

Theoretical considerations on the constitutive properties of the SPH bulk viscosity

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Abstract—The constitutive properties of the SPH bulk viscosity are discussed in this paper. To this aim, a continuum macroscopic fluid domain is initially modeled as a Hamiltonian system of discrete particles, for which the inter-particle dissipative forces are required to be radial in order to conserve the angular momentum. The resulting system of particles is then reconverted to the continuum domain via the framework of the SPH model. Since a SPH consistent approximation of the Newtonian viscous term in the momentum equation incorporates both inter-particle radial as well as non-radial terms, it is postulated that the latter must be null. In the present work it is shown that this constraint implies that first and second viscosities are equal, resulting in a positive value for the bulk viscosity, in contradiction with the Stokes' hypothesis, i.e., the zeroing of the bulk viscosity. Moreover, it is found that this postulate leads to bulk viscosity coefficients close to values found in the experimental literature for monoatomic gases and common liquids such as water.

I. INTRODUCTION

Due to their simplicity and the wide range of applications, in which they are representative of the involved physics, Newtonian fluids are the most commonly used fluid model in Physics, Chemistry and Engineering. The form of the Newtonian fluid constitutive relationship is derived starting from the idea of a Stokesian fluid (see e.g. [1]), meaning that stresses are a function of the rate-of-deformation tensor and the thermodynamic state of the system. This function is then linearized with respect to the rate-of-deformation tensor. Isotropy and homogeneity are further imposed, leading to the finalized Newtonian fluid constitutive model, in which shear and bulk viscosity coefficients play a central role.

In 1845 Stokes [2] hypothesized that the bulk viscosity coefficient could be assumed to be zero in most cases. This was done as a matter of convenience so that, for compressible flows, the normal isotropic stresses would be related only to the pressure field, and hence only to the thermodynamics of the system (see again [1]). There has been wide research, and interesting discussions in the literature, on this so-called Stokes' hypothesis (see e.g. [3]), claiming that it is correct in principle only for monatomic gases, as derived from the kinetic theory. However, as early as the 1950s, Truesdell [4] had already questioned that the Stokes hypothesis could be consistently derived from the kinetic theory of gases, and Landau and Lifshitz [5] directly argued the general

incorrectness of this assumption by using purely energetic arguments.

More recently, Rajagopal [6] has argued, from a phenomenological point of view, that the bulk viscosity can never be truly zero for realistic fluids, including monatomic gases. Moreover, experimental research (see e.g. [7], [8]) shows that the bulk viscosity is in most cases actually larger than the dynamic viscosity for liquids, e.g. twice larger in the common cases of water or methanol. Summarizing, it seems that the Stokes' hypothesis is questionable, and this translates into an ongoing debate on how to define reasonable values for the bulk viscosity coefficient and how to apply them in computational fluid dynamics simulations.

In particular, there are numerical methods such as SPH which are able to model incompressibility using a weakly compressible approach, for which the onset of spurious dissipation in general [9], [10], and spurious bulk viscosity in particular [11], [12] are sensitive topics. With the latter in mind, the Stokes' hypothesis is investigated herein by modeling a macroscopic fluid domain as a Hamiltonian system of discrete particles and, consistently, coming back to the continuum in the framework of the SPH method, leading to an exact relationship between bulk and shear viscosities. As the main original contribution of this research, we show that, for the elementary but general model presented here, shear and bulk viscosities cannot be independently modeled, and that the Stokes' hypothesis is thus inconsistent with the underlying dynamics of the fluid particles. The formulation of the SPH model from a bottom-up perspective permits us to clearly introduce underlying physical principles that ultimately support the internal consistency of the SPH model for a fluid.

II. MODELING FLUIDS AS MACROSCOPIC SYSTEMS OF DISCRETE PARTICLES

Let us consider a macroscopic system of N fluid particles in a physical space of n dimensions. Each particle represents a moving fluid element. The generic i -th particle has a position \mathbf{r}_i , velocity \mathbf{u}_i , internal energy per unit mass e_i , entropy per unit mass s_i and mass m_i . The latter is supposed to be constant with time.

Although the system is formulated in terms of particles, it is essential to realize that, on the one hand, their collective motion corresponds to the one of a fluid with well defined macroscopic properties and, as a consequence, their simulation allows one to describe the motion of a fluid comparable with experimental observations. On the other hand, the particles have to be considered as representative of lumps of a large amount of molecules which ultimately determine the physical properties of the system. This perspective permits us to consider each particle as a thermodynamic system in itself, and thus thermodynamic relations are valid at the particle level.

It is further assumed that only central forces between pairs of particles, directed along the line connecting their centers of mass, are acting as interparticle forces. No coupling between the translational motion of the particles and the possible vibrational or rotational degrees of freedom is hence considered and, therefore, their dynamics is disregarded.

The decoupling between translation and the intrinsic rotation of the fluid particles implies that the conservation of the angular momentum imposes constraints on the form of the interaction between particles. Together with Galilean invariance, these are the two conditions that permit us to define the minimal SPH model from fundamental mechanical principles. It is shown later that the definition of this minimal model for a fluid implies that shear and bulk viscosities cannot be independently modeled or, in other words, that Stokes' hypothesis would lead to an intrinsic contradiction if applied to SPH based on these two conditions.

