Shear-viscosity-independent bulk-viscosity term in smoothed particle hydrodynamics

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An angular momentum conservative pure bulk viscosity term for smoothed particle hydrodynamics (SPH) is proposed in the present paper. This formulation permits independent modeling of shear and bulk viscosities, which is of paramount importance for fluids with large bulk viscosity in situations where sound waves or large Mach numbers are expected. With this aim a dissipative term proportional to the rate of change of the volume is considered at the particle level. The equations of motion are derived from the minimization of a Lagrangian combined with an appropriate dissipation function that depends on this rate of change of particle volume, in analogy with the corresponding entropy production contribution in fluids. Due to the Galilean invariance of the formulation, the new term is shown to exactly conserve linear momentum. Moreover, its invariance under solid-body rotations also ensures the conservation of angular momentum. Two verification cases are proposed: the one-dimensional propagation of a sound pulse and a two-dimensional case, modeling the time decay of an accelerating-decelerating pipe flow. The SPH solutions are compared to exact ones, showing that the newly proposed term behaves indeed as a viscosity associated only with the local expansion-compression of the fluid. In view of these considerations, we conclude that the method presented in this paper allows for setting up a bulk viscosity independently of the shear one and as large as any particular problem may require. At the same time, together with the prescribed momentum conservation to reproduce the Navier-Stokes equation, the new term also keeps the angular momentum conservation required to properly model free interfaces or overall rotations of the bulk fluid.

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I. INTRODUCTION

Smoothed particle hydrodynamics (SPH) is a consolidated technique to simulate macroscopic flows through a Lagrangian description of the fluid dynamics [1]. Within the context of the ongoing developments in this methodology, in a recent article [2] Colagrossi *et al.* derived dissipative terms in SPH departing from a dissipation function expressed in terms of the relative particle velocities. The concept of *dissipation function* was already introduced by Rayleigh [3] and generalized by Onsager to various nonequilibrium thermodynamic processes [4,5]. Examples of recent applications of the dissipation function can be found in Refs. [6,7]. Within this framework, Colagrossi *et al.* showed that it was Monaghan and Gingold's expression [8] for the two-body dissipative interaction that conserves both linear and angular momentum and produces a viscous stress in the simulated fluid. When analyzing the hydrodynamic limit of this model, i.e., $kd \ll 1$, where k is a characteristic wave number of the field spatial dependence and d is the interparticle characteristic distance, one realizes that this formulation introduces contributions to the Navier-Stokes equation proportional to the symmetric traceless tensor $\overline{\nabla \mathbf{v}}^{\circ}$, but also unavoidably to the field divergence $\nabla \cdot \mathbf{v}$. These two contributions emerge from one single expression for the dissipative interaction. Therefore, this choice implies that Monaghan and Gingold's term gives rise to both, shear μ and bulk κ viscosities, but that these contributions are not independent but satisfy a fixed proportionality $\mu = 3\kappa/5$ [2], being in fact both of the same order. This dependence of shear and bulk vicosities was also highlighted in the astrophysical context by Lodato and Price [9], who discussed various existing options to model the right dissipation in an evolution problem.

Colagrossi *et al.* [2] also showed that if exact angular momentum conservation is not required, the expression proposed by Morris *et al.* [10] in the context of creeping flow, contains an additional degree of freedom as the friction between particles is split into one contribution along their

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relative velocity and another orthogonal to it. However, this additional contribution influences the transport properties of the system in such a way that $\mu > 3\kappa/5$, to the price of sacrificing the angular momentum conservation. The latter property may not be required for creeping flow motions in bounded environments, but is necessary to model vorticity relaxation near free surfaces. For example, if angular momentum is not conserved, then the overall rotation of a drop of fluid in vacuo spuriously dies out if Morris' expression is used. The top-down approach, which derives the interparticle dissipative forces from the discretization of the continuum field [11,12], has the same limitation of a maximum value for the bulk viscosity, necessary to avoid a negative contribution to the entropy production.

Therefore, if incompressible flows in general situations are to be modeled within SPH with a weakly compressible approach, then what Ref. [2] teaches us is that choosing the expression of Morris *et al.* [10] allows one to avoid the consideration of any compressible dissipation to the expense of the loss of angular momentum conservation. Choosing instead Monaghan and Gingold's [8] expression guarantees conservation of angular momentum but introduces a compressible viscosity of the same order as the shear viscosity. This effect, however, is not relevant if the Mach number is sufficiently small, and consequently $d\rho/dt \simeq 0$ (see, e.g., Ref. [13]), which can be achieved in practical cases by sufficiently reducing the fluid compressibility. Moreover, the consistency of the model within the framework of Morris *et al.* formulation can be recovered by introducing the particle spin (see Müller *et al.* [14], who proposed such an approach to improve a smoothed dissipative particle dynamics model), as a way to close the balance of the total angular momentum. Momentum transfer between translational and rotational motions then occurs, but the final outcome of the model is that the inequality $\mu > 3\kappa/5$ still holds.

In the present paper we address the question of whether it is possible to introduce an additional dissipation interaction at the particle level to overcome the limiting relative value of bulk versus shear viscosities and, at the same time, that the force conserves linear but also angular momentum. Proposing an appropriate form of the dissipation function we derive a particle-particle dissipative force term that strictly contributes only to the bulk viscosity, leaving the shear viscosity unchanged. However, despite the fact that the force is pairwise additive, it is multibody in nature since its calculation involves the relative velocity of third particles in the neighborhood of the interacting ones. Therefore, the new term introduced in this article will be relevant in systems with large bulk viscosity, like CO_2, particularly for situations involving Mach numbers near or larger than one, or where sound propagation and attenuation is the target.

In this article we also show that the concept of dissipation function can be applied to general formulations of dissipative interactions for complex fluids within the framework of SPH. The advantage of the formulation of the particle equations of motion from a minimum principle involving the Lagrangian lies in that the underlying conservation principles can be enforced in the layout of the problem [12,15]. In this article we have extended this concept to the dissipative interactions introducing the dissipation function, along the lines of the pioneering works of Lord Rayleigh [3] and Onsager [4,5]. Within the conditions of validity of the dissipation function as a generator of dissipative interactions, if is invariant under pure translations and solid body rotations, the conjugate momenta will be conserved by the derived equations of motion, including the dissipative forces. Hence, as Dirac remarked (quoted by Monaghan [12]), basing the equations of motion in a Lagrangian (here extended with the Rayleigh dissipation function) allows new physical interactions to be included consistently. Therefore, the bottom-up formulation of SPH permits us to enforce general physical properties for the system that will have their projection into the continuum macroscopic behavior in a way that may be very difficult to infer from a top-down perspective based on the continuum [16].

The article is organized as follows. In Sec. II we introduce the SPH framework, including the Monaghan-Gingold term, and we derive the new contribution to the dissipation force for a general system with arbitrary shear and bulk viscosities. The hydrodynamic limit of the model is derived in Sec. III and is shown to be equivalent to a Newtonian bulk viscosity term. We are able to derive expressions relating the macroscopic bulk viscosity with the parameters of the model for the particle-particle interaction. The passage from continuum to discrete, which is not unequivocal in SPH, is discussed in Sec. IV. One-dimensional and two-dimensional numerical verification cases are proposed in Sec. V. Some conclusions are enumerated and future work threads proposed to close the paper.

II. DERIVATION OF THE MULTIBODY FORCE FOR THE BULK VISCOSITY

A. The SPH approximation to the hydrodynamic fields

Let us consider an ensemble of N particles representing fluid elements located at positions $\mathbf{r}_i$, $i = 1, \ldots, N$ with velocities $\mathbf{u}_i$ and masses m_i. Since the particles are considered as macroscopic objects, we can define the internal energy per unit of mass e_i and the particle entropy per unit of mass s_i. In SPH, fields are associated to corresponding physical properties carried by particles, or defined from the immediate neighborhood. The main example or the latter is the particle mass density [11,17]

$$\rho_i = m_i \sum_{j=1}^{N} W(r_{ij}; h), \tag{1}$$

where W is a weight function referred to as kernel. Here, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and $r_{ij} = |\mathbf{r}_{ij}|$. The kernel is a positive definite integrable smooth function with a characteristic length h (see Ref. [18] for a recent discussion on the choice of kernels' characteristic length), which will be omitted in the notation where no confusion could occur. In this article, this kernel is isotropic and its volume integral is normalized; i.e.,

$$\int d\mathbf{r}\, W(r) = 1. \tag{2}$$

The spatial gradient of the kernel satisfies

$$\boldsymbol{\nabla}_i W(r_{ij}) = \mathbf{e}_{ij} \frac{dW}{dr_{ij}} \equiv -\mathbf{e}_{ij} r_{ij} F(r_{ij}) = -\boldsymbol{\nabla}_j W(r_{ij}), \tag{3}$$

