta\right)\frac{F_{ij}}{d_id_j},\\ b_{ij}+\frac{a_{ij}}{3} &= 5\left(\frac{\eta}{3}+\zeta\right)\frac{F_{ij}}{d_id_j},\\ c_{ij} &= 2\kappa\frac{F_{ij}}{d_id_j}. \end{aligned} \tag{61}$$

Through Eqs. (60) these forms implies the following amplitudes for the thermal noise

$$\begin{aligned} A_{ij} &= \left[8k_B\frac{T_iT_j}{T_i+T_j}\left(\frac{5\eta}{3}-\zeta\right)\frac{F_{ij}}{d_id_j}\right]^{1/2},\\ B_{ij} &= \left[8k_B\frac{T_iT_j}{T_i+T_j}\left(\frac{5\eta}{3}+8\zeta\right)\frac{F_{ij}}{d_id_j}\right]^{1/2},\\ C_{ij} &= \left[4\kappa k_BT_iT_j\frac{F_{ij}}{d_id_j}\right]^{1/2}. \end{aligned} \tag{62}$$

In summary, by postulating the noise terms (49) with amplitudes (62), the fluctuation-dissipation theorem leads to a dissipation which is exactly the same as the dissipation in the SDPD deterministic model, Eqs. (30).

We finally write the stochastic differential equations (38) for our model. The term $k_B\partial M/\partial x$ is computed in the Appendix and the final equations are

$$\begin{aligned} d\mathbf{r}_i &= \mathbf{v}_i dt,\\ m\,d\mathbf{v}_i &= \sum_j\left[\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right]F_{ij}\mathbf{r}_{ij}dt-\sum_j(1-d_{ij})a_{ij}\mathbf{v}_{ij}dt\\ &\quad-\sum_j(1-d_{ij})\left(\frac{a_{ij}}{3}+b_{ij}\right)\mathbf{e}_{ij}\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}dt+m\,d\tilde{\mathbf{v}}_i,\\ T_idS_i &= \frac{1}{2}\sum_j\left(1-d_{ij}-\frac{T_j}{T_i+T_j}\frac{k_B}{C_i}\right)\left[a_{ij}\mathbf{v}_{ij}^2+\left(\frac{a_{ij}}{3}+b_{ij}\right)\right.\\ &\quad\left.\times(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})^2\right]dt-\frac{2k_B}{m}\sum_j{}'\frac{T_iT_j}{T_i+T_j}\left(\frac{10}{3}a_{ij}+b_{ij}\right)dt\\ &\quad-2\kappa\sum_j\frac{F_{ij}}{d_id_j}T_{ij}dt-2\kappa\frac{k_B}{C_i}\sum_j{}'\frac{F_{ij}}{d_id_j}T_jdt+T_id\tilde{S}_i. \end{aligned} \tag{63}$$

The prime in Σ_j' restricts the index j to be different from i. We have introduced in Eq. (63) the dimensionless quantity

$$d_{ij}=\frac{T_iT_j}{(T_i+T_j)^2}\left[\frac{k_B}{C_i}+\frac{k_B}{C_j}\right], \tag{64}$$

where C_i is the heat capacity at constant volume of particle i. Note that C_i is an extensive quantity and, therefore, for large fluid particles the dimensionless ratio k_B/C_i is very small. In the limit $k_B\rightarrow 0$, one recovers the deterministic equations (30), which are a discretization of the Navier-Stokes equations. Therefore, the set of equations (63) can be understood as a discrete Lagrangian version of fluctuating hydrodynamics [9].

The stochastic differential equations (63) will produce, at equilibrium, a distribution of the variables given by the Einstein distribution function (43). This is automatically ensured by the GENERIC structure of these equations.

The stochastic differential equations (63) conserve energy exactly. In order to prove this, it is necessary to use Itô calculus,

$$dE=\frac{\partial E}{\partial x}dx+\frac{1}{2}\frac{\partial^2E}{\partial x\partial x}d\tilde{x}d\tilde{x}. \tag{65}$$

A straightforward algebra using Eqs. (63) leads to $dE=0$. Finally, Eqs. (63) take a much compact form for the particular case in which the bulk viscosity vanishes, $\zeta=0$. In this case, $A_{ij}=B_{ij}$ in Eqs. (62) and the thermal fluctuations (49) have also a much simpler structure.

