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Discussion of Stokes' hypothesis through the smoothed particle hydrodynamics model

Andrea Colagrossi[*]

CNR-INSEAN, Marine Technology Research Institute,

Rome, Italy and

Ecole Centrale Nantes,

LHEEA Lab., Nantes, France

Danilo Durante

CNR-INSEAN, Marine Technology Research Institute, Rome, Italy

Josep Bonet Avalos

Department d'Enginyeria Química, ETSEQ,

Universitat Rovira i Virgili, Tarragona, Spain

Antonio Souto-Iglesias

CEHINAV, DMFPA, ETSIN,

Universidad Politécnica de Madrid, Madrid, Spain

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Abstract

Stokes' hypothesis, the zeroing of the bulk viscosity in a Newtonian fluid, is 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 Smoothed Particle Hydrodynamics (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 cited Stokes' hypothesis. 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.

*Electronic address: andrea.colagrossi@cnr.it

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. Aris [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 Aris [1]). There has been wide research, and interesting discussions in the literature, on this so-called Stokes' hypothesis (see e.g. Buresti [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. Rosenhead [7], Dukhin and Goetz [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 new numerical methods, such as Smoothed Particle Hydrodynamics (SPH), which are able to model incompressible Navier-Stokes dynamics using a weakly compressible approach, for which the onset of spurious dissipation in general [9, 10], and spurious bulk viscosity [11, 12] related terms and dissipation in particular, 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.

For the sake of clearness, we apprise the reader that the indexes i, j are referred to the particle labels, while vectors and tensors are always written in their implicit form without using indexes of coordinates.

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 $\boldsymbol{r}_i$, velocity $\boldsymbol{u}_i$, 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 (r_i, u_i) defined, at a certain time t, as

$$\mathcal{L} = \sum_j \left[m_j \frac{u_j^2}{2} - m_j U(t, r_j) - m_j e(\rho_j, s_j) \right], \tag{II.1}$$

where U is a generic energy potential per unit of mass whose gradient gives the force field $f = -\partial U/\partial r$, 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:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial u_i} \right) - \frac{\partial \mathcal{L}}{\partial r_i} = Q_i^V + Q_i, \tag{II.2}$$

where Q_i^V are the generalized dissipative forces acting among the particles and Q_i are the non-dissipative forces due to the kinematic constraints. Due to the dissipative nature of Q_i^V, the inequality $(Q_i^V \cdot u_i) < 0$ must hold. Eventual dissipative forces related to kinematic constraints, such as those derived from no-slip boundary conditions, can be included in Q_i^V. A specific investigation on energetic considerations related to forces originating from kinematic restrictions in fixed and moving boundaries, in the SPH context, can be found in [15, 16]).

In order to close the system of ODEs (II.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

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the variations of the specific internal energy as a consequence of variations of the density field:

$$p_i = -\left.\frac{\partial e_i}{\partial v_i}\right|_s = \rho_i^2 \left.\frac{\partial e_i}{\partial \rho_i}\right|_s, \qquad v_i := \frac{1}{\rho_i}. \tag{II.3}$$

Notice that we consider only variations with $s = const$ 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:

$$T_i = \left.\frac{\partial e_i}{\partial s_i}\right|_V. \tag{II.4}$$

Under the above assumptions, substituting (II.1) in (II.2), we get:

$$m_i \frac{d\boldsymbol{u}_i}{dt} - m_i \boldsymbol{f}_i + \sum_j m_j \left.\frac{\partial e_j}{\partial \rho_j}\right|_s \frac{\partial \rho_j}{\partial \boldsymbol{r}_i} = Q_i^V + Q_i, \tag{II.5}$$

and using equations (II.3) it becomes:

$$m_i \frac{d\boldsymbol{u}_i}{dt} - m_i \boldsymbol{f}_i + \sum_j m_j \frac{p_j}{\rho_j^2} \frac{\partial \rho_j}{\partial \boldsymbol{r}_i} = Q_i^V + Q_i. \tag{II.6}$$

The last term in the left-hand side in equation (II.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 need to define a density field connected with the particle mass distribution (see section II A).