where $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ is a unit vector. With this definition Eq. (3), F is positively definite function. Within the same framework, one can define the particle number density as

$$c_i = \sum_j W(r_{ij}). \tag{4}$$

The definition of c_i allows us to introduce an estimate of the volume surrounding the ith particle, namely,

$$V_i \equiv \frac{1}{c_i} = \frac{1}{\sum_j W(r_{ij})}. \tag{5}$$

In SPH, to reproduce smooth fields, insensitive to the underlying particulate nature of the description, it is required that $V_i \ll h^D$, i.e., that the number of particles ν in a given particle environment determined by the range of the kernel h, must be large enough, i.e., $\nu \sim ch^D \gg 1$. Here D is the dimensionality of the space. Otherwise, the local fields show large fluctuations at short wavelengths of the fields, revealing the aforementioned particulate nature of the model. Moreover, to recover the hydrodynamic behavior as described by the Navier-Stokes equation the so-called hydrodynamic limit must be invoked [19]. The latter states that the characteristic wavelengths of the fields must be much larger than h so that spatial variations of the fields up to $\mathcal{O}(k^2)$ are sufficient to describe the dynamics, k being the field wave number. Hence, if $L \sim 1/k$ is the characteristic length for the variation of a hydrodynamic field, then the continuous limit description should be reached when $h/L \sim kh \to 0$ with $V_i/h^D \to 0$ [20–22]. The latter limit will be discussed in the next section.

Following the approach of Ref. [2], the conservative dynamics of the system can be derived from the Lagrangian

$$\mathcal{L}[\dot{\mathbf{r}}_i, \mathbf{r}_i] = \sum_i \left[\frac{1}{2} m_i \dot{r}_i^2 - m_i U(t, \boldsymbol{r}_i) - m_i e(\rho_i, s_i) \right], \tag{6}$$

where the first term on the right-hand side of this equation is the kinetic energy of the particles. U is a general external potential field such as gravity and $\dot{\mathbf{r}}_i = \mathbf{u}_i$. e_i is the internal energy, which is considered to be a function only on the particle thermodynamic properties ρ_i and s_i in the present model.

Together with the Lagrangian, following Ref. [7] we define the dissipation function, often referred to as Rayleighian, as

$$\Phi_D[\mathbf{u}_i] = \frac{1}{2} \sum_{i,j>i} \eta F(r_{ij}) r_{ij} (\mathbf{e_{ij}} \cdot \mathbf{u}_{ij})^2 V_i V_j + \frac{1}{2} \sum_i \zeta V_i^3 \dot{c}_i^2. \tag{7}$$

The first contribution to the dissipation function has already been proposed in Ref. [2] and gives rise to the Monaghan and Gingold's force. The second one is the new contribution proposed. Formally, it takes the form of an entropy production due to a divergence fluid field since the continuity equation states that $dc/dt = -c\nabla \cdot \mathbf{v}$. Thus, $V_i \dot{c}_i$ is an approximation of a local divergence field. To have an intuitive idea of the nature of the newly introduced term, let us use the continuity equation into the new term and write

$$\frac{1}{2} \sum_i \zeta V_i^3 \dot{c}_i^2 \sim \frac{1}{2} \sum_i \zeta V_i^3 c_i^2 (\nabla \cdot \mathbf{v})_i^2 \sim \frac{1}{2} \int dV \, \zeta \, (\nabla \cdot \mathbf{v})^2 \tag{8}$$

where we have used that $c_i V_i = 1$ and that $\sum_i V_i (\nabla \cdot \mathbf{v})_i^2 \simeq \int dV \, (\nabla \cdot \mathbf{v})^2$, as $\sum_i V_i \sim \int dV \sim V$, the latter being the total volume of the system. Therefore, this contribution to the dissipative function effectively has the form of the entropy produced in the system due to the fluid bulk viscosity ζ. The relevant property of the formulation of this contribution from the dissipation function is that the form of the interparticle force obtained will be consistent with the general concepts behind the theory of irreversible processes in fluids [23], as intended. The factor V_i^3 is introduced here by convenience, to make the resulting contribution to the bulk viscosity independent of the particle number density, as demonstrated in the next section, but that can also be gathered from Eq. (8). Notice that the factor $V_i V_j$ in Monaghan and Gingold's contribution has the same effect of making the coefficient independent of the particle number density.

Notice that in Eqs. (6) and (7) we have made the distinction between the independent variables in the Lagrangian $\dot{\mathbf{r}}_i, \mathbf{r}_i$ and the ones in the Rayleighian $\mathbf{u}_i$, which either set must be considered as mutually independent, although at the end one assumes $\dot{\mathbf{r}}_i = \mathbf{u}_i$. Moreover, the dissipation function must be a quadratic function of the velocities. Under these conditions, the dynamics of the system is given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i} \right) - \frac{\partial \mathcal{L}}{\partial \mathbf{r}_i} = -\frac{\partial}{\partial \mathbf{u}_i} \Phi_D, \tag{9}$$

where the generalized dissipative forces are obtained from differentiation of Φ_D with respect to $\mathbf{u}_i$; i.e.,

$$\mathbf{f}_i^v = -\frac{\partial}{\partial \mathbf{u}_i} \Phi_D. \tag{10}$$

Following Ref. [2], one can arrive to the equation of motion for the dynamics of the ensemble of particles, which reads

$$m_i \frac{d\boldsymbol{u}_i}{dt} = \sum_{j \neq i} \left[\frac{p_j V_j^2 + p_i V_i^2}{V_i V_j} \right] \mathbf{e}_{ij} r_{ij} F(r_{ij}) V_i V_j + m_i \mathbf{g}_i + \mathbf{f}_i^v. \tag{11}$$

Since $F(0) = 0$ for common kernels, the restriction $j \neq i$ in the summation in this equation, and in the ones that follow in the rest of the paper, could be removed.

Making use of the properties of e_i and translational invariance, one can write the conservative interparticle force $\mathbf{f}_i^C$ in Eq. (11) as

$$\begin{aligned} \mathbf{f}_i^C &\equiv -\sum_j m_j \frac{\partial e_j}{\partial \mathbf{r}_i} = -\sum_j m_j \frac{\partial e_j}{\partial \rho_j}\bigg|_s \frac{\partial \rho_j}{\partial \boldsymbol{r}_i} \\ &= \sum_{j \neq i} \left[\frac{p_j V_j^2 + p_i V_i^2}{V_i V_j} \right] \mathbf{e}_{ij} r_{ij} F(r_{ij}) V_i V_j, \end{aligned} \tag{12}$$

where we have used the fact that the particle pressure $p_i \equiv -m_i \partial e_i / \partial V_i|_s$. In this derivation we have considered that s_i is intrinsically carried by the particles and is not a function of the environment, as the local mass density ρ_i is. Notice that

$\mathbf{f}_i^C$ is defined here as the reversible (adiabatic) variation of the internal energy of the particle e_i. To have a model with a complete thermodynamic description, the energy balance has to be also provided (see, e.g., Eq. (12) in Ref. [2]).

The contribution due to the external potential is given by

$$\mathbf{g}_i = -\frac{\partial U}{\partial \mathbf{r}_i}, \tag{13}$$

which is a pure acceleration in view of the fact that we have defined U as an energy per unit of mass. Therefore, the dynamics of the system takes the form

$$\frac{d\mathbf{p}_i}{dt} = \mathbf{f}_i^C + \mathbf{f}_i^v + m_i \mathbf{g}_i, \tag{14}$$

where we have introduced the particle momentum as $\mathbf{p}_i \equiv m_i \mathbf{u}_i$.