V. DISCUSSION

By following the smoothed particle hydrodynamics methodology, we have discretized the Navier-Stokes equations with the aid of a novel interpolant that ensures the explicit fulfillment of the second law. This allows to introduce thermal fluctuations in a consistent way through the fluctuation-dissipation theorem and allows to apply SPH to mesoscopic scales where these fluctuations are important.

The model is very similar to the original dissipative particle dynamics model, although in a much improved form. There are several advantages of the present model with respect to the original formulation of DPD. The introduction of the volume of the particles as a thermodynamic variable allows one to formulate a thermodynamically consistent model in which the conservative forces of the original DPD algorithm are actually given in terms of pressure forces. This allows one to introduce arbitrary equations of state in the model. In particular, equations of state of the van der Waals type describing liquid-vapor transitions can be used. A recent work by Pagonabarraga and Frenkel has considered the introduction of a van der Waals equation of state, but the model is limited to isothermal situations and does not conserve exactly total energy [14]. With the model presented here it is now possible to study thermal effects in the generation of bubbles and droplets in nonequilibrium liquid-vapor coexistence. In addition, the introduction of a volume variable for each fluid particle introduces a physical length scale allowing for a clear interpretation of the size of the dissipative particles and the scales that are being explored in actual simulations. Another great benefit of the model presented over the classic DPD model is the fact that a direct connection between the model parameters and the transport coefficients of the fluid is given. In the original DPD model it was necessary to follow an indirect route by means of kinetic theory in order to relate the model parameters with the transport coefficients of the fluid being modeled [15]. Note that we provide specific functional forms for the weight function to be used in the DPD model, and the form in which the weight function appears in the pressure force and viscous force terms are not identical ($r_{ij}F_{ij}/d_id_j$ in the former, F_{ij}/d_id_j in the later).

The GENERIC framework allows to introduce modifications of the model that respect the thermodynamic consistency. As an example, we consider the XSPH model introduced by Monaghan in order to avoid interpenetration of particles at high mach numbers [2]. The proposal of Monaghan is to substitute the equation of motion (11) by

$$\dot{\mathbf{r}}_i=\mathbf{v}_i-\sum_j\frac{2}{d_i+d_j}\mathbf{v}_{ij}W_{ij}=\sum_j\Delta_{ij}\mathbf{v}_j, \tag{66}$$

where

$$\Delta_{ij}=\frac{2}{d_i+d_j}W_{ij}+\delta_{ij}\left(1-\frac{2}{d_i+d_j}W_{ij}\right). \tag{67}$$

This modification produces updates of the positions which take into account the surrounding velocity of the fluid and reduces interpenetration in actual simulations. If we want to introduce this equation of motion for the positions, the antisymmetric structure of the matrix L enforces to have the following set of reversible equations:

$$\begin{pmatrix}\dot{\mathbf{r}}_i\\ \dot{\mathbf{v}}_i\\ \dot{S}_i\end{pmatrix}=\sum_j\frac{\mathbf{1}}{m}\begin{pmatrix}\mathbf{0} & \mathbf{1}\Delta_{ij} & \mathbf{0}\\ -\mathbf{1}\Delta_{ij} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & 0\end{pmatrix}\begin{pmatrix}\frac{(\boldsymbol{\nabla}P)_i}{d_i}\\ m\mathbf{v}_j\\ T_j\end{pmatrix}. \tag{68}$$

This L matrix is antisymmetric and satisfies the incompressibility of the flow in x space. The resulting equation of motion for the velocity becomes

$$m\dot{\mathbf{v}}_i=-\frac{(\boldsymbol{\nabla}P)_i}{d_i}-\sum_j\frac{2}{d_i+d_j}W_{ij}\left[\frac{(\boldsymbol{\nabla}P)_i}{d_i}-\frac{(\boldsymbol{\nabla}P)_j}{d_j}\right], \tag{69}$$

where $(\boldsymbol{\nabla}P)_i/d_i$ is given in Eq. (22). Thus we see that an additional term in the momentum equation arises by virtue of the modification of the position equation. This term conserves total momentum and total energy.