Aiming at proving this statement, in the present section let us combine the analysis performed in the three works of Monaghan [11], Colagrossi et al. [13] and Violeau [14]. A novel interpretation of these works is conducted in this section, allowing us to build a formalism in which the discussion on the bulk viscosity in SPH is properly framed. Such formalism permits us in turn to analyze the most commonly used SPH viscous terms as particular cases of a general form for the dissipative term, something missing in the literature.

As far as the conservative dynamics is concerned, the particle system considered can be described in the framework of the Lagrangian and Hamiltonian mechanics. The Lagrangian \mathcal{L} is a state function of its N generalized coordinates $(\mathbf{r}_i, \mathbf{u}_i)$ defined, at a certain time t , as

$$\mathcal{L} = \sum_j \left[m_j \frac{u_j^2}{2} - m_j U(t, \mathbf{r}_j) - m_j e(\rho_j, s_j) \right], \quad (1)$$

where U is a generic energy potential per unit of mass whose gradient gives the force field $\mathbf{f} = -\partial U/\partial \mathbf{r}$, such as e.g. gravity. The last term in the right-hand side contains the internal energy e related to the thermodynamic part of the particle-particle interaction. The internal energy is supposed to be a function of the density and entropy fields through a suitable equation of state $e = e(\rho, s)$.

Since the system is also subject to non-conservative forces,

its dynamics is given by the equation:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \mathbf{u}_i} \right) - \frac{\partial \mathcal{L}}{\partial \mathbf{r}_i} = \mathbf{Q}_i^V + \mathbf{Q}_i, \quad (2)$$

where \mathbf{Q}_i^V are the generalized dissipative forces acting among the particles and \mathbf{Q}_i are the non-dissipative forces due to the kinematic constraints. Due to the dissipative nature of \mathbf{Q}_i^V , the inequality $(\mathbf{Q}_i^V \cdot \mathbf{u}_i) < 0$ must hold. Eventual dissipative forces related to kinematic constraints, such as those derived from no-slip boundary conditions, can be included in \mathbf{Q}_i^V . Regarding SPH, investigations on energetic considerations related to forces originating from kinematic restrictions in boundaries can be found in [15], [16]).

In order to close the system of ODEs (2) we need to specify how the thermodynamics of the system, through the internal energy of a particle, e_i , reversibly changes along with its motion. In accordance with the first law of thermodynamics, the pressure p_i of a particle is obtained through the variations of the specific internal energy as a consequence of variations of the density field:

$$p_i = - \left. \frac{\partial e_i}{\partial v_i} \right|_s = \rho_i^2 \left. \frac{\partial e_i}{\partial \rho_i} \right|_s, \quad v_i := \frac{1}{\rho_i}. \quad (3)$$

Notice that we consider only variations with $s = \text{const}$ due to the fact that the Lagrangian dynamics is only concerned with the reversible mechanical work involved with the motion of the particles.

In accordance with the second law of thermodynamics the temperature T_i of a particle is obtained as the variation of the specific internal energy as a consequence of variations of the entropy field:

$$T_i = \left. \frac{\partial e_i}{\partial s_i} \right|_v. \quad (4)$$

Under the above assumptions, substituting (1) in (2):

$$m_i \frac{d\mathbf{u}_i}{dt} - m_i \mathbf{f}_i + \sum_j m_j \left. \frac{\partial e_j}{\partial \rho_j} \right|_s \frac{\partial \rho_j}{\partial \mathbf{r}_i} = \mathbf{Q}_i^V + \mathbf{Q}_i, \quad (5)$$

and using equations (3) it becomes:

$$m_i \frac{d\mathbf{u}_i}{dt} - m_i \mathbf{f}_i + \sum_j m_j \frac{p_j}{\rho_j^2} \frac{\partial \rho_j}{\partial \mathbf{r}_i} = \mathbf{Q}_i^V + \mathbf{Q}_i. \quad (6)$$

The last term in the left-hand side in equation (6) represents the particle interactions due to the pressure forces, related to the compression-expansion work when considering the particles as thermodynamic entities, as previously defined. In order to make this term explicit, we will later define a density field connected with the particle mass distribution.

Since the pressure field is influenced by the entropy, an equation for the time variation of s is necessary to close the system of equations (6). To define it, let us consider the total energy of the system as given by:

$$\mathcal{E} = \sum_i \left[m_i \frac{u_i^2}{2} + m_i U(t, \mathbf{r}_i) + m_i e(\rho_i, s_i) \right]. \quad (7)$$

Differentiating it with respect to the time and considering the conservation of \mathcal{E} we get:

$$\dot{\mathcal{E}} = \sum_i \left[m_i \mathbf{u}_i \cdot \frac{d\mathbf{u}_i}{dt} - m_i \mathbf{u}_i \cdot \mathbf{f}_i + m_i \frac{de_i}{dt} \right] \equiv \sum_i \mathcal{Q}_i \cdot \mathbf{u}_i. \quad (8)$$