B. Analysis of the dissipative forces

The presence of two terms in Eq. (7) permits us to split the force also into two contributions. The first one is the Monaghan and Gingold's force, as expected

$$\mathbf{f}_i^{\mathrm{MG}} = -\sum_{j\neq i} \eta F(r_{ij})\, r_{ij} (\mathbf{u}_{ij}\cdot \mathbf{e}_{ij})\, \mathbf{e}_{ij} V_i V_j. \tag{15}$$

The new contribution requires the derivative of the local number density; i.e.,

$$\frac{dc_i}{dt} = \sum_j W'(r_{ij}) \frac{dr_{ij}}{dt} = -\sum_{j\neq i} F(r_{ij})\, r_{ij}\, \mathbf{e}_{ij}\cdot \mathbf{u}_{ij}. \tag{16}$$

Then, the related force in Eq. (7) is obtained by differentiating with respect to $\mathbf{u}_i$, and using this latter result

$$\begin{aligned}
\mathbf{f}_i^{\mathrm{Bulk}} &= -\frac{\partial}{\partial \mathbf{u}_i}\left(\frac{1}{2}\zeta \sum_j V_j^3\, \dot{c}_j^2\right) \\
&= \sum_j \zeta V_j^3\, \dot{c}_j \left(\frac{\partial}{\partial \mathbf{u}_i} \sum_{k\neq j} F(r_{jk})\, r_{ij}\, \mathbf{e}_{jk}\cdot \mathbf{u}_{jk}\right) \\
&= \sum_j \zeta \left(V_j^3\, \dot{c}_j\right) \sum_{k\neq j} F(r_{jk})\, r_{ij}\, \mathbf{e}_{jk} (\delta_{ij} - \delta_{ik}).
\end{aligned} \tag{17}$$

Hence, using the symmetry $F(r_{ij})\,\mathbf{e}_{ij} = -F(r_{ji})\,\mathbf{e}_{ji}$ one arrives at the central result of this article, namely,

$$\mathbf{f}_i^{\mathrm{Bulk}} = \sum_{j\neq i} \zeta \left[V_j^3 \dot{c}_j + V_i^3 \dot{c}_i\right] F(r_{ij})\, r_{ij}\, \mathbf{e}_{ij}. \tag{18}$$

The first and most obvious property of $\mathbf{f}_i^{\mathrm{Bulk}}$ is that is null in an incompressible system. This is due to the fact that the force is proportional to $\dot{c}_i$, in view of Eq. (18). Thus, its presence in the dynamics of the ensemble of particles does not modify the shear viscosity, as we will prove below. Therefore, Eq. (18) introduces a genuine contribution to the bulk viscosity alone. Moreover, the expression found is already symmetric with respect to the permutation of particle indices, as a result of the translational invariance of the dissipation function Eq. (7).

Second, while the force given by Monaghan and Gingold [Eq. (15)] depends only on the relative velocity of the interacting particles, the form given in Eq. (18) depends on velocities of third particles in the immediate environment of the interacting particles. It is thus many body in nature. By inspection of Eq. (18) one can see that it is still pair-wise additive.

Third, according to Eq. (18) by permuting the indices we arrive at the conclusion that

$$\mathbf{f}_{ij}^{\mathrm{Bulk}} = \zeta \left[V_j^3 \dot{c}_j + V_i^3 \dot{c}_i\right] F(r_{ij})\, r_{ij}\, \mathbf{e}_{ij} = -\mathbf{f}_{ji}^{\mathrm{Bulk}}. \tag{19}$$

Thus, the total force on the center of mass of the pair is zero and, therefore, the total momentum of the system will be a conserved quantity under the action of this force.

Fourth, due to the aforementioned invariance of the dissipation function under solid-body rotations, the derived interparticle force is directed along the relative vector between particle centers, and thus the torque induced by this force over the pair is also zero, i.e.,

$$\mathbf{r}_i \times \mathbf{f}_{ij}^{\mathrm{Bulk}} + \mathbf{r}_j \times \mathbf{f}_{ji}^{\mathrm{Bulk}} = (\mathbf{r}_i - \mathbf{r}_j) \times \mathbf{f}_{ij}^{\mathrm{Bulk}} \;\propto\; \mathbf{r}_{ij} \times \mathbf{e}_{ij} = 0, \tag{20}$$

which indicates that the total angular momentum of the system will be also conserved.

Finally, we want to point out that the introduction of random forces to describe fluid fluctuations should require the definition of a specific contribution coupled to the new term. This analysis will be presented elsewhere.

III. FROM THE DISCRETE TO THE CONTINUUM

To obtain the relationship between the SPH particle dynamic parameters and the macroscopic transport coefficients of the "continuum" fluid represented by the ensemble of moving particles, we have to introduce the macroscopic fields and take the hydrodynamic limit, i.e., that the spatial variation of the fields $L \sim 1/k$ is much longer than the characteristic range of the kernel h [24]. For the purposes of this article it is sufficient to focus on the momentum conservation and the Navier-Stokes equation.

A. Macroscopic field densities

We can introduce the field densities from the knowledge of the properties of the particles. These magnitudes are intrinsically different from the weighted densities given in Eqs. (1) and (4), which are properties defined at the particle level. Let us introduce in the first place the particle number density $n(\mathbf{r}, t)$ as

$$n(\mathbf{r}, t) \equiv \sum_{i=1}^{N} \delta[\mathbf{r} - \mathbf{r}_i(t)]. \tag{21}$$

A general property ψ_i carried by the particles allows us to define a field Ψ from the relation

$$\Psi(\mathbf{r}, t) \equiv \sum_{i=1}^{N} \psi_i\, \delta[\mathbf{r} - \mathbf{r}_i(t)]. \tag{22}$$

However, in the framework of SPH the fields are extrapolated and smoothed out by using the kernel W, according to

$$\Psi^{\mathrm{SPH}}(\mathbf{r}, t) \equiv \int d\mathbf{r}'\, W(|\mathbf{r} - \mathbf{r}'|) \sum_{i=1}^{N} \psi_i\, \delta[\mathbf{r}' - \mathbf{r}_i(t)]$$

$$= \sum_{i=1}^{N} \psi_i \, W(|\mathbf{r} - \mathbf{r}_i|). \tag{23}$$

This difference between the *particulate* field Eq. (22) and the smoothed SPH field Eq. (23) is irrelevant in the hydrodynamic limit, where the field Ψ is expected to slowly vary with the distance. The relevance of the kernel becomes apparent only at the level of particle interactions, as we have indicated in Sec. II, but it is not relevant for the derivation of the transport coefficients of the ensemble of particles.

The effect of the uneven distribution of the particles in space is reflected by the pair distribution function $g(\mathbf{r} - \mathbf{r}')$, which is defined from the relation [19]

$$\sum_{i=1}^{N} \sum_{j \neq i} \delta[\mathbf{r} - \mathbf{r}_i(t)] \delta[\mathbf{r}' - \mathbf{r}_j(t)] \equiv n(\mathbf{r}, t)\, n(\mathbf{r}', t)\, g(\mathbf{r} - \mathbf{r}'). \tag{24}$$

In Eq. (24) no average is considered, contrary to the usual statistical mechanical analysis of liquids, because no thermal agitation is present in the model. Thus, strictly speaking, $g(r)$ depends locally and instantaneously on the actual distribution of particles. However, if the conditions mentioned in Sec. II are satisfied, then we can assume that $g(\mathbf{r} - \mathbf{r}') \simeq g(|\mathbf{r} - \mathbf{r}'|) \simeq 1 - 1/N \simeq 1$ all over the bulk fluid. Moreover, $g(r)$ will only be different from 1 when $|\mathbf{r} - \mathbf{r}'| < h$, as the range of interaction of SPH particles is h. Furthermore, in view of Eq. (12), SPH particles interact through soft potentials (i.e., the interaction energy is finite when particles overlap). It is thus expected that the minimum of g will be shallow at particle-particle overlap, namely, $g(|\Delta r| \to 0) > 0$. Finally, if the number of particles is very large as to have $ch^D \gg 1$, then the interaction between two particles such that $|\mathbf{r}_i - \mathbf{r}_j| < h$ is screened by the presence of third particles interacting with both. Thus, the local structure of the ensemble introduced by the direct particle-particle interaction is confined to an effective distance $V_i^{1/D}$. Hence, for the hypothesis $g(|\Delta r|) \simeq 1$, usually assumed in SPH method, to be correct, the limit $V_i \ll h^D$ needs to be considered. In this work we keep $g(r)$ within the analysis instead of replacing it by 1 to obtain general expressions for systems where the limit $V_i \ll h^D$ is only marginally satisfied and the particulate nature of the model may be relevant.

Particle number density and the corresponding field are related in the following way:

$$c_i = \sum_{j=1}^{N} W(r_{ij}) = \int d\mathbf{r}'\, W(|\mathbf{r}_i - \mathbf{r}'|) \sum_j \delta(\mathbf{r}' - \mathbf{r}_j)$$
$$\simeq \int d\mathbf{r}'\, W(|\mathbf{r}_i - \mathbf{r}'|) n(\mathbf{r}', t). \tag{25}$$

Due to the fact that the kernel W is a short-ranged function, in the hydrodynamic long-wavelength limit, a multipolar expansion can be carried out. Effectively, writing $\mathbf{r}' = \mathbf{r}_i + \Delta\mathbf{r}'$ and using translational invariance of the bulk system, up to second order in the gradients $\mathcal{O}(kh)^2$ we can write

$$c_i \simeq n(\mathbf{r}_i) + \tfrac{1}{2}\mathbf{C}_2 : \nabla\nabla\, n(\mathbf{r}', t)\big|_{\mathbf{r}'=\mathbf{r}_i} + \ldots, \tag{26}$$

with the multipolar coefficients given by

$$\mathbf{C}_q = \int d\Delta\mathbf{r}\ \Delta\mathbf{r}\Delta\mathbf{r}\overset{(q)}{\cdots}\Delta\mathbf{r}\Delta\mathbf{r}\, W(|\Delta\mathbf{r}|). \tag{27}$$

Notice that $C_0 = 1$ due to the normalization of the kernel, and all the odd-q multipoles vanish due to the kernel isotropy.