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APPENDIX A

We demonstrate here the identity Eq. (25). First we note that the function $F(r)$ satisfies the property

$$\int d\mathbf{r}F(r)\mathbf{r}\mathbf{r}=\mathbf{1} \tag{A1}$$

as can be proved from

$$\int d\mathbf{r}\mathbf{r}\boldsymbol{\nabla}W(r)=-\mathbf{1}. \tag{A2}$$

This identity follows by partial integration and the normalization (6). Equation (A1) implies

$$\begin{gathered}\int d\mathbf{r}F(r)\mathbf{r}\cdot\mathbf{r}=3,\\ \int_0^h drF(r)r^4=\frac{3}{4\pi}.\end{gathered} \tag{A3}$$

By Taylor expanding $A(\mathbf{r}')$ around $\mathbf{r}$ we obtain

$$\begin{aligned}A(\mathbf{r}')=&A(\mathbf{r})+\boldsymbol{\nabla}A(\mathbf{r})\cdot(\mathbf{r}-\mathbf{r}')\\ &+\frac{1}{2}\boldsymbol{\nabla}\boldsymbol{\nabla}A(\mathbf{r}):(\mathbf{r}-\mathbf{r}')(\mathbf{r}-\mathbf{r}')+\cdots.\end{aligned} \tag{A4}$$

We substitute this expression in

$$\begin{aligned}&\int d\mathbf{r}'[A(\mathbf{r}')-A(\mathbf{r})]F(|\mathbf{r}'-\mathbf{r}|)\left[\frac{(\mathbf{r}'-\mathbf{r})^\alpha(\mathbf{r}'-\mathbf{r})^\beta}{(\mathbf{r}'-\mathbf{r})^2}\right]\\ &=\frac{1}{2}\nabla^{\alpha'}\nabla^{\beta'}A(\mathbf{r})\int d\mathbf{r}'F(|\mathbf{r}'-\mathbf{r}|)\\ &\quad\times\left[\frac{(\mathbf{r}'-\mathbf{r})^{\alpha'}(\mathbf{r}'-\mathbf{r})^{\beta'}(\mathbf{r}'-\mathbf{r})^\alpha(\mathbf{r}'-\mathbf{r})^\beta}{(\mathbf{r}'-\mathbf{r})^2}\right]+\mathcal{O}(\nabla^4Ah^2)\\ &=\frac{1}{2}\nabla^{\alpha'}\nabla^{\beta'}A(\mathbf{r})\int d\mathbf{q}F(q)\left[\frac{\mathbf{q}^{\alpha'}\mathbf{q}^{\beta'}\mathbf{q}^\alpha\mathbf{q}^\beta}{q^2}\right]+\mathcal{O}(\nabla^4Ah^2),\end{aligned} \tag{A5}$$

where the change of variables $\mathbf{q}=\mathbf{r}'-\mathbf{r}=(x,y,z)$ has been made. The first derivative term in Eq. (A4) produces a third order tensor that vanish by isotropy. The fourth order tensor is easily computed in spherical coordinates. The only surviving components are of the form

$$\int d\mathbf{q}F(q)\frac{xxxx}{q^2}=\frac{3}{5},$$

$$\int d\mathbf{q}F(q)\frac{xxyy}{q^2}=\frac{1}{5}, \tag{A6}$$

where use has been made of Eq. (A3). Therefore, the contraction of the isotropic fourth order tensor with the second derivatives of $A(\mathbf{r})$ becomes simply

$$\int d\mathbf{r}'[A(\mathbf{r}')-A(\mathbf{r})]F(|\mathbf{r}'-\mathbf{r}|)\left[\frac{(\mathbf{r}'-\mathbf{r})^\alpha(\mathbf{r}'-\mathbf{r})^\beta}{(\mathbf{r}'-\mathbf{r})^2}\right]$$
$$=\frac{1}{5}\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}A(\mathbf{r})\delta^{\alpha\beta}+\frac{2}{5}\nabla^\alpha\nabla^\beta A(\mathbf{r})+\mathcal{O}(\nabla^4Ah^2), \tag{A7}$$

from which Eq. (25) in the text follows.

APPENDIX B: CALCULATION OF M AND $\partial M/\partial x$

We compute the following preliminary results by using the Itô formulas (53)

$$\mathrm{tr}[d\mathbf{W}_{ii'}]\mathrm{tr}[d\mathbf{W}_{jj'}]=3[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{i'j}]dt,$$

$$\mathrm{tr}[d\mathbf{W}_{ii'}]d\overline{\mathbf{W}}_{jj'}^{\alpha\alpha'}=0,$$

$$d\overline{\mathbf{W}}_{ii'}^{\alpha\alpha'}d\overline{\mathbf{W}}_{jj'}^{\beta\beta'}=[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{i'j}]\left[\frac{1}{2}(\delta^{\alpha\beta}\delta^{\alpha'\beta'}+\delta^{\alpha'\beta}\delta^{\alpha\beta'})-\frac{1}{3}\delta^{\alpha\alpha'}\delta^{\beta\beta'}\right]dt. \tag{B1}$$