The time derivative of e_i can be expressed as:

$$\frac{de_i}{dt} = \frac{\partial e_i}{\partial \rho_i} \Big|_s \frac{d\rho_i}{dt} + \frac{\partial e_i}{\partial s_i} \Big|_V \frac{ds_i}{dt} = \frac{p_i}{\rho_i^2} \sum_j \left[\frac{\partial \rho_i}{\partial \mathbf{r}_j} \cdot \mathbf{u}_j \right] + T_i \frac{ds_i}{dt}, \quad (9)$$

where equations (3) and (4) have been used together with the continuity equation:

$$\frac{d\rho_i}{dt} = \sum_j \left[\frac{\partial \rho_i}{\partial \mathbf{r}_j} \cdot \mathbf{u}_j \right]. \quad (10)$$

Multiplying eq. (6) by \mathbf{u}_i and substituting in (8) together with eq. (9), we finally get:

$$\sum_i \left[\mathcal{Q}_i^V \cdot \mathbf{u}_i + m_i T_i \frac{ds_i}{dt} \right] = 0. \quad (11)$$

Equation (11) states that the work done by the dissipative forces increases the entropy of the system, which is translated into an increase of the temperature of the particles.

Based on the above considerations, an equation governing the change of entropy of each particle is proposed:

$$m_i T_i \frac{ds_i}{dt} = -\mathbf{u}_i \cdot \mathcal{Q}_i^V + \mathbf{q}_i, \quad (12)$$

where we have introduced \mathbf{q}_i to describe the heat flux exchanged by particle i with the surroundings. In addition of its modelling, not treated in this work (the reader is addressed to *e.g.* [11], [17]), the \mathbf{q}_i should satisfy the condition $\sum_i \mathbf{q}_i = 0$ in order to maintain the overall energy conservation.

Notice that, unlike in a Dissipative Particle Dynamics (DPD) model (see *e.g.* [18], [19]), in the SPH context the fluid particles are large enough so as not to observe thermal agitation. Hence, the case where all the terms \mathcal{Q}_i and \mathcal{Q}_i^V are set to zero effectively corresponds to a discrete model of an inviscid fluid. Extensions of the original SPH model to include the thermal agitation initiated in ref. [20], referred to as SDPD for Smoothed Dissipative Particle Dynamics, and have been applied to simulate the diffusion motion of colloidal suspensions of rigid particles [21]. Additional considerations on energy aspects of the Lagrangian framework in particle methods can be found in [22], [23] and [24].

A. Density field approximation within the SPH model

In SPH, a density field is associated to a discrete mass distribution chosen arbitrarily (see *e.g.* [25]). Here, following [20], the density of a generic i -th particle is defined as:

$$\rho_i = m_i \sum_j W(\mathbf{r}_j - \mathbf{r}_i; h), \quad (13)$$

where W is the kernel and h the smoothing length. Notice that in (13) the mass of the particle is left out of the summation. W

monotonously decreases with the distance $r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j|$. The kernel considered in this study is spherical, thus depending only on r_{ij} . Hereinafter we adopt the notation $W_{ij} = W(r_{ij}; h)$. Regarding the spatial derivative of W , due to the above properties it is possible to write:

$$\nabla_i W_{ij} = (\mathbf{r}_i - \mathbf{r}_j) \frac{1}{r_{ij}} \frac{dW}{dr_{ij}} = -\mathbf{r}_{ij} F(r_{ij}). \quad (14)$$

Because of W 's properties, the function $F(r_{ij})$ is always positive. Furthermore, W integrates to one and the following relations hold:

$$\int_0^\infty r^{n-1} W(r) dr = C_n, \quad \int_0^\infty F(r) r^{n+1} dr = -C_n n, \\ C_1 = 1/2, \quad C_2 = 1/(2\pi), \quad C_3 = 1/(4\pi). \quad (15)$$

Through eq. (13), the mass m_i is ‘‘smoothed’’ in the neighborhood of the particle i accounting for the positions of the surrounding particles through the weights given by W_{ij} . As a consequence, a particle volume V_i can be assigned to the i -th particle as:

$$V_i = 1/ \sum_j W_{ij}. \quad (16)$$

Consequently, a geometrical size of the particle can be assigned as:

$$\Delta r_i = \sqrt[n]{V_i}. \quad (17)$$

In the following, the average size of the particles will be indicated with Δr . When performing the limit $\Delta r \rightarrow 0$, it is understood that the number of particles goes to infinity and that the volume of all particles decreases homogeneously.

It is important to underline that the volumes (16) are not connected to any tessellation of the geometrical space covered by the particles set. Indeed the volume subdivision obtained with (16) is not a Partition-of-Unity or, in other words, the sum $\sum_j V_j$ does not coincide with the geometrical volume occupied by the system, but is an estimate obtained from the local particle density, which is expected not to significantly differ from the physical volume. The volumes V_i are referred to in [20] as ‘‘thermodynamic volumes’’, but actually this is only an indirect way to determine the particle’s density, which is a physical property necessary to eventually determine the particle’s pressure needed for the dynamic evolution, according to eq. (6). However, thanks to the properties (15) of W , the Partition-of-Unity is recovered in the limit $\Delta r/h \rightarrow 0$.