For the local volume one can further write

$$V_i \simeq \frac{1}{n(\mathbf{r}_i)}\left(1 - \frac{1}{2n(\mathbf{r}_i)}\mathbf{C}_2 : \nabla\nabla n(\mathbf{r}', t)|_{\mathbf{r}'=\mathbf{r}_i} + \ldots\right). \tag{28}$$

In a homogeneous system $n = N/V$, and if $V_i \ll h^D$, then $c_i \simeq n(\mathbf{r}_i)$, but their values may differ near interfaces. Therefore, for long-wavelength variations of the fields, $kh \ll 1$, we expect that c_i and $n(\mathbf{r}_i)$ are practically the same. The momentum density is given by

$$\mathbf{j}(\mathbf{r}, t) \equiv \sum_{i=1}^{N} \mathbf{p}_i\, \delta[\mathbf{r} - \mathbf{r}_i(t)]. \tag{29}$$

Differentiating Eq. (29) one can write

$$\frac{\partial}{\partial t}\mathbf{j}(\mathbf{r}, t) = \sum_{i=1}^{N} [\dot{\mathbf{p}}_i - \nabla \cdot \mathbf{u}_i\mathbf{p}_i]\, \delta[\mathbf{r} - \mathbf{r}_i(t)], \tag{30}$$

with $\mathbf{u}_i = \mathbf{p}_i/m_i$. Making use of Eq. (14), we find

$$\frac{\partial}{\partial t}\mathbf{j}(\mathbf{r}, t) = \sum_i \left(\mathbf{f}_i^C + m_i\mathbf{g}_i - \nabla \cdot \mathbf{u}_i\mathbf{p}_i\right) \delta[\mathbf{r} - \mathbf{r}_i(t)]$$
$$+ \sum_i \sum_{j \neq i} \big[-\eta F(r_{ij})\, r_{ij}(\mathbf{u}_{ij} \cdot \mathbf{e}_{ij}) V_i V_j$$
$$+ \zeta\left(V_j^3 \dot{c}_j + V_i^3 \dot{c}_i\right) F(r_{ij})\, r_{ij}\, \mathbf{e}_{ij}\big]\, \delta[\mathbf{r} - \mathbf{r}_i(t)]. \tag{31}$$

Introducing $\int d\mathbf{r}'\, \delta(\mathbf{r}' - \mathbf{r}_j) = 1$, together with Eq. (24), we can write

$$\frac{\partial}{\partial t}\mathbf{j}(\mathbf{r}, t) = -\nabla P(\mathbf{r}) + \rho(\mathbf{r})\mathbf{g}(\mathbf{r}) - \nabla \cdot \rho(\mathbf{r})\mathbf{v}(\mathbf{r})$$
$$+ \nabla \cdot \sigma^{\mathrm{MG}} + \nabla \cdot \sigma^{\mathrm{Bulk}}. \tag{32}$$

In this equation, we have defined the convective contribution from the relation

$$\sum_i \mathbf{u}_i\mathbf{p}_i\, \delta(\mathbf{r} - \mathbf{r}_i) \equiv \rho(\mathbf{r})\mathbf{v}(\mathbf{r}), \tag{33}$$

and we made use of Eq. (28) replacing $\mathbf{r}_i$ by the field point $\mathbf{r}$. Notice that we have introduced the velocity field $\mathbf{v}$ from Eq. (33), although we are implicitly assuming that the particle velocity $\mathbf{u}_i \simeq \mathbf{v}(\mathbf{r}_i)$. Moreover, the particle-particle interaction force gives the system pressure,

$$-\nabla P = \sum_i \sum_{j \neq i} \left[\frac{p_j V_j^2 + p_i V_i^2}{V_i V_j}\right]$$
$$\times F(r_{ij})\, r_{ij}\, \mathbf{e}_{ij}\, V_i V_j\, \delta[\mathbf{r} - \mathbf{r}_i(t)]. \tag{34}$$

The contribution due to the external fields is straightforwardly given by

$$\rho(\mathbf{r})\mathbf{g}(\mathbf{r}) \equiv \sum_i m_i\mathbf{g}_i\, \delta[\mathbf{r} - \mathbf{r}_i(t)] = \mathbf{g}(\mathbf{r}) \sum_i m_i \delta[\mathbf{r} - \mathbf{r}_i(t)]. \tag{35}$$

Furthermore, we can define the two contributions to the viscous stress, i.e.,

$$\nabla \cdot \sigma^{\mathrm{MG}} = -\sum_i \sum_{j\neq i} \eta F(r_{ij})\, r_{ij}(\mathbf{u}_{ij}\cdot \mathbf{e}_{ij}) V_i V_j\, \delta[\mathbf{r}-\mathbf{r}_i(t)], \tag{36}$$

where σ^{MG} stands for the contribution to the stress tensor due to the Monoghan and Gingold's expression, and

$$\nabla \cdot \sigma^{\mathrm{Bulk}} = \sum_i \sum_{j\neq i} \zeta \left[V_j^3 \dot{c}_j + V_i^3 \dot{c}_i\right] F(r_{ij})\, r_{ij}\, \mathbf{e}_{ij}\, \delta[\mathbf{r}-\mathbf{r}_i(t)], \tag{37}$$

where σ^{Bulk} refers to the contribution to the stress tensor arising from the new term. The stress tensor σ^{Bulk} should not be regarded as the only contribution to the bulk viscosity as the Monaghan and Gingold's expression also produces a residual contribution.

B. Identification of the different contributions to the viscosities

To develop further the right-hand side of Eq. (31), using the fact that both W and F are short ranged (h), we can introduce the multipolar expansions, as in Eq. (26). From Eq. (34) we insert the identity $\int d\mathbf{r}'\delta(\mathbf{r}-\mathbf{r}')=1$ and use Eq. (24) to obtain

$$-\nabla P(\mathbf{r}) = -\int d\mathbf{r}' [p(\mathbf{r}+\Delta\mathbf{r}')V^2(\mathbf{r}+\Delta\mathbf{r}') + p(\mathbf{r})V^2(\mathbf{r})]\Delta\hat{\mathbf{r}} \times F(\Delta r')\,\Delta r'\, g(\Delta r') n(\mathbf{r}+\Delta\mathbf{r}') n(\mathbf{r}), \tag{38}$$

where the negative sign arises from the fact that the unit vector $\mathbf{e}_{ij} \to -\Delta\hat{\mathbf{r}}$ since in the pass to the continuum we have $\mathbf{r}_i \to \mathbf{r}$ and $\mathbf{r}_j \to \mathbf{r}'$ with $\mathbf{r}' = \mathbf{r}+\Delta\mathbf{r}'$, while $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Hence, introducing the multipolar expansion and collecting terms up to second order in the gradients,

$$-\nabla P(\mathbf{r}) = -\int d\Delta\mathbf{r} F(\Delta r')\,\Delta r'\, g(\Delta r')\Delta\hat{\mathbf{r}}\Delta\mathbf{r} \cdot\nabla[p(\mathbf{r})V^2(\mathbf{r})n^2(\mathbf{r})]. \tag{39}$$

Despite the apparent complexity of this expression, in the hydrodynamic limit and for a sufficiently homogeneous system $V_i \ll h^D$, i.e., $g(\Delta r')\simeq 1$, the macroscopic pressure coincides with the particle pressure, since $V(\mathbf{r})\simeq 1/n(\mathbf{r})$, cf. Eq. (28) and

$$\begin{aligned}\int d\Delta\mathbf{r}' F(\Delta r')\Delta\mathbf{r}'\Delta\mathbf{r}' &= \frac{4\pi}{3}\int_0^\infty d\Delta r'\, F(\Delta r')(\Delta r')^4 \\ &= -\frac{4\pi}{3}\int_0^\infty d\Delta r'\,(\Delta r')^3 \frac{dW(\Delta r')}{d\Delta r'} = 1.\end{aligned} \tag{40}$$

The last equality follows after partial integration and the fact that W is normalized, together with $W(\Delta r\to\infty)\to 0$. In evaluating this expression we have used that the angular integral of the isotropic second rank tensor yields

$$\mathbf{I}^{\mathrm{3D}}_{\alpha\beta} = \int d\Delta\hat{\mathbf{r}}\,\Delta\hat{\mathbf{r}}_\alpha\Delta\hat{\mathbf{r}}_\beta = \frac{4\pi}{3}\delta_{\alpha\beta}. \tag{41}$$

Therefore, if the system is locally homogeneous enough, then it follows that the macroscopic pressure gradient is given by the particle expression for the pressure p_i; i.e.,

$$-\nabla P(\mathbf{r}) \simeq -\nabla p(\mathbf{r}). \tag{42}$$

For completeness we provide the general expression in the hydrodynamic limit, for situations were only marginally $V_i \leqslant h^D$, i.e.,

$$-\nabla P(\mathbf{r}) = -\left(\frac{4\pi}{3}\int d\Delta r F(\Delta r')g(\Delta r')(\Delta r)^4\right)\nabla p(\mathbf{r}), \tag{43}$$

where use has been made of the fact that $V\simeq 1/n$, according to Eq. (28).