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 (II.6). To define it, let us consider the total energy of the system as given by:

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

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

$$\dot{\mathcal{E}} = \sum_i \left[m_i \boldsymbol{u}_i \cdot \frac{d\boldsymbol{u}_i}{dt} - m_i \boldsymbol{u}_i \cdot \boldsymbol{f}_i + m_i \frac{d e_i}{dt} \right] \equiv \sum_i Q_i \cdot \boldsymbol{u}_i. \tag{II.8}$$

The time derivative of the internal energy can be expressed as:

$$\frac{d e_i}{dt} = \left.\frac{\partial e_i}{\partial \rho_i}\right|_s \frac{d\rho_i}{dt} + \left.\frac{\partial e_i}{\partial s_i}\right|_V \frac{d s_i}{dt} = \frac{p_i}{\rho_i^2} \sum_j \left[\frac{\partial \rho_i}{\partial \boldsymbol{r}_j} \cdot \boldsymbol{u}_j \right] + T_i \frac{d s_i}{dt}, \tag{II.9}$$

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

$$\frac{d\rho_i}{dt} = \sum_j \left[\frac{\partial \rho_i}{\partial \boldsymbol{r}_j} \cdot \boldsymbol{u}_j \right].$$

(II.10)

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

$$\sum_i \left[Q_i^V \cdot \boldsymbol{u}_i + m_i T_i \frac{ds_i}{dt} \right] = 0.$$

(II.11)

Equation (II.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 to close this section:

$$m_i T_i \frac{ds_i}{dt} = -\boldsymbol{u}_i \cdot Q_i^V + \boldsymbol{q}_i,$$

(II.12)

where we have introduced $\boldsymbol{q}_i$ 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 $\boldsymbol{q}_i$ should satisfy the condition $\sum_i \boldsymbol{q}_i = 0$ 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 Q_i and 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]. In this last reference, for instance, it is indicated that the average thermal velocity of the particles scales as $\sqrt{k_B T/M}$, where M is the mass of the fluid particle and k_B is the Boltzmann constant. In agreement with our previous statement, if the particles are sufficiently large, their thermal motion can be ignored.

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 the SPH model a density field is associated to a discrete mass distribution chosen arbitrarily (see *e.g.* Grenier et al. [25]). Here, following the work of Español and Revenga [20], the density

of the generic i-th particle is defined as:

$$\rho_i = m_i \sum_j W(\boldsymbol{r}_j - \boldsymbol{r}_i; h),$$ (II.13)

where W is a weight function often referred to as "kernel" function. Notice that in (II.13) the mass of the particle is left out of the summation. W is a positive smooth function which converges in the weak sense to the Dirac delta measure when its characteristic length h tends to zero. W monotonously decreases with the distance $r_{ij} = |\boldsymbol{r}_{ij}| = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. The kernel considered in this study is spherical, thus depending only on r_{ij}. Hereinafter we adopt the notation $W_{ij} = W(r_{ij}; h)$, the dependence on h being implicitly assumed. Regarding the spatial derivative of W, due to the above properties it is possible to write:

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

where the dependence of F on h is again implicit. Because of the W's properties, the function $F(r_{ij})$ is always positive. Furthermore, the integral over the space of W is equal to one and the following useful relations hold:

$$\int_0^\infty r^{n-1} W(r)\, dr = C_n, \qquad \int_0^\infty F(r)\, r^{n+1}\, dr = -C_n\, n,$$

$$C_1 = \frac{1}{2}, \qquad C_2 = \frac{1}{(2\pi)}, \qquad C_3 = \frac{1}{(4\pi)},$$ (II.15)

where n is the dimension of the geometrical space considered.