It is also convenient to compute the following object:

$$\left[A_{ii'}d\overline{\mathbf{W}}_{ii'}^{\alpha\alpha'}+B_{ii'}\frac{\delta^{\alpha\alpha'}}{3}\mathrm{tr}[d\mathbf{W}_{ii'}]\right]\times\left[A_{jj'}d\overline{\mathbf{W}}_{jj'}^{\beta\beta'}+B_{jj'}\frac{\delta^{\beta\beta'}}{3}\mathrm{tr}[d\mathbf{W}_{jj'}]\right]$$
$$=[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{i'j}]\left[A_{ii'}A_{jj'}\frac{1}{2}(\delta^{\alpha\beta}\delta^{\alpha'\beta'}+\delta^{\alpha'\beta}\delta^{\alpha\beta'})+(B_{ii'}B_{jj'}-A_{ii'}A_{jj'})\frac{1}{3}\delta^{\alpha\alpha'}\delta^{\beta\beta'}\right]dt. \tag{B2}$$

Now we are in the position of computing the correlations of the random forces $d\tilde{\mathbf{v}}_i, d\tilde{S}_i$. By using Eqs. (49) and (B2) one obtains

$$m^2\frac{d\tilde{\mathbf{v}}_i^\alpha d\tilde{\mathbf{v}}_j^\beta}{dt}=\delta_{ij}\left[\sum_k\frac{A_{ik}^2}{2}(\delta^{\alpha\beta}+\mathbf{e}_{ik}^\alpha\mathbf{e}_{ik}^\beta)\right]+\delta_{ij}\left[\sum_k\frac{B_{ik}^2-A_{ik}^2}{3}\mathbf{e}_{ik}^\alpha\mathbf{e}_{ik}^\beta\right]-\frac{A_{ij}^2}{2}(\delta^{\alpha\beta}+\mathbf{e}_{ij}^\alpha\mathbf{e}_{ij}^\beta)-\frac{B_{ij}^2-A_{ij}^2}{3}\mathbf{e}_{ij}^\alpha\mathbf{e}_{ij}^\beta,$$

$$-mT_j\frac{d\tilde{\mathbf{v}}_i^\alpha d\tilde{S}_j}{dt}=\delta_{ij}\left[\sum_k\frac{A_{ik}^2}{2}\left(\frac{\mathbf{v}_{ik}^\alpha}{2}+\mathbf{e}_{ik}\cdot\frac{\mathbf{v}_{ik}}{2}\mathbf{e}_{ik}^\alpha\right)\right]+\delta_{ij}\left[\sum_k\frac{B_{ik}^2-A_{ik}^2}{3}\mathbf{e}_{ik}^\alpha\mathbf{e}_{ik}\cdot\frac{\mathbf{v}_{ik}}{2}\right]+\frac{A_{ij}^2}{2}\left(\frac{\mathbf{v}_{ij}^\alpha}{2}+\mathbf{e}_{ij}\cdot\frac{\mathbf{v}_{ij}}{2}\mathbf{e}_{ij}^\alpha\right)+\frac{B_{ij}^2-A_{ij}^2}{3}\mathbf{e}_{ij}^\alpha\mathbf{e}_{ij}\cdot\frac{\mathbf{v}_{ij}}{2},$$

$$-mT_i\frac{d\tilde{S}_i d\tilde{\mathbf{v}}_j^\alpha}{dt}=\delta_{ij}\left[\sum_k\frac{A_{ik}^2}{2}\left(\frac{\mathbf{v}_{ik}^\alpha}{2}+\mathbf{e}_{ik}\cdot\frac{\mathbf{v}_{ik}}{2}\mathbf{e}_{ik}^\alpha\right)\right]+\delta_{ij}\left[\sum_k\frac{B_{ik}^2-A_{ik}^2}{3}\mathbf{e}_{ik}^\alpha\mathbf{e}_{ik}\cdot\frac{\mathbf{v}_{ik}}{2}\right]-\frac{A_{ij}^2}{2}\left(\frac{\mathbf{v}_{ij}^\alpha}{2}+\mathbf{e}_{ij}\cdot\frac{\mathbf{v}_{ij}}{2}\mathbf{e}_{ij}^\alpha\right)-\frac{B_{ij}^2-A_{ij}^2}{3}\mathbf{e}_{ij}^\alpha\mathbf{e}_{ij}\cdot\frac{\mathbf{v}_{ij}}{2},$$