As far as the viscous stresses are concerned, let us consider Eq. (36) and introduce the pair distribution function as in Eq. (38). One has

$$\begin{aligned}\nabla\cdot\sigma^{\mathrm{MG}} = -\int d\Delta\mathbf{r}'\eta F(\Delta r')\,\Delta r'\,\Delta\hat{\mathbf{r}}'\Delta\hat{\mathbf{r}}' \\ \cdot[\mathbf{v}(\mathbf{r})-\mathbf{v}(\mathbf{r}+\Delta\mathbf{r}')] \\ \times V(\mathbf{r})n(\mathbf{r})V(\mathbf{r}+\Delta\mathbf{r}')n(\mathbf{r}+\Delta\mathbf{r}')g(\Delta r').\end{aligned} \tag{44}$$

After the multipolar expansion one obtains up to second order in the gradients

$$\begin{aligned}\nabla\cdot\sigma^{\mathrm{MG}} \simeq \frac{\eta}{2}\int d\Delta\mathbf{r}'\, F(\Delta r')g(\Delta r')(\Delta r')^3 \\ \times \Delta\hat{\mathbf{r}}'\Delta\hat{\mathbf{r}}'\Delta\hat{\mathbf{r}}'\Delta\hat{\mathbf{r}}' \vdots \{n^2(\mathbf{r})V^2(\mathbf{r})\nabla\nabla\mathbf{v}(\mathbf{r}) \\ + (\nabla[n^2(\mathbf{r})V^2(\mathbf{r})])\nabla\mathbf{v}(\mathbf{r})\}.\end{aligned} \tag{45}$$

The integration of the isotropic fourth rank tensor can be carried out to give

$$\begin{aligned}\mathbf{I}^{\mathrm{3D}}_{\alpha\beta\gamma\nu} &= \int d\Delta\hat{\mathbf{r}}'\,\Delta\hat{\mathbf{r}}'_\alpha\Delta\hat{\mathbf{r}}'_\beta\Delta\hat{\mathbf{r}}'_\gamma\Delta\hat{\mathbf{r}}'_\nu \\ &= \frac{4\pi}{15}(\delta_{\alpha\beta}\delta_{\gamma\nu}+\delta_{\alpha\gamma}\delta_{\beta\nu}+\delta_{\alpha\nu}\delta_{\beta\gamma}).\end{aligned} \tag{46}$$

After evaluating the triple contraction in Eq. (45) one finds

$$\begin{aligned}\nabla\cdot\sigma^{\mathrm{MG}} &= \nabla\cdot\mu(\nabla\mathbf{v}+(\nabla\mathbf{v})^T+\mathbf{1}\nabla\cdot\mathbf{v}) \\ &= \nabla\cdot\mu\left(2\overset{\circ}{\overline{\nabla\mathbf{v}}}+\tfrac{5}{3}\mathbf{1}\nabla\cdot\mathbf{v}\right),\end{aligned} \tag{47}$$

where $(\nabla\mathbf{v})^T$ is the transposed of $\nabla\mathbf{v}$, we have introduced the symmetric traceless velocity gradient tensor $\overset{\circ}{\overline{\nabla\mathbf{v}}}$ and $\mathbf{1}$ is the identity matrix. The prefactor is the shear viscosity of the model and is given by the expression

$$\mu \equiv \eta\frac{2\pi}{15}\int_0^\infty d\Delta r'\,\Delta r'^5\, F(\Delta r')\, g(\Delta r'), \tag{48}$$

where use has been made of the fact that $Vn\simeq 1$ in view of Eq. (28). Again, in a sufficiently locally homogeneous system $V_i \ll h^D$, this expression reduces to

$$\mu \equiv \eta\frac{2\pi}{15}\int_0^\infty d\Delta r'\,\Delta r'^5\, F(\Delta r'). \tag{49}$$

As we can see from Eq. (47) this calculation leads us to the aforementioned result that the Monaghan and Gingold's expression produces also a bulk viscosity whose magnitude is proportional to the one of the shear viscosity, namely, $\lambda^{\mathrm{MG}} = 5\mu/3$.

The new contribution to the viscous dissipation can be transformed to introduce the pair distribution function and the local densities, as before. From Eq. (37)

$$\nabla \cdot \sigma^{\text{Bulk}} = -\zeta \int d\Delta\mathbf{r}' F(\Delta r') \Delta r' g(\Delta r') \times [V^3(\mathbf{r}+\Delta\mathbf{r}')\dot{c}(\mathbf{r}+\Delta\mathbf{r}') + V^3(\mathbf{r})\dot{c}(\mathbf{r})] \times \Delta\hat{\mathbf{r}}' n(\mathbf{r}) n(\mathbf{r}+\Delta\mathbf{r}'), \tag{50}$$

with the additional complexity introduced by the multibody nature of the force, i.e.,

$$\dot{c}(\mathbf{r}) = \int d\Delta\mathbf{r}'\, F(\Delta r)\, \Delta r'\, g(\Delta r)\, \Delta\hat{\mathbf{r}}' \cdot[\mathbf{v}(\mathbf{r}) - \mathbf{v}(\mathbf{r}+\Delta\mathbf{r})] n(\mathbf{r}+\Delta\mathbf{r}), \tag{51}$$

according to Eq. (16). Again, introducing a multipolar expansion and retaining terms up to second order in the gradients one arrives at the expression

$$\nabla \cdot \sigma^{\text{Bulk}} = \nabla(\lambda \nabla \cdot \mathbf{v}), \tag{52}$$

where

$$\lambda \equiv \zeta \left[\frac{4\pi}{3} \int_0^\infty d\Delta r'\, \Delta r'^4\, F(\Delta r')\, g(\Delta r')\right]^2. \tag{53}$$

Again, use has been made of the fact that $Vn \simeq 1$. If the limit $V_i \ll h^D$ is assumed, then the expression for this dissipative coefficient takes the simpler form

$$\lambda \equiv \zeta \left[\frac{4\pi}{3} \int_0^\infty d\Delta r\, \Delta r^4\, F(\Delta r)\right]^2 = \zeta, \tag{54}$$

according to Eq. (40).

As we can see from Eq. (52), the new contribution to the dissipation projects only onto $\nabla \cdot \mathbf{v}$, showing that it is possible to separately model shear and bulk viscosities with arbitrary relative values, keeping the conservation of both linear and angular momenta, which was the main objective of this article.

IV. FROM THE CONTINUUM TO THE DISCRETE

In the previous section we have deduced the macroscopic hydrodynamic equations for a SPH fluid starting from the formulation of particle interactions only. These particle properties included conservative and dissipative forces as well. While the conservative forces due to pressure need to be of a particular form, to recover the appropriate meaning of the pressure in the macroscopic system [cf. Eqs. (34), (38), (40), and (42)], the dissipative force can be defined in many different ways, all leading to the same type of viscous dissipation, although the dependence of the viscosity coefficients on model parameters may be rather different. The formulation in terms of the dissipation function is then an instrument for exploring a pleiad of possible, equally consistent at the macroscopic level, expressions for the fluid viscosities, including specific kernels as well as density dependent viscosities. The key ingredient for this bottom-up formulation is that the appropriate conservation laws, such as total momentum, angular momentum and energy, are maintained at the particle level by the algorithm. For comparison it is thus instructive to also explore the derivation of the additional bulk viscosity from a top-down perspective, starting for the continuum equations.

The choice of Eq. (18) as dissipative force is motivated by the requirement that the corresponding contribution to the bulk viscosity is independent of the particle density [cf. Eq. (54)], as it is also customary for the shear viscosity in the form of Monaghan and Gingold term in Eq. (49) but also implicitly for the pressure term in Eq. (12). However, it should be now obvious for the reader that other forms could have been chosen for the dissipation forces, including the use of kernels other than W and its gradient F, with an interaction range different from h, although here, for the simplicity of the formulation, we have used the same kernel in all the interactions, as is customary in SPH.