An example of a kernel function can be:

$$W_{ij} = \frac{1}{\pi^{\frac{n}{2}} h^n} \exp\left(-\frac{r_{ij}^2}{h^2}\right) \qquad \Rightarrow \qquad F(r_{ij}) = \frac{2}{\pi^{\frac{n}{2}} h^{n+2}} \exp\left(-\frac{r_{ij}^2}{h^2}\right),$$

for which the function F is, in particular, strictly positive.

Through eq. (II.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:

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

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

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

In the following, the average size of the particles will be indicated with Δr. When performing the limit $\Delta r \to 0$, it is understood that the number of particles goes to infinity and that the volume of all particles decreases homogeneously in such a way that the standard deviation of the distribution Δr_i goes to zero.

It is important to underline that the volumes (II.16) are not connected to any tessellation of the geometrical space covered by the particles set. Indeed the volume subdivision obtained with (II.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. For this reason, Español and Revenga [20] call the volumes V_i in (II.16) "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. (II.6). However, thanks to the properties (II.15) of W, the Partition-of-Unity is recovered in the limit $\Delta r/h \to 0$.

As remarked in Mas-Gallic and Raviart [26], Quinlan et al. [27] and Di Lisio et al. [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 $\Delta r/h \to 0$, 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 $h \to 0$.

It has to be mentioned that there are particle based schemes in which the particle volumes are identified using a Voronoi tessellation procedure [29]. Furthermore, in the latter reference the rotational degree of freedom has been also incorporate in the dynamics equations. We will however restrict ourselves herein to state-of-the-art SPH schemes, in which the above potential enhancements have not yet been sufficiently investigated.

B. SPH equation for the motion of particles

Introducing (II.13) in (II.6), the general case, accounting for dissipative forces, leads to

$$
m_i \frac{d\boldsymbol{u}_i}{dt} - m_i \boldsymbol{f}_i + \left[\sum_j m_j \frac{p_j}{\rho_j^2} m_j \nabla_i W_{ij} + m_i \frac{p_i}{\rho_i^2} m_i \sum_j \nabla_i W_{ij} \right] = Q_i^V + Q_i .
\tag{II.18}
$$

Substituting the particle volumes (II.16), the ODEs representing the dynamics of the particle system is finally given by:

$$m_i \frac{du_i}{dt} = -\sum_j \left(p_j V_j^2 + p_i V_i^2 \right) \nabla_i W_{ij} + m_i f_i + Q_i^V + Q_i \qquad \text{(II.19)}$$

Rearranging the different terms, the i-th particle acceleration is given by:

$$\frac{du_i}{dt} = \frac{1}{\rho_i} \sum_j \left[\frac{p_j V_j^2 + p_i V_i^2}{V_i V_j} \right] r_{ij} F(r_{ij}) V_j + f_i + \frac{Q_i^V + Q_i}{m_i}. \qquad \text{(II.20)}$$

Considering the limit from discrete particles to continuum media, $i.e.$ $h \to 0$ and $\Delta r/h \to 0$, it is possible to show (see $e.g.$ Colagrossi et al. [30]) that equation (II.20) converges, as it should, to the standard Euler momentum conservation equation for an inviscid fluid (i.e. $Q^V = 0$):

$$\frac{du}{dt} = -\frac{1}{\rho} \nabla p + f, \qquad \text{(II.21)}$$

where the effects related to the generalized forces, 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 (II.2), the dissipative forces need to be modeled. Following the pioneering work of Rayleigh, reviewed in detail by Greiner [31], dissipative forces 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, $u_{ij} = u_i - u_j$:

$$\Phi_D = \frac{1}{2} \sum_i \sum_j u_{ij} \cdot \mathbb{A}_{ij}(r_{ij}) \cdot u_{ij}, \qquad \text{(II.22)}$$