As remarked in [26], [27] and [28], when considering the limit process from the discrete particle system to a continuous model, two limits need to be taken into account: (i) the limit $\Delta r/h \rightarrow 0$, which states that the particles sizes need to go to zero faster than the kernel length, and (ii) the limit linked to the kernel length scale $h \rightarrow 0$.

B. SPH equation for the motion of particles

Introducing (13) in (6) and substituting the particle volumes (16), the general case leads to:

$$\frac{d\mathbf{u}_i}{dt} = \frac{1}{\rho_i} \sum_j \left[\frac{p_j V_j^2 + p_i V_i^2}{V_i V_j} \right] \mathbf{r}_{ij} F(r_{ij}) V_j + \mathbf{f}_i + \frac{\mathbf{Q}_i^V + \mathbf{Q}_i}{m_i}. \quad (18)$$

Considering the limit from discrete particles to continuum media, *i.e.* $h \rightarrow 0$ & $\Delta r/h \rightarrow 0$, it is possible to show (see *e.g.* [29]) that equation (18) converges, as it should, to the Euler momentum conservation equation for an inviscid fluid (*i.e.* $\mathbf{Q}^V = 0$):

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \nabla p + \mathbf{f}, \quad (19)$$

where the effects related to the generalized forces, \mathbf{Q}_i , and their eventual links with the boundary conditions, are, for the sake of simplicity, disregarded.

C. Dissipative force in a Lagrangian particle model

In order to close the ODEs for the dynamics of the particle system (2), the dissipative forces need to be modeled. Following the pioneering work of Rayleigh, reviewed in detail by Grenier et al. [30], dissipative forces \mathbf{Q}_i^V can be derived from a variational principle involving the so-called dissipation function Φ_D . The dissipation function may be expressed as a quadratic form of the relative particle velocities, $\mathbf{u}_{ij} = \mathbf{u}_i - \mathbf{u}_j$:

$$\Phi_D = \frac{1}{2} \sum_i \sum_j \mathbf{u}_{ij} \cdot \mathbb{A}_{ij}(r_{ij}) \cdot \mathbf{u}_{ij}, \quad (20)$$

where the \mathbb{A}_{ij} are symmetric tensors with respect to the particle indexes, $\mathbb{A}_{ij} = \mathbb{A}_{ji}$, to ensure the action-reaction principle. Moreover, to comply with the requirements of the second principle of thermodynamics, Φ_D must be positive definite [31] (see appendix in [32]). According to this assumption, the generalized force in the equation (2) takes the form [30]:

$$\mathbf{Q}_i^V = -\frac{\partial \Phi_D}{\partial \mathbf{u}_i} = -\sum_j \mathbb{A}_{ij}(r_{ij}) \cdot \mathbf{u}_{ij}, \quad (21)$$

where we have implicitly assumed that $\mathbb{A}_{ij}(r_{ij})$ are symmetric matrices themselves, *i.e.* $\mathbb{A}_{ij}(r_{ij}) = \mathbb{A}_{ij}^T(r_{ij})$ that, apart from these general considerations, have to be appropriately specified. From now on, the dependence of these matrices on the distance modulus will be implicitly assumed.

Following [14], a first constraint comes from imposing that the friction forces must be null if the particle system moves with a rigid body motion. This constraint reduces the possible choice of the tensor \mathbb{A}_{ij} to the following form:

$$\mathbb{A}_{ij} = \boldsymbol{\gamma}_{ij} \otimes \mathbf{r}_{ij}, \quad (22)$$

where $\boldsymbol{\gamma}_{ij}$ is an antisymmetric vector with respect to indexes i, j to comply with the symmetry of \mathbb{A}_{ij} .

A second constraint follows from enforcing the conservation of the total angular momentum on the particle system; in such a case the vector $\mathbb{A}_{ij} \cdot \mathbf{u}_{ij}$ must be collinear with \mathbf{r}_{ij} , hence :

$$\mathbb{A}_{ij} = \mathbf{r}_{ij} \otimes \boldsymbol{\gamma}'_{ij}, \quad (23)$$

where $\boldsymbol{\gamma}'_{ij}$ is another antisymmetric vector.

It must be stressed that this is a key point of the present work. Indeed the collinearity of the elementary dissipative forces $\mathbb{A}_{ij} \mathbf{u}_{ij}$ with the vector position \mathbf{r}_{ij} means that we are treating the interactions between the particles similarly to what happens at the atomistic scale. This is linked to the assumption that rotation in the particles cannot be excited by the forces considered, thus implying that, in order to ensure angular momentum conservation, the constraint (23) must be satisfied.

Having to hold the conditions (23) and (22) simultaneously, the vectors $\boldsymbol{\gamma}_{ij}$ must linearly depend on \mathbf{r}_{ij} , namely $\boldsymbol{\gamma}_{ij} = \gamma_{ij} \mathbf{r}_{ij}$, through some scalar coefficients γ_{ij} , so that the final form of the matrices is obtained:

$$\mathbb{A}_{ij} = \gamma_{ij}(r_{ij}) (\mathbf{r}_{ij} \otimes \mathbf{r}_{ij}), \quad (24)$$

where the symmetry of the scalars γ_{ij} follows from the symmetry properties of \mathbb{A}_{ij} with respect to the particles indexes (*i.e.* $\gamma_{ij} = \gamma_{ji}$).