In the usual deductive top-down procedure in SPH (cf. Ref. [12] and references therein), one starts by associating the viscous terms with forces per unit volume exerted between the particles, namely,

$$\rho\mathbf{g} = \mu\, \nabla^2\boldsymbol{u} + (\lambda+\mu)\, \nabla\, (\nabla \cdot \boldsymbol{u}), \tag{55}$$

where, as in Eq. (13), $\mathbf{g}$ is a force per unit of mass, i.e., a pure acceleration. In Ref. [2] it was shown that using Monaghan and Gingold's viscous term is equivalent at the continuous level to having the force per unit volume term

$$\rho\mathbf{g}^{\text{MG}} = \mu\, \nabla^2\mathbf{v} + 2\mu\, \nabla\, (\nabla \cdot \mathbf{v}), \tag{56}$$

in the momentum equation, which automatically implies $\lambda = \mu$. Thus, to introduce an additional contribution that acts only on $\nabla \cdot \mathbf{v}$, one can write Eq. (55) to be equal to

$$\rho\mathbf{g} = \rho\mathbf{g}^{\text{MG}} + \lambda^{\text{SPH}}\, \nabla\, (\nabla \cdot \mathbf{v}), \tag{57}$$

which combines Eq. (56) with an independent term on the gradient of the velocity divergence. The additional term depends on a new parameter (let us call it λ^{SPH}) to introduce a correct second viscosity. A viscous term allowing for this is proposed taking advantage of continuity equation, leading to

$$\rho\mathbf{g} = \rho\mathbf{g}^{\text{MG}} - \lambda^{\text{SPH}} \nabla\left(\frac{1}{\rho}\frac{d\rho}{dt}\right). \tag{58}$$

Then, discretizing this last equation with plain SPH in a particle set leads to the expression

$$\rho_i\, \mathbf{g}_i = -2\mu\, (n+2) \sum_j F(r_{ij})\, (\boldsymbol{u}_{ij} \cdot \boldsymbol{e}_{ij})\, \boldsymbol{e}_{ij}\, V_j + \lambda^{\text{SPH}} \sum_j \left(\frac{\dot{\rho}_j}{\rho_j}\right) F(r_{ij})\, \boldsymbol{e}_{ij}\, V_j. \tag{59}$$

As usual in the top-down procedure, the structure of the last term in the previous equation does not satisfy crucial physical properties; in particular, total momentum conservation. This is due to the fact that the process of discretization of the continuum equations is not unequivocal, and can be done in different ways. Here we explore two different possibilities and their connection with the formulation given in the previous section.

Multiplying Eq. (59) by the particle volume, we have a force to be applied onto particle i, where the last term has been symmetrized by using that the integral of the kernel gradient is zero,

$$\mathbf{f}_i = -\mu\, (n+2) \sum_j F(r_{ij})\, (\boldsymbol{u}_{ij} \cdot \boldsymbol{e}_{ij})\, \boldsymbol{e}_{ij}\, V_i\, V_j$$

$$+\lambda^{\mathrm{SPH}}\sum_j\left(\frac{\dot\rho_i}{\rho_i}+\frac{\dot\rho_j}{\rho_j}\right)F(r_{ij})\,\boldsymbol{e}_{ij}\,V_i\,V_j. \tag{60}$$

This last expression conserves linear and angular momentum for the particle motion. Since the Lagrangian evolution of the volume of a fluid element is governed by the volumetric strain rate equation:

$$\frac{1}{V}\frac{dV}{dt}=\boldsymbol{\nabla}\cdot\mathbf{v}, \tag{61}$$

using the definition $c=1/V$, then

$$-V\,\dot c=\boldsymbol{\nabla}\cdot\mathbf{v}. \tag{62}$$

This allows us to write Eq. (60) as

$$\mathbf{f}_i=-\mu\,(n+2)\sum_j F(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{e}_{ij})\,\boldsymbol{e}_{ij}\,V_i\,V_j$$
$$+\lambda^{\mathrm{SPH}}\sum_j(V_i\dot c_i+V_j\dot c_j)F(r_{ij})\,\boldsymbol{e}_{ij}\,V_i\,V_j, \tag{63}$$

with the second part of the term becoming another choice for a bulk viscosity term, similar to the one in Eq. (18), which also conserves linear and angular momentum exactly and that remarkably gives the same contribution to the macroscopic viscosity, Eq. (54). Let us denote it as

$$\mathbf{f}_i^{\mathrm{Bulk}}=\lambda^{\mathrm{SPH}}\sum_j(V_i\dot c_i+V_j\dot c_j)F(r_{ij})\,\boldsymbol{e}_{ij}\,V_i\,V_j. \tag{64}$$

As it happens with different consistent choices in various SPH formulas (see, e.g., Ref. [12] Sec. 2.2 for a discussion on SPH discretizations for the continuity equation), there may be some advantages in using one or another formula in a particular problem (e.g., multiphase with high density ratios, hypersonic gas dynamics, etc.), an aspect to be investigated in the future.

Equating (55) and (57), the free parameter λ^{SPH} is obtained from the physical viscosities as

$$\lambda^{\mathrm{SPH}}=\lambda-\mu, \tag{65}$$

with the same meaning as the ζ parameter introduced in the discrete analysis.

Since the bulk viscosity, κ, is defined as

$$\kappa=\lambda+\frac{2\,\mu}{n}, \tag{66}$$

then

$$\lambda^{\mathrm{SPH}}=\kappa-\left(1+\frac{2}{n}\right)\mu, \tag{67}$$

and, therefore, there is no upper limit for representing any actual physical bulk viscosity with this model. Such bulk viscosity can be achieved by adjusting the parameter λ^{SPH} as a function of the physical shear and bulk viscosities with Eq. (67), then applying, at the discrete level, Monaghan and Gingold formula for the viscous term, and Eq. (18) or (64) for the additional compressible viscosity dissipation.

According to Eq. (67), assuming Stokes hypothesis, i.e., the zeroing of the bulk viscosity, κ, in a Newtonian fluid [2], leads to a negative value of the new contribution coefficient, λ^{SPH}. This fact violates the second principle for the novel term, unless its contributions to the volumetric dissipation and the Monaghan and Gingold one are considered as part of the same dissipation mechanism, which they are.

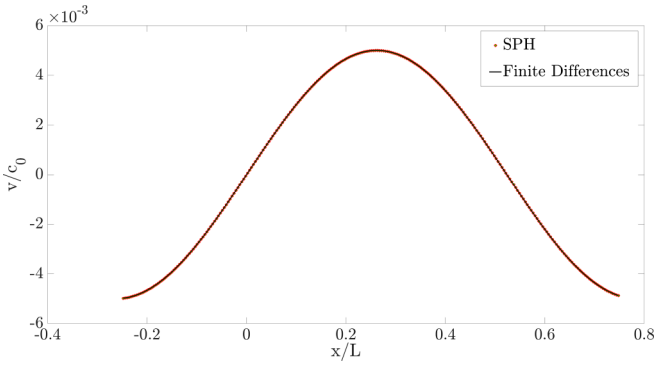


FIG. 1. Sinusoidal pulse. Initial velocity field, $n=256$.

To end this section, let us consider the last term in Eq. (58) and discretize it following a different strategy. Effectively, as it is customarily done to obtain Eq. (12) from the continuum [12] we can write

$$-\lambda^{\mathrm{SPH}}\boldsymbol{\nabla}\left(\frac{\dot\rho}{\rho}\right)=-\lambda^{\mathrm{SPH}}\rho\left[\boldsymbol{\nabla}\left(\frac{\dot\rho}{\rho^2}\right)+\frac{\dot\rho}{\rho^3}\boldsymbol{\nabla}\rho\right]. \tag{68}$$

Applying the rules of discretization as before, multiplying by the particle volume, one arrives at

$$\mathbf{f}_i=-\mu\,(n+2)\sum_j F(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{e}_{ij})\,\boldsymbol{e}_{ij}\,V_i\,V_j$$
$$+\lambda^{\mathrm{SPH}}\sum_j\left(V_i^3\dot c_i+V_j^3\dot c_j\right)F(r_{ij})\,\boldsymbol{e}_{ij}. \tag{69}$$

This expression for the contribution to the bulk viscosity is the same as derived in Eq. (18).

V. NUMERICAL VERIFICATION

The periodic propagation of a sinusoidal sound wave and the time decay of a two-dimensional accelerating-decelerating pipe flow are used as verification cases.