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 [32] (see appendix A). According to this assumption, the generalized force in the equation (II.2) takes the form[31]:

$$Q_i^V = -\frac{\partial \Phi_D}{\partial u_i} = -\sum_j \mathbb{A}_{ij}(r_{ij}) \cdot u_{ij}, \qquad \text{(II.23)}$$

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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 Violeau [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:

$$\mathbb{A}_{ij} = \boldsymbol{\gamma}_{ij} \otimes \boldsymbol{r}_{ij}, \qquad (\text{II}.24)$$

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 $\mathbb{A}_{ij} \cdot \boldsymbol{u}_{ij}$ must be collinear with $\boldsymbol{r}_{ij}$, hence :

$$\mathbb{A}_{ij} = \boldsymbol{r}_{ij} \otimes \boldsymbol{\gamma}'_{ij}, \qquad (\text{II}.25)$$

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 $\mathbb{A}_{ij}\boldsymbol{u}_{ij}$ with the vector position $\boldsymbol{r}_{ij}$ 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 (II.25) must be satisfied.

In a more intuitive way, the dissipation force may be assumed collinear to the relative velocity, by defining the matrices as $\mathbb{A}_{ij} = \gamma_{ij}\,\boldsymbol{I}$ where $\boldsymbol{I}$ is the identity matrix and γ_{ij} is a certain scalar. Even if this choice does not comply with the former constraints, it will be shown that it is widely exploited in a well known SPH viscosity formulation (see Colagrossi et al. [13], Morris et al. [33]). We will examine this point at the end of this section and in the next one.

Having to hold the conditions (II.25) and (II.24) simultaneously, the vectors $\boldsymbol{\gamma}_{ij}$ must linearly depend on $\boldsymbol{r}_{ij}$, namely $\boldsymbol{\gamma}_{ij} = \gamma_{ij}\boldsymbol{r}_{ij}$, through some scalar coefficients γ_{ij}, so that the final form of the matrices is obtained:

$$\mathbb{A}_{ij} = \gamma_{ij}(r_{ij})\,(\boldsymbol{r}_{ij} \otimes \boldsymbol{r}_{ij}), \qquad (\text{II}.26)$$

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. $\gamma_{ij} = \gamma_{ji}$).

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The specification (II.26) of $\mathbb{A}_{ij}$ allows to express the dissipation function and the related force as:

$$\Phi_D = \frac{1}{2}\sum_i\sum_j \gamma_{ij}(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{r}_{ij})^2 \qquad \Rightarrow \qquad Q_i^V = -\sum_j\gamma_{ij}(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{r}_{ij})\,\boldsymbol{r}_{ij}\,. \qquad \text{(II.27)}$$

Similarly to the derivation of the pressure forces (see eq. (II.19)), 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:

$$Q_i^V = -\sum_j\hat{\gamma}_{ij}(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{r}_{ij})\,\boldsymbol{r}_{ij}\,V_i\,V_j\,. \qquad \text{(II.28)}$$

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 $\Delta r \to 0$, the specific force:

$$\boldsymbol{f}^V(\boldsymbol{r}_i) = \frac{Q_i^V}{V_i} = \sum_j \hat{\gamma}_{ij}(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{r}_{ij})\,\boldsymbol{r}_{ij}\,V_j \qquad \text{(II.29)}$$

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

$$\hat{\gamma}_{ij}(r_{ij}) = \frac{g_{ij}(r_{ij})}{r_{ij}^2} \qquad \text{with} \qquad \lim_{r_{ij}\to 0} g_{ij}(r_{ij}) = g_{ii} > 0\,, \qquad \text{(II.30)}$$

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 the appendix A; for a deeper discussion see [14]). The suitability of the choice (II.30) is further inspected in the next section where the limits $\Delta r/h \to 0$ and $h \to 0$ of the field $\boldsymbol{f}^V$ are solved.