$$T_iT_j\frac{d\tilde{S}_i d\tilde{S}_j}{dt}=\delta_{ij}\left\{\sum_k\frac{A_{ik}^2}{2}\left[\left(\frac{\mathbf{v}_{ik}}{2}\right)^2+\left(\mathbf{e}_{ik}\cdot\frac{\mathbf{v}_{ik}}{2}\right)^2\right]\right\}+\delta_{ij}\left[\sum_k\frac{B_{ik}^2-A_{ik}^2}{3}\left(\mathbf{e}_{ik}\cdot\frac{\mathbf{v}_{ik}}{2}\right)^2\right]+\frac{A_{ij}^2}{2}\left(\left(\frac{\mathbf{v}_{ij}}{2}\right)^2+\left(\mathbf{e}_{ij}\cdot\frac{\mathbf{v}_{ij}}{2}\right)^2\right]+\frac{B_{ij}^2-A_{ij}^2}{3}\left(\mathbf{e}_{ij}\cdot\frac{\mathbf{v}_{ij}}{2}\right)^2+\delta_{ij}\sum_k C_{ik}^2-C_{ij}^2. \tag{B3}$$

From these expressions (B3), the components of the matrix M in Eq. (56) are readily obtained. We now need to compute the elements of the vector $k_B\partial M/\partial x$ in Eq. (38). This vector has the form

$$k_B\sum_j \frac{\partial}{\partial x_j}\mathbf{M}_{ij} = k_B\sum_j \begin{pmatrix} 0 \\ \displaystyle\sum_j \frac{\partial}{\partial \mathbf{v}_j}\frac{d\tilde{\mathbf{v}}_i d\tilde{\mathbf{v}}_j}{2k_B dt} + \sum_j \frac{\partial}{\partial S_j}\frac{d\tilde{\mathbf{v}}_i d\tilde{S}_j}{2k_B dt} \\ \displaystyle\sum_j \frac{\partial}{\partial \mathbf{v}_j}\frac{d\tilde{S}_i d\tilde{\mathbf{v}}_j}{2k_B dt} + \sum_j \frac{\partial}{\partial S_j}\frac{d\tilde{S}_i d\tilde{S}_j}{2k_B dt} \end{pmatrix}. \tag{B4}$$

We compute each term separately,

$$k_B\sum_j \frac{\partial}{\partial \mathbf{v}_j}\frac{d\tilde{\mathbf{v}}_i d\tilde{\mathbf{v}}_j}{2k_B dt} = 0$$

$$k_B\sum_j \frac{\partial}{\partial S_j}\frac{d\tilde{\mathbf{v}}_i d\tilde{S}_j}{2k_B dt} = \frac{1}{m}\sum_j d_{ij}\left(a_{ij}\mathbf{v}_{ij} + \left[\frac{a_{ij}}{3} + b_{ij}\right]\mathbf{v}_{ij}\cdot\mathbf{e}_{ij}\mathbf{e}_{ij}\right), \tag{B5}$$

where we have introduced

$$d_{ij} = \frac{T_i T_j}{(T_i + T_j)^2}\left[\frac{k_B}{C_i} + \frac{k_B}{C_j}\right]. \tag{B6}$$

Note that d_{ij} is a dimensionless quantity involving the heat capacity at constant volume of cell i, C_i, which is defined from

$$\frac{\partial T_i}{\partial S_i} = \frac{T_i}{C_i}. \tag{B7}$$

The next term is

$$k_B\sum_j \frac{\partial}{\partial \mathbf{v}_j}\cdot\frac{d\tilde{S}_i d\tilde{\mathbf{v}}_j}{2k_B dt} = -\frac{2k_B}{mT_i}\sum_{j\neq i}\left[\frac{10}{3}a_{ij} + b_{ij}\right]\frac{T_i T_j}{T_i + T_j} \tag{B8}$$

and, finally, the last term is

$$k_B\sum_j \frac{\partial}{\partial S_j}\cdot\frac{d\tilde{S}_i d\tilde{S}_j}{2k_B dt} = -\frac{2\kappa}{T_i}\frac{k_B}{C_i}\sum_j \frac{F_{ij}}{d_i d_j}T_j - \frac{1}{2T_i}\sum_j\left(\frac{T_j}{T_i + T_j}\frac{k_B}{C_i} + d_{ij}\right) \times\left[a_{ij}\mathbf{v}_{ij}^2 + \left(\frac{a_{ij}}{3} + b_{ij}\right)(\mathbf{v}_{ij}\cdot\mathbf{e}_{ij})^2\right]. \tag{B9}$$

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