A. Sinusoidal sound pulse

The setup is the same used by Ott and Schnetter [25] to test a new algorithm for muliphasic SPH. Their same periodic one-dimensional domain $[-0.5, 1.5)$ is proposed. The width of the domain is therefore $L=2$. A fluid with reference density ρ_0 and numerical sound speed c_0 equal to one (in consistent units) is considered.

The governing equations are the compressible one dimensional continuity and momentum equation, with the bulk viscosity as the only contribution to dissipation due to the one-dimensional nature of the problem:

$$\frac{d\rho}{dt}=-\rho\frac{\partial v}{\partial x}, \tag{70}$$

$$\rho\frac{dv}{dt}=-\frac{\partial p}{\partial x}+\kappa\frac{\partial^2 v}{\partial x^2}. \tag{71}$$

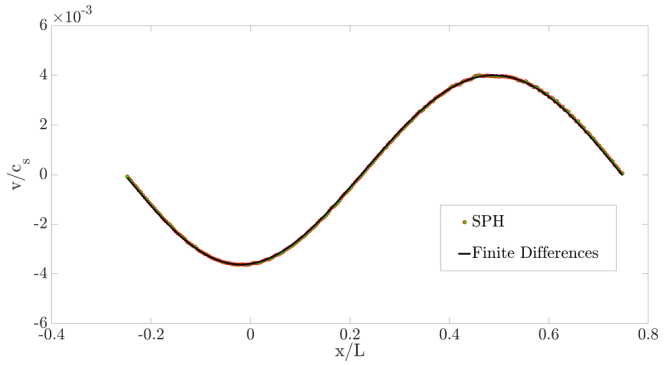


FIG. 2. Sinusoidal pulse. Velocity field, $n = 256$, $t/(L/c_0) \approx 1.22$.

Pressure p is linked to density with a linear isentropic barotropic equation of state:

$$p = c_0^2 \rho. \tag{72}$$

An initial density field is defined by perturbing the reference field with a sinusoidal function of wavelength equal to L, as

$$\frac{\rho(x)}{\rho_0} = 1 + A \sin\left(2\pi \frac{x}{L}\right), \tag{73}$$

with $A = 0.005$.

An initial velocity field, consistent with the density disturbance through the linearized sound propagation equations, representing a pressure pulse traveling to the right, is defined as

$$v(x) = c_s\left(\frac{\rho(x)}{\rho_0} - 1\right). \tag{74}$$

A test with $A\rho_0 c_0 L/\kappa = 0.05$ is discussed next. The reference solution, considered exact, is obtained with a straightforward finite-difference (FD) 1D Eulerian discretization of Eqs. (70) and (71).

Wendland's C2 kernel is used [26]. The ratio between the initial interparticle distance Δx and the smoothing length h is taken as 0.25, low enough to obtain representative SPH summations. A leap-frog time integration scheme is used [27]. The time integration step is defined based on stability criteria (see Ref. [28] for a recent investigation on the optimal value of this variable). Cases, with $n = 64$, 128, 256, and 512 particles are considered. Therefore, by taking $\Delta x = 2/n$, then $kh \sim h/W = 0.62$, 0.31, 0.16, and 0.08, respectively. Hence, the larger the n the closer the sought hydrodynamic limit $kh \to 0$. The mass of each particle is defined at time zero consistently with the density field. Equation (18) is used for the bulk viscosity term. Since the volume of particles is very similar during the time evolution, the impact of substituting this formula by the alternative Eq. (63) is negligible.

To compare SPH and the reference FD solution, the time evolution of the kinetic energy of one period will be inspected. In Fig. 1, the initial velocity field, and an example of a given particle discretization are shown. In Fig. 2 the velocity field is shown when its maximum has already noticeably decreased (20%). Time is made nondimensional with the residence time defined by the sound speed c_0 and the wavelength L. In Fig. 3 the time evolution of the kinetic energy is plotted. As can be appreciated, the agreement with the reference solution improves for increasing resolution.

B. Time decay of an accelerating-decelerating pipe flow

As a test case in two dimensions, the time decay of an accelerating-decelerating pipe flow is proposed. The fluid domain is $(x, y) \in [-x_0, x_0] \times [0, L]$ with walls at $y = 0$ and $y = L$ and inflow/outflow conditions at $x = \pm x_0$, respectively. We assume the state equation to be linear, that is $p = c_0^2(\rho - \rho_0) + p_b$ (where p_b is a background pressure) and the velocity to be $\boldsymbol{v} = [u(t, x, y), 0]$. Then, the continuity and the Navier-Stokes equation simplify as follows:

$$\begin{aligned} &\rho_t + (\rho u)_x = 0, \\ &u_t + u u_x = -c_0^2 \frac{\rho_x}{\rho} + f + (\lambda' + \nu) u_{xx} + \nu (u_{yy} + u_{xx}), \end{aligned} \tag{75}$$

where $\lambda' = \lambda/\rho$ and $\nu = \mu/\rho$ are assumed to be constant, and f is an external body force. The previous to last term in the right-hand side of Eq. (75) is the action of the bulk viscosity.

For the body force, the following field is chosen:

$$f = b\left[\frac{U_0^2}{2} \frac{\sinh(2bx)}{\cosh(bx_0)^2} \sin(ky)^2 \exp(-2\nu\alpha^2 k^2 t) - c_0^2 \tanh(bx)\right],$$

where $k = \pi/L$ (L is the wavelength in the y direction) and

$$\alpha = \sqrt{\frac{\sigma + 2}{\sigma + 3}}, \quad b = \frac{k}{\sqrt{\sigma + 2}\sqrt{\sigma + 3}}, \quad \sigma = \frac{\lambda}{\mu}. \tag{76}$$

The following solution for the velocity is obtained:

$$u(t,x,y) = U_0 \frac{\cosh(bx)}{\cosh(bx_0)} \sin(ky) \exp(-\nu\alpha^2 k^2 t), \quad \rho(t,x,y) = \frac{\rho_0}{\cosh(bx)}, \tag{77}$$

where U_0 represents the maximum velocity, which is attained at the initial instant (namely, $t = 0$) for $(x, y) = (\pm x_0, L/2)$. Note that the density depends neither on time nor on the variable y.

The Reynolds number for this test case is defined as $\mathrm{Re} = U_0 L/\nu$ and is set equal to 50. Regarding the speed of sound, c_0, it is set equal to $2U_0$, and hence the Mach number is $\mathrm{Ma} = 0.5$.

Several values of the ratio $\sigma = \lambda/\mu$ are considered, namely, $\sigma = -1, 0, 1, 10$, and the related initial velocity fields are displayed in Fig. 4. The case $\sigma = -1$ implies a null bulk viscosity or, in other words, that the Stokes' hypothesis is verified for this 2D test.

Considering the solution Eq. (77), the viscous forces on the right-hand side of Eq. (75) can be reshaped as

$$\begin{aligned} f_v :&= [(\lambda' + \nu)u_{xx} + \nu(u_{yy} + u_{xx})] = \nu u[(\sigma + 2)b^2 - k^2] \\ &= -\nu k^2 u\left[1 - \frac{1}{(\sigma + 3)}\right]. \end{aligned} \tag{78}$$

This equation shows how the viscous forces are affected by the parameter σ (i.e., by the ratio λ/μ).

In all the simulations the particles are initially positioned on a Cartesian lattice with spacing Δx, and the volumes of all particles equal to $(\Delta x)^2$. However, it is important to underline that the flow studied in this section is characterized by a divergence velocity field equal to

$$\nabla \cdot \mathbf{v}\,(t,x,y) = U_0\, b \frac{\sinh(bx)}{\cosh(bx_0)} \sin(ky) \exp(-\nu\alpha^2 k^2 t), \tag{79}$$

which, for the chosen parameters, induces a considerable change on the particles' volumes during the time evolution [see Eq. (61)]. To tackle this behavior numerically, the splitting and merging procedure described in Ref. [29] has been implemented to limit the relative variations on the particles' volumes and the related interpolation errors.

The time decay of the velocity field at the center of the fluid domain and of the total kinetic energy of the fluid are shown in Fig. 5. In all the simulations the agreement between the analytic and numerical solutions is good.