The specification (24) of \mathbb{A}_{ij} allows to express:

$$\mathbf{Q}_i^V = -\sum_j \gamma_{ij}(r_{ij}) (\mathbf{u}_{ij} \cdot \mathbf{r}_{ij}) \mathbf{r}_{ij}. \quad (25)$$

Similarly to the derivation of the pressure forces (see eq. (18)), also the dependence of the dissipative forces on the volume of the particles must be consistently introduced in order to preserve the momenta conservation as:

$$\mathbf{Q}_i^V = -\sum_j \hat{\gamma}_{ij}(r_{ij}) (\mathbf{u}_{ij} \cdot \mathbf{r}_{ij}) \mathbf{r}_{ij} V_i V_j. \quad (26)$$

The dependence of the dissipation force between particles on their relative distance r_{ij} implies that the coefficients $\hat{\gamma}_{ij}(r_{ij})$ must be specified in a coherent way. Indeed, in the limit $\Delta r \rightarrow 0$, the specific force:

$$\mathbf{f}^V(\mathbf{r}_i) = \frac{\mathbf{Q}_i^V}{V_i} = \sum_j \hat{\gamma}_{ij}(r_{ij}) (\mathbf{u}_{ij} \cdot \mathbf{r}_{ij}) \mathbf{r}_{ij} V_j \quad (27)$$

must remain finite. This argument suggests that $\hat{\gamma}_{ij}$ must diverge with the square of the distance r_{ij} , *i.e.*,

$$\hat{\gamma}_{ij}(r_{ij}) = \frac{g_{ij}(r_{ij})}{r_{ij}^2} \quad \text{with} \quad \lim_{r_{ij} \rightarrow 0} g_{ij}(r_{ij}) = g_{ii} > 0, \quad (28)$$

where the condition of positiveness of g_{ii} guarantees the positive definiteness of the tensor \mathbb{A}_{ij} . This latter condition is consistent with the total energy decreasing with time and must be fulfilled, in any case, independently from the argument used to define a particular form of the matrices (for details see see [14] and the appendix in [32]).

By substituting the latter definition in the expression (25), the final form of the dissipative force is obtained:

$$\mathbf{Q}_i^V = -\sum_j g_{ij}(r_{ij}) (\mathbf{u}_{ij} \cdot \mathbf{e}_{ij}) \mathbf{e}_{ij} V_i V_j, \quad (29)$$

where $\mathbf{e}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$ are unit vectors.

D. The dissipation forces in the SPH model and the related intrinsic bulk viscosity

Now the problem stands in finding a suitable way to express the coefficients g_{ij} . Similarly to what is done for the pressure forces, the SPH Kernel function is also used to model the dissipative forces.

To simplify the problem at hand, it may be foremost assumed that g_{ij} does not depend on the specific couple of particles considered, but only on their relative distance: $g_{ij}(r_{ij}) = g(r_{ij})$. Moreover, it may be considered that in equation (18) the pressure force term between two generic particles is collinear with the relative distance \mathbf{r}_{ij} and proportional to the product of the SPH Kernel gradient $F(r_{ij})$ with the particle volumes, so that a similar relation may be assumed valid for the dissipative force:

$$g(r_{ij}) = C F(r_{ij}), \quad (30)$$

where the value of the coefficient C , which has the same dimensions of a dynamic viscosity, is uniform in the flow field and $F(r_{ij})$ is strictly positive for each pair i, j . Assuming the form (30), the dissipative force becomes:

$$\mathbf{Q}_i^V = -C \sum_j F(r_{ij}) (\mathbf{u}_{ij} \cdot \mathbf{e}_{ij}) \mathbf{e}_{ij} V_i V_j. \quad (31)$$

In order to close the procedure, the constant C in eq. (31) must be addressed. To this aim, the passage from a discrete to a continuum description with the procedure followed in [13] is again brought forth, in which the limit $\Delta r/h \rightarrow 0$ is firstly considered and the limit $h \rightarrow 0$ is performed as a second step.

After the first limit passage, the summation in (31) is converted into an integral where the generic particle position \mathbf{r}_i becomes a generic point \mathbf{r} of the fluid domain Ω whereas the inter-particle \mathbf{r}_{ij} becomes the vector \mathbf{r}' ; the specific force defined in eq. (27) is then given by:

$$\mathbf{f}^V(\mathbf{r}) = C \int_{\Omega} F(r') \frac{[\mathbf{u}(\mathbf{r} + \mathbf{r}') - \mathbf{u}(\mathbf{r})] \cdot \mathbf{r}'}{r'^2} \mathbf{r}' dV', \quad (32)$$

where the fluid domain Ω is here considered unbounded.

In such a condition the relative velocity is expanded using a Taylor series:

$$\mathbf{u}(\mathbf{r} + \mathbf{r}') - \mathbf{u}(\mathbf{r}) = \nabla \mathbf{u}|_{\mathbf{r}} \cdot \mathbf{r}' + \frac{1}{2} \mathbf{r}' \cdot \mathbf{H}_r \cdot \mathbf{r}' + O(r'^3), \quad (33)$$

where \mathbf{H} is the Hessian tensor.