By substituting the latter definition in the expression (II.27), the final form of the dissipation function and the related dissipative force is obtained:

$$\Phi_D = \frac{1}{2}\sum_i\sum_j g_{ij}(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{e}_{ij})^2\,V_i\,V_j\,, \qquad Q_i^V = -\sum_j g_{ij}(r_{ij})\,(\boldsymbol{u}_{ij}\cdot\boldsymbol{e}_{ij})\,\boldsymbol{e}_{ij}\,V_i\,V_j\,, \qquad \text{(II.31)}$$

where $\boldsymbol{e}_{ij} = \boldsymbol{r}_{ij}/|\boldsymbol{r}_{ij}|$ 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 (II.20) 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. In this case, we can write:

$$g(r_{ij}) = C\, F(r_{ij})\,, \tag{II.32}$$

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. Although being the common practice in SPH and in the smoothed DPD formulations [11, 20], in purity, it is not strictly necessary that the same kernel has to be used for the pressure term and the dissipative forces. Actually, some SPH implementations [34, 35] and all Moving Particle Semi-Implicit formulations (MPS is a technique equivalent to incompressible SPH) use such different kernels [36, 37]. However, as will be later seen, the results here obtained are independent of such function, and therefore, using the same function F for both terms does not affect the generality of present analysis while lightening the notation.

Assuming the form (II.32), dissipation function and the related dissipative force becomes:

$$\Phi_D = \frac{C}{2} \sum_i \sum_j F(r_{ij})\, (\mathbf{u}_{ij} \cdot \mathbf{e}_{ij})^2\, V_i\, V_j\,, \qquad Q_i^V = -C \sum_j F(r_{ij})\, (\mathbf{u}_{ij} \cdot \mathbf{e}_{ij})\, \mathbf{e}_{ij}\, V_i\, V_j\,. \tag{II.33}$$

In order to close the procedure, the constant C in eq. (II.33) needs to be addressed. To this purpose we consider again the passage from a discrete to a continuum description with the procedure followed in Colagrossi et al. [13]. In the latter, the limit $\Delta r/h \to 0$ is firstly considered and the limit $h \to 0$ is performed as a second step.

After the first limit passage, the summation in (II.33) 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. (II.29) is then given by:

$$\mathbf{f}^V(\mathbf{r}) \;=\; C \int_\Omega F(r') \frac{[\mathbf{u}(\mathbf{r} + \mathbf{r}') - \mathbf{u}(\mathbf{r})] \cdot \mathbf{r}'}{r'^2} \mathbf{r}'\, dV'\,, \tag{II.34}$$

where the fluid domain Ω is here considered unbounded.

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

$$\boldsymbol{u}(\boldsymbol{r} + \boldsymbol{r}') - \boldsymbol{u}(\boldsymbol{r}) = \nabla \boldsymbol{u}|_r \cdot \boldsymbol{r}' + \frac{1}{2} \boldsymbol{r}' \cdot \mathbb{H}_r \cdot \boldsymbol{r}' + O(r'^3),$$ (II.35)

where $\mathbb{H}$ is the Hessian tensor.

By substituting the expression (II.35) into (II.34), the following definition is obtained :

$$\boldsymbol{f}^V(\boldsymbol{r}) = C \left[\int_\Omega \frac{\boldsymbol{r}' \otimes \boldsymbol{r}' \otimes \boldsymbol{r}'}{r'^2} F(r') \, dV' \right] \mathbb{D}_r + \frac{C}{2} \left[\int_\Omega \frac{\boldsymbol{r}' \otimes \boldsymbol{r}' \otimes \boldsymbol{r}' \otimes \boldsymbol{r}'}{r'^2} F(r') \, dV' \right] \mathbb{H}_r + O(h),$$ (II.36)

where $\mathbb{D}$ 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 (II.36) is analyzed in detail by Colagrossi et al. [13]. Evaluating it, using spherical coordinates, they were able to split it in various independent factors, which, combined with the anti-symmetry of $\boldsymbol{r} \, F(r)$, enabled them to demonstrate it is null.