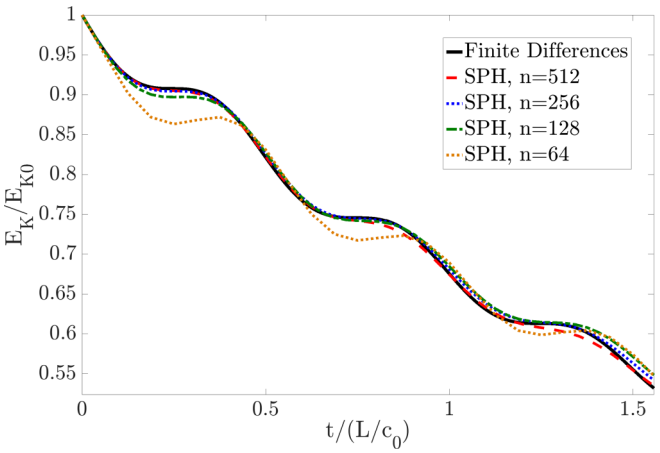


FIG. 3. One-dimensional sinusoidal pulse propagation. $A\rho_0 c_0 L/\kappa = 0.05$, $\Delta x/h = 0.25$. Kinetic energy; time history.

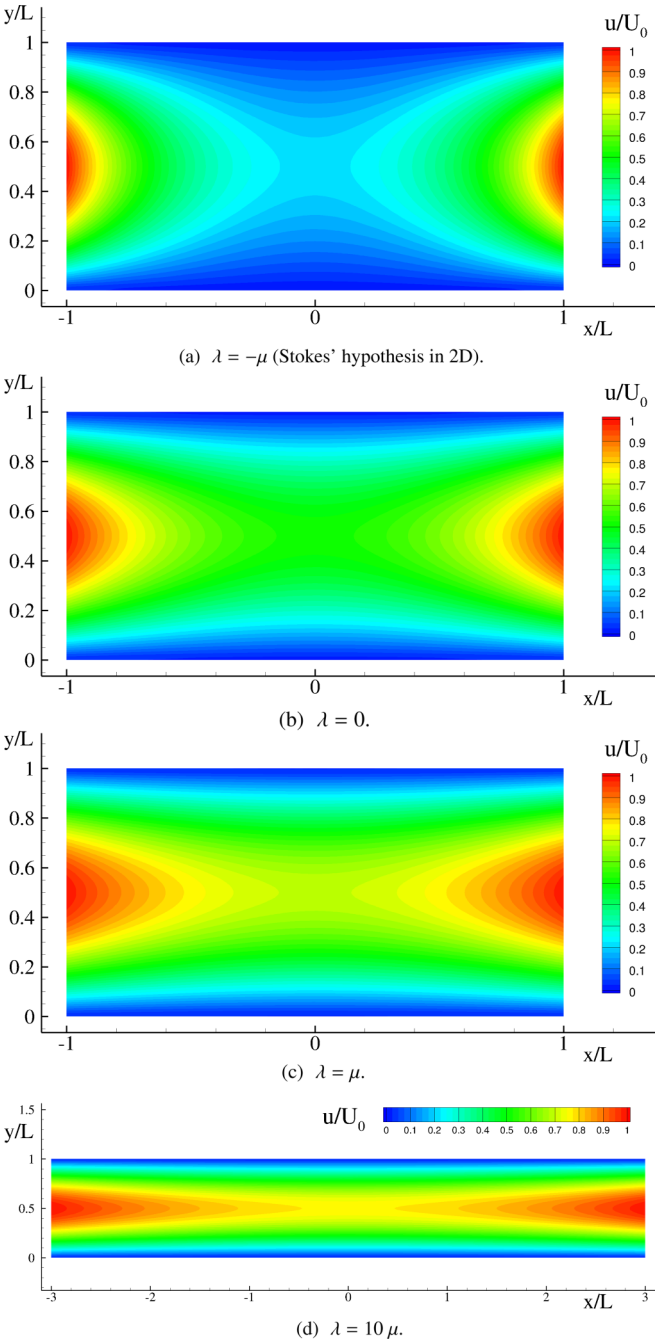
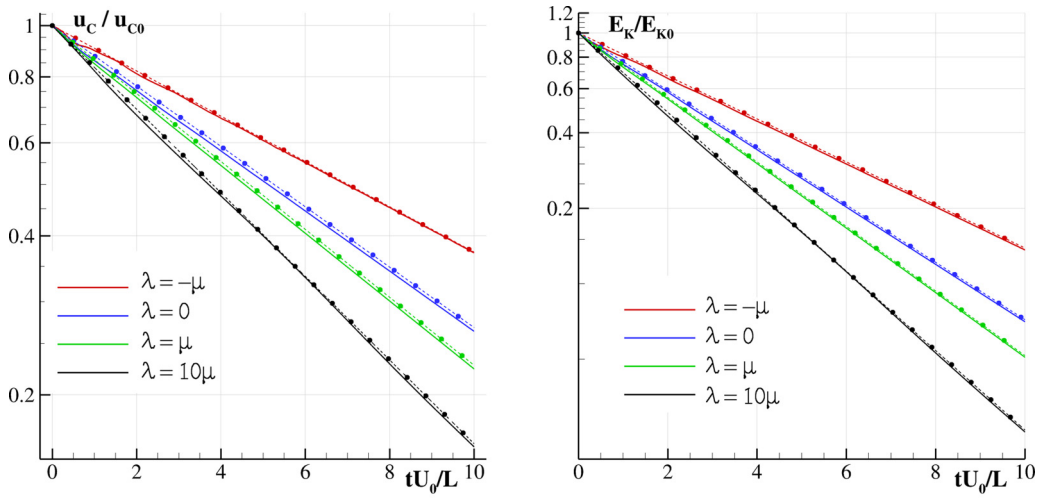


FIG. 4. Pipe flow: initial velocity field for $\mathrm{Re} = 50$ and different values of the ratio $\sigma = \lambda/\mu$.



(a) Velocity. (b) Kinetic energy.

FIG. 5. Pipe flow: time decay of the velocity at the center of the fluid domain and of the total kinetic energy for different values of the ratio $\sigma = \lambda/\mu$. The dash-dotted lines represent the analytical solutions, while the solid lines are the SPH solutions.

VI. CONCLUSIONS

A pure bulk viscosity term for smoothed particle hydrodynamics has been proposed in the present paper. The main characteristics of the new term are, on the one hand, that bulk viscosity can be modeled independently of the shear viscosity and, on the other hand, that the interparticle interaction conserves the angular momentum, in addition to the necessary linear momentum conservation. The key element of our proposed additional contribution is that the new term is proportional to the rate of change of volume of the volume element, here defined as a local estimate from the collective motion of the particles. Effectively, from the definition of the local particle density we have defined an estimate of the particle volume. The time evolution of the latter, in analogy with the continuity equation, permits us to define an estimator of $\nabla \cdot \mathbf{v}$, from which we eventually produce the dissipation term leading to this contribution to the bulk viscosity of the fluid, independently of other sources of viscous dissipation related to the shear viscosity, such as the Monaghan and Gingold's classical friction force. By construction, the newly proposed bulk viscosity term conserves the linear momentum, as required to produce the macroscopic behavior embedded into the Navier-Stokes equation. However, it also conserves the angular momentum, which is a crucial property to describe free interfaces in a dynamically consistent way, as well as situations involving free rotations of parts of the fluid. Nonconserving interactions, such as the one of Morris *et al.*, produce a spurius damping of the overall angular momentum.

From a technical point of view, we have formulated the equations for the SPH model from a bottom-up perspective, defining the interations between the particles, along the lines of Ref. [2] and references therein. As a novelty, however, we have introduced the dissipative interactions from the dissipation function, formulated along the lines of the works of Rayleigh and Onsager, which allows us to define complex dissipative behavior in a consistent manner if the restrictive conditions of validity of the minimum principle are satisfied [4,5]. The use of the dissipation function has additional advantages with regards to other approaches. In particular, the dissipation function Φ_D in Eq. (7) is Galilean invariant. As a result, the resulting force has the appropriate momentum conservation as well as is symmetric with respect to the permutation of particle indices, requiring no further symmetrization as often occurs in top-down approaches. Similarly, the angular momentum conservation of the obtained force term stems from the solid-body rotational invariance of the dissipation function.

In this article we have also explored an alternative derivation starting from the continuous Newtonian viscous term. Within this top-down analysis, together with the SPH Monaghan and Gingold shear and bulk viscosity terms, we have derived also a similar additional contribution to the bulk viscosity at the discrete level. Notably, the discretization uses the continuity equation, which is also the main starting point of the bottom-up approach described in this article. Although equivalent, the functional form of the terms in Eqs. (18) and (64) are substantially different. They produce the same macroscopic bulk viscosity, but they can present particular aspects that may be relevant depending on the applications.

Two verification cases have been proposed: the one-dimensional propagation of a sound pulse, and a two-dimensional case, modeling the time decay of an accelerating-decelerating pipe flow. The SPH solutions have been compared to exact ones, showing that the newly proposed term behaves indeed as a viscosity associated only with the local expansion-compression of the fluid. It remains as future work to apply this term for complex 3D problems in which bulk viscosity plays a relevant role.

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