By substituting the expression (33) into (32), the following definition is obtained :

$$\mathbf{f}^V(\mathbf{r}) = C \left[\int_{\Omega} \frac{\mathbf{r}' \otimes \mathbf{r}' \otimes \mathbf{r}'}{r'^2} F(r') dV' \right] \mathbf{D}_r + \frac{C}{2} \left[\int_{\Omega} \frac{\mathbf{r}' \otimes \mathbf{r}' \otimes \mathbf{r}' \otimes \mathbf{r}'}{r'^2} F(r') dV' \right] \mathbf{H}_r + O(h), \quad (34)$$

where \mathbf{D} is the rate of deformation tensor.

For an unbounded domain, thanks to the kernel function isotropy, the error passes from first to second order. The first

term in the right-hand side of (34) is analyzed in detail in [13], where, using spherical coordinates, it was split in various independent factors, and demonstrated to be null.

Defining the following fourth order tensor:

$$\mathbb{G} := \frac{C}{2} \int_{\Omega} \frac{\mathbf{r}' \otimes \mathbf{r}' \otimes \mathbf{r}' \otimes \mathbf{r}'}{r'^2} F(r') dV' \quad (35)$$

the dissipation force field at the position \mathbf{r} can be rewritten as:

$$\mathbf{f}^V(\mathbf{r}) = \mathbb{G} \mathbf{H}_r + O(h^2) \quad (36)$$

The tensor \mathbb{G} does not depend on the particular Kernel function used, provided the normalization relations (15) are fulfilled.

As demonstrated in [13], the relation (36) becomes:

$$\mathbf{f}^V(\mathbf{r}) = \frac{C}{2(n+2)} \nabla^2 \mathbf{u}(\mathbf{r}) + \frac{C}{(n+2)} \nabla (\nabla \cdot \mathbf{u})(\mathbf{r}) + O(h^2). \quad (37)$$

Finally, considering the limit $h \rightarrow 0$ and comparing the above expression with the viscous force for a Newtonian fluid:

$$\mathbf{f}^V = \mu \nabla^2 \mathbf{u} + (\mu + \lambda) \nabla (\nabla \cdot \mathbf{u}), \quad (38)$$

the meaning of the quantity $C = 2(n+2)\mu$ becomes evident.

Furthermore, from this analysis, it results that the secondary viscosity λ is equal to μ , and therefore the bulk viscosity κ :

$$\kappa = \lambda + \frac{2\mu}{n}, \quad (39)$$

in the SPH model is fixed to the value:

$$\kappa = \mu (1 + 2/n) \quad \boxed{\text{Bulk viscosity in the SPH model}} \quad (40)$$

Therefore, the bulk viscosity is $\kappa = 2\mu$ and $\kappa = 5\mu/3$ in a 2D and a 3D framework respectively. (40) indicates that in the customary formulation of the SPH model based on interparticle central forces, bulk and shear viscosity cannot be independently modeled.

E. The Monaghan-Cleary-Gingold's and the Morris' formulations

Coming back to the particle system, once the constant C is derived, the dissipative force (31) acting on the generic particle i is given by the formula:

$$\mathbf{Q}_i^V = -\mu 2(n+2) \sum_j F(r_{ij}) (\mathbf{u}_{ij} \cdot \mathbf{e}_{ij}) \mathbf{e}_{ij} V_i V_j, \quad (41)$$

which resembles the formula derived for the SPH model by Monaghan&Gingold [33]. In that work the authors derived an artificial viscous term for stabilizing the SPH model around shock waves setting the constant $C = \alpha c h$ where α is a non-dimensional parameter and c is the speed of sound of the considered medium. Furthermore, in that work the inter-particle force is set equal to zero when $(\mathbf{u}_{ij} \cdot \mathbf{r}_{ij})$ is positive, in order to mimic a Neumann-Richtmyer viscosity (see [34]).

The authors paid attention to writing an expression which, on the one hand, is invariant for Galilean transformations and, on the other, conserves the angular momentum of the particle system. Again, the use of these two constraints led these authors to analogous conditions as expressed in (22-23), and arrive in eq. (41) to the same structure as given in (29).

It is interesting to underline that, only after many years, Prof. Monaghan, Dr. Cleary and other researchers found the link between the artificial bulk viscosity, introduced for numerical stability reasons, and the real viscous force for the kind of Newtonian fluid they were implicitly implementing, modifying the original formula into the aforementioned eq. (41) (see *e.g.* [35], [36], [11], [37], and in particular [38] for a genealogy of the various SPH viscous formulae). It is also interesting to mention that even in the weakly compressible formulations, the bulk viscosity term has usually been neglected in the governing equations, on the grounds that since the velocity divergence should be small, the term could be considered negligible. A relevant outcome of present research is to highlight the fact that such bulk viscosity term is actually present when using the Monaghan-Cleary-Gingold's formula, and, as will be later seen, with actual values similar to those found in a number of important fluids.