Defining the following fourth order tensor:

$$\mathbb{G} := \frac{C}{2} \int_\Omega \frac{\boldsymbol{r}' \otimes \boldsymbol{r}' \otimes \boldsymbol{r}' \otimes \boldsymbol{r}'}{r'^2} F(r') \, dV'$$ (II.37)

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

$$\boldsymbol{f}^V(\boldsymbol{r}) = \mathbb{G} \, \mathbb{H}_r + O(h^2)$$ (II.38)

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

As demonstrated in Colagrossi et al. [13], the relation (II.38) becomes:

$$\boldsymbol{f}^V(\boldsymbol{r}) = \frac{C}{2(n+2)} \nabla^2 \boldsymbol{u}(\boldsymbol{r}) + \frac{C}{(n+2)} \nabla (\nabla \cdot \boldsymbol{u})(\boldsymbol{r}) + O(h^2).$$ (II.39)

where n stands for the dimensionality of the space. Finally considering the limit $h \rightarrow 0$ and comparing the above expression with the viscous force for a Newtonian fluid:

$$\boldsymbol{f}^V = \mu \, \nabla^2 \boldsymbol{u} + (\mu + \lambda) \nabla (\nabla \cdot \boldsymbol{u}),$$ (II.40)

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:

$$\kappa = \lambda + \frac{2\mu}{n},$$ (II.41)

in the SPH model is fixed to the value:

$$\kappa = \mu \left(1 + 2/n\right) \qquad \boxed{\text{Bulk viscosity in the SPH model}} \qquad \text{(II.42)}$$

Therefore, the bulk viscosity is $\kappa = 2\mu$ and $\kappa = 5\mu/3$ in a 2D and a 3D framework respectively. (II.42) 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 dissipation function and dissipative force (II.33) acting on the generic particle i is given by the formula:

$$\Phi_D = \mu \, (n + 2) \sum_i \sum_j F(r_{ij}) \, (\boldsymbol{u}_{ij} \cdot \boldsymbol{e}_{ij})^2 \, V_i \, V_j \, , \qquad Q_i^V = -\mu \, 2(n + 2) \sum_j F(r_{ij}) \, (\boldsymbol{u}_{ij} \cdot \boldsymbol{e}_{ij}) \, \boldsymbol{e}_{ij} \, V_i \, V_j \, ,$$
$$\text{(II.43)}$$

which resembles the formula derived for the SPH model by Monaghan and Gingold [38]. 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 $(\boldsymbol{u}_{ij} \cdot \boldsymbol{r}_{ij})$ is positive, in order to mimic a Neumann-Richtmyer viscosity (see Wilkins [39]).

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 (II.24-II.25), and arrive in eq. (II.43) to the same structure as given in (II.31).

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. (II.43) (see *e.g.* [40], [41], [11], [42], and in particular [43] 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

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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. [33]. In this case the dissipation forces among the particles are supposed to be collinear with the relative velocity $\boldsymbol{u}_{ij}$, which is equivalent to merely define the matrices $\mathbb{A}_{ij}(r_{ij})$ in (II.22) as:

$$\mathbb{A}_{ij}(r_{ij}) = \gamma_{ij}(r_{ij}) \, \boldsymbol{I} \,, \tag{II.44}$$

$$\gamma_{ij}(r_{ij}) = g_{ij}(r_{ij}) \, V_i \, V_j \,, \tag{II.45}$$

where $\boldsymbol{I}$ is the identity matrix. It is worth to stress that, unlike the former case, none of the two constraints (II.25) and (II.24) are satisfied. However, the condition of positive definiteness of the matrices must hold also in this case. Through the same assumption of (II.32) for the function g_{ij}, the viscous force is written as follows:

$$Q_i^V = -C \sum_j F(r_{ij}) \, \boldsymbol{u}_{ij} \, V_i \, V_j \tag{II.46}$$

This form of the dissipative force obviously violates the conservation of angular momentum. Considering again the limit $\Delta r/h \to 0$ the continuous viscous dissipation force field is:

$$\boldsymbol{f}^V(\boldsymbol{r}) \,=\, C \int_\Omega F(r')[\boldsymbol{u}(\boldsymbol{r}' + \boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r})] \, dV' \tag{II.47}$$

By expanding in Taylor series the velocity difference in the integrand, as in the (II.35, the following expression is obtained:

$$\boldsymbol{f}^V(\boldsymbol{r}) = C \, \nabla\boldsymbol{u}|_r \cdot \int_\Omega \boldsymbol{r}' F(r') \, dV' \,+\, \left[\frac{C}{2} \int_\Omega (\boldsymbol{r}' \otimes \boldsymbol{r}') \, F(r') \, dV'\right] \mathbb{H}_r \,+\, O(h) \tag{II.48}$$

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:

$$\mathbb{M} := \int_\Omega (\boldsymbol{r}' \otimes \boldsymbol{r}') \, F(r') \, dV' \tag{II.49}$$

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

$$\boldsymbol{f}^V(\boldsymbol{r}) \,=\, \frac{C}{2} \, \mathbb{H}_r \, \boldsymbol{I} \,+\, O(h^2) \,=\, \frac{C}{2} \, \boldsymbol{\nabla}^2 \boldsymbol{u}(\boldsymbol{r}) \,+\, O(h^2) \tag{II.50}$$

Summarizing, considering the limit $h \to 0$ 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 (II.25) and (II.24), 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 (II.46) should not be applied to viscous free-surface flows (it renders inaccurate dissipation in the integral limit), where SPH has become a competitive alternative to mesh based CFD solvers. 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, with this viscous term rendering accurate dissipation even in the presence of a free surface. The theoretical predictions related to both terms are confirmed with numerical computations for the decay of a viscous standing wave also in [13].

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 $\boldsymbol{u}_{ij}$ leads to models that exhibit the same drawbacks as discussed above for the purely SPH models within Morris formulation [20]. The effect of these drawbacks do not manifest in problems involving rather incompressible fluids, without shock waves and free surfaces [21, 44]. 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. [45] 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 $\boldsymbol{u}_{ij}$. For such a general model, shear and bulk viscosities could be, in principle, independently chosen.

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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:

$$\boldsymbol{f}^V = \mu \nabla^2 \boldsymbol{u} + (\mu + \lambda) \nabla (\nabla \cdot \boldsymbol{u}), \qquad \text{(III.51)}$$

and discretizing it through convolution integrals with the Kernel function introduced for the SPH model in II A. This approach has been developed by Español and Revenga [20] where the authors write a viscous term which is a combination of the two formulations (II.43) and (II.46) derived in the previous section. Indeed, integral interpolations of second derivative of the velocity field can be obtained combining the four eq. (II.34), (II.39), (II.47) and (II.50):

$$\frac{1}{2} \nabla^2 \boldsymbol{u}(\boldsymbol{r}) + \nabla (\nabla \cdot \boldsymbol{u})(\boldsymbol{r}) = \underbrace{(n+2) \int_\Omega F(r') \frac{[\boldsymbol{u}(\boldsymbol{r}+\boldsymbol{r}') - \boldsymbol{u}(\boldsymbol{r})] \cdot \boldsymbol{r}'}{r'^2} \boldsymbol{r}' \, dV'}_{\Psi_1} + O(h^2) \qquad \text{(III.52)}$$

$$\nabla^2 \boldsymbol{u}(\boldsymbol{r}) = \underbrace{2 \int_\Omega F(r')[\boldsymbol{u}(\boldsymbol{r}' + \boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r})] \, dV'}_{\Psi_2} + O(h^2) \qquad \text{(III.53)}$$

These two formulas allow for the calculation of second derivatives of the velocity field using the value of $\boldsymbol{u}$ within the fluid domain. In this context we are using such approximations of the second order spatial differential operators, without taking care of any consideration that should regard the nature of the particles system used. Combining the above formulas, it is possible to approximate the viscous term (III.51) as:

$$\boldsymbol{f}^V = \mu \Psi_2 + (\mu + \lambda) \left[\Psi_1 - \frac{1}{2} \Psi_2 \right] + O(h^2) = (\mu + \lambda) \Psi_1 + \frac{(\mu - \lambda)}{2} \Psi_2 + O(h^2) \qquad \text{(III.54)}$$

Discretizing this formula on the particles set, the dissipation force on the generic particle i is:

$$Q_i^V = -(\mu + \lambda)(n + 2) \sum_j F(r_{ij}) (\boldsymbol{u}_{ij} \cdot \boldsymbol{e}_{ij}) \boldsymbol{e}_{ij} V_i V_j + (\lambda - \mu) \sum_j F(r_{ij}) \boldsymbol{u}_{ij} V_i V_j. \qquad \text{(III.55)}$$

This formula permits to take into account both the primary and the secondary viscosities. However, as commented in the previous section, the second term in the right-hand side is not invariant in a Galilean transformation and it does not preserve the angular momentum of the particles system. To recover both these properties, the only solution is to set $\lambda = \mu$ or, in other words, to set the bulk viscosity $\kappa = \lambda + 2\mu/n$ equal to:

$$\kappa = \mu (1 + 2/n) \qquad \boxed{\text{Bulk viscosity in the SPH model}}. \qquad \text{(III.56)}$$

IV. DISCUSSION

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 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 [46, 47] 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 [48] 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 CO_2 or N_2O [48] 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

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relevant role in determining the actual ratio of bulk to shear viscosity for this type of fluids (see e.g. [49]).

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 (II.25) and (II.24) 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 et al. [50], based on a Boltzmann-like equation for the DPD system, the dissipative contribution is found to satisfy exactly the same ratio (II.42) (cf. eq. (78) of [50]). The same ratio was also found later in ref. [51], 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 et al. [50], $\kappa_K = 2\mu_K/n$ (cf. eq. (70) of this last reference), even providing a different ratio than equation (II.42), 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. [44]'s numerical calculations of the transport coefficients using correlation functions [52] led to values of bulk viscosity of the same order like the shear one, in line with the referred DPD estimates.

Analogous situations are encountered in Kinetic Theory of gases. Let us take, for example, the Enskog calculation for a hard sphere gas in two dimensions. It is found that

$$\mu_E = \nu_0 \left[\frac{1}{\chi(\phi)} + 2\phi \left(1 + \frac{8}{\pi} \right) \chi(\phi)\,\phi^2 \right] \tag{IV.57}$$

$$\kappa_E = \nu_0 \frac{16\,\chi(\phi)\phi^2}{\pi} \tag{IV.58}$$

with

$$\nu_0 \equiv \frac{1}{2\sigma} \left(\frac{mT}{\pi} \right)^{1/2} \tag{IV.59}$$

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In the above expressions, ϕ is the volume fraction of the gas and $\chi(\phi)$ is the correlation function at contact, namely at a distance σ, where σ is the diameter of the hard spere. We observe from the above expressions that both viscosities depend on an only coefficient ν_0, which indicates that both viscosities cannot be independently modeled. The proportionality between both coefficients depends, however, on the state of the system through the volume fraction of particles. Further analysis based on Kinetic Theory is an interesting research line to be considered after the present work.

Another interesting consideration is that granular fluids under central forces in the quasielastic limit behave in the same way [53] regarding the joint modeling of bulk and shear viscosities although, for large restitution coefficients, the proportionality ratio depends also on this coefficient (see also [54]).

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 particular, for the weakly-compressible SPH practitioners, 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.

V. CONCLUSIONS

In the present article the previous works by Español and Revenga [20