Another formulation widely used within the SPH framework is the one introduced by Morris et al. [39]. In this case the dissipation forces among the particles are supposed to be collinear with the relative velocity \mathbf{u}_{ij} , which is equivalent to merely define the matrices $\mathbf{A}_{ij}(r_{ij})$ in (20) as:

$$\mathbf{A}_{ij}(r_{ij}) = \gamma_{ij}(r_{ij}) \mathbf{I}, \quad (42)$$

$$\gamma_{ij}(r_{ij}) = g_{ij}(r_{ij}) V_i V_j, \quad (43)$$

where \mathbf{I} is the identity matrix. It is worth to stress that, unlike the former case, none of the two constraints (23) and (22) are satisfied. However, the condition of positive definiteness of the matrices must hold also in this case. Through the same assumption of (30) for the function g_{ij} , the viscous force is written as follows:

$$\mathbf{Q}_i^V = -C \sum_j F(r_{ij}) \mathbf{u}_{ij} V_i V_j \quad (44)$$

This form of the dissipative force obviously violates the conservation of angular momentum. In the limit $\Delta r/h \rightarrow 0$, the viscous dissipation force field becomes:

$$\mathbf{f}^V(\mathbf{r}) = C \int_{\Omega} F(r') [\mathbf{u}(\mathbf{r}' + \mathbf{r}) - \mathbf{u}(\mathbf{r})] dV' \quad (45)$$

By expanding in Taylor series the velocity difference in the integrand, as in the (33), the following expression is obtained:

$$\mathbf{f}^V(\mathbf{r}) = C \nabla \mathbf{u}_r \cdot \int_{\Omega} \mathbf{r}' F(r') dV' + \left[\frac{C}{2} \int_{\Omega} (\mathbf{r}' \otimes \mathbf{r}') F(r') dV' \right] \mathbf{H}_r + O(h) \quad (46)$$

for an unbounded domain the first term on the right-hand side is zero and the error becomes $O(h^2)$. The second order tensor in the second term:

$$\mathbf{M} := \int_{\Omega} (\mathbf{r}' \otimes \mathbf{r}') F(r') dV' \quad (47)$$

results to be equal to the identity tensor, i.e. $\mathbf{M} = \mathbf{I}$, once considered the normalization relations (15). The dissipation force field at the position \mathbf{r} can be rewritten as:

$$\mathbf{f}^V(\mathbf{r}) = \frac{C}{2} \mathbf{H}_r \mathbf{I} + O(h^2) = \frac{C}{2} \nabla^2 \mathbf{u}(\mathbf{r}) + O(h^2) \quad (48)$$

Summarizing, considering the limit $h \rightarrow 0$ and comparing the above formula with the viscous force for an incompressible Newtonian fluid, we finally get $C = 2\mu$.

This means that with this second formulation of the viscous forces, where the dissipation forces among the particles are supposed to be collinear with the relative velocity, it is not possible to take into account the viscosity related to the compressibility. Therefore, the lack of conservation of the angular momentum in the inter particle dissipative interaction, which led us to the conditions (23) and (22), yields a model that does not naturally display a bulk viscosity.

Independently of this matter, it is shown in [13] that, due to consistency issues, the Morris et al. formulation (44) should not be applied to viscous free-surface flows (it renders inaccurate dissipation in the integral limit). Moreover, this aspect does not depend on whether a weakly compressible or a pure incompressible model is used. On the other hand, in the same reference [13] it is shown that this inconsistency is fortunately not present when the Monaghan-Cleary-Gingold's term is used.

The conclusions derived in this article can also be extended to the SDPD context. This implies that non-conservation of the angular momentum due to the collinearity of the dissipative forces with the relative velocity between particles \mathbf{u}_{ij} leads to models that exhibit the same drawbacks as discussed above for the purely SPH models within Morris formulation [20]. Therefore, to construct a model in which the shear and bulk viscosities could be independently modeled, the particles have to admit a larger number of degrees of freedom coupled with the overall motion of the system. Recently, in ref. [40] a SDPD model involving the dynamic coupling between translation and the intrinsic rotation of the particles (spin) was developed to study the motion of vesicles in a fluid. This model permits the conservation of the total angular momentum even though the friction forces depend on the relative velocity between particles \mathbf{u}_{ij} . Bender et al. [41], in the context of computer graphics, developed an alternative angular momentum conservative SPH formulation to generate flow fields with enhanced turbulence levels. To this aim, they included the particle rotation as a material variable whose evolution in time is tracked, as velocity and density.

III. DISCRETIZATION OF THE NEWTONIAN VISCOUS TERM THROUGH INTEGRAL INTERPOLATION

The analysis performed in the previous section can be made in a second way, considering the viscous term of the Navier-Stokes equation (38), and discretizing it through convolution integrals with the Kernel function introduced for the SPH model in II-A. This approach has been developed in [20], where the authors write a viscous term which is a combination of the two formulations (41) and (44) derived in the previous section, and leads to the same conclusion regarding the relative value of bulk and shear viscosity. The reader is referred to [32] for further details.

IV. DISCUSSION & CONCLUSIONS

Considering a macroscopic model for a fluid as a discrete set of particles with interactions that conserve linear and angular momentum and that are invariant to Galilean transformation, a consistent discretization of the continuous Newtonian viscous term written in the SPH method has been established. It has been deduced that such consistently constructed model leads to a certain intrinsic relation between the bulk and shear viscosities, namely $\kappa = (1 + 2/n) \mu$, which in addition implies that κ and μ are of the same order of magnitude. Therefore, invoking Stokes' hypothesis, $\kappa = 0$, for a SPH model is not consistent with the linear and angular momentum conservation.

Moreover, against the general validity of Stokes' hypothesis, there is experimental evidence (e.g., [7], [8]) indicating that the bulk viscosity is of the order of the dynamic viscosity for common liquids such as water ($\kappa/\mu = 2.70$) and alcohols such as methanol ($\kappa/\mu = 1.47$), ethanol ($\kappa/\mu = 1.30$), 2-propanol ($\kappa/\mu = 1.32$), etc. These facts are in support of the present prediction, $\kappa/\mu = 1.67$.

It has to be remarked that in the model considered, the SPH particles are not allowed to rotate neither vibrate around their center of mass. More precisely, they inherit the property assumed for the Hamiltonian particle model referred to the particles' inability to couple their rotation and vibration modes with the translational one. Since monoatomic gases (the only stable ones in standard temperature and pressure conditions are the noble gases) and monoatomic liquids (mercury is the only monoatomic liquid at standard ambient conditions), are likely to have translational motions decoupled from rotations and vibrations in a wide range of thermodynamic conditions, it is reasonable to expect, from the arguments given in this article, that their bulk viscosity is not zero but of the same order of magnitude as their shear viscosity. As a matter of fact, references such as [42], [43] document similar values of shear and bulk viscosity ($\kappa/\mu \sim 1$) for fluids such as argon, xenon and krypton in near saturation conditions, and the theoretical work [44] predicts that $\kappa/\mu \sim 1.5$ for mercury, close to the one obtained in the present research.

Regarding the relative magnitude of shear and bulk viscosities, there is also experimental evidence about Newtonian fluids with ratios between bulk and shear viscosity much larger than unity (of the order of 10 for Toluene and Hexane in liquid form [7], [8] or of the order of a thousand for CO₂ or N₂O [44] polyatomic gases). This challenges Stokes' hypothesis but also questions the range of validity of the ratio obtained in the present article for the simple SPH model. Such experiments thus suggest that the referred particle's "internal" degrees of freedom must play a relevant role in determining the actual ratio of bulk to shear viscosity for this type of fluids (see e.g. [45]).

Therefore, the intrinsic relationship between shear and bulk viscosities seems to lie in the decoupling between translation and the dynamics of internal degrees of freedom of the particles, together with the need to comply with general

physical laws such as the conservation of linear and angular momentum. The general proof of this statement goes beyond the range of validity of the analysis given in this article, but similar conclusions are also encountered in analogous studies. Effectively, if one takes the standard DPD model as an example, it also represents a fluid in which bulk and shear viscosities are related. As compared with the present SPH model, DPD particles are subject to thermal agitation, unlike SPH. Although the two models share the presence of dissipative forces satisfying constraints (23) and (22) and, consequently, preserve angular momentum, the DPD fluid has an additional so-called kinetic contribution to the viscous dissipation. The viscosities of the standard DPD model are hence given by the sum of the regular dissipative contribution and the referred kinetic one. Following the analysis of Marsh [46], based on a Boltzmann-like equation for the DPD system, the dissipative contribution is found to satisfy exactly the same ratio (40) (cf. eq. (78) of [46]). The same ratio was also found later in ref. [47], for the energy conserving DPD, but using linear response theory.

Notwithstanding that the kinetic contribution has no counterpart in SPH, a DPD estimate of this contribution found by Marsh [46], $\kappa_K = 2\mu_K/n$ (cf. eq. (70) of this last reference), even providing a different ratio than equation (40), indicates that the kinetic contribution related bulk and shear viscosities are also proportional, and of the same order. Within the context of SDPD, Bian et al. [48]'s numerical calculations of the transport coefficients using correlation functions [49] led to values of bulk viscosity of the same order like the shear one, in line with the referred DPD estimates.

It has to be finally mentioned that the influence of bulk viscosity terms in the dynamics is negligible in most cases. The reasons are, first, the small relative value of κ times the velocity divergence as compared to the work done by the pressure due to compression-expansion, when it comes to modifying normal forces [3], and, second, the small relative value of the viscous dissipation due to bulk viscosity when compared to the one due to shear, in nearly incompressible flows [12]. Clarifying this small relative importance while also understanding that in fluids like water the coefficients themselves are however of the same order, is in our opinion a relevant contribution of present investigations for researchers which deal with bulk viscosity terms in their numerical approximations to the conservation equations. In addition to the considerations presented in this paper, some details not discussed herein can be found in [32].

Finally, for the weakly-compressible SPH practitioners present in this workshop, this paper can be useful in order to understand the SPH bulk viscosity term not as a spurious side-effect of the weakly-compressibility assumption, but as yet another case in which the SPH model is able to retain fundamental physical aspects of the problems at hand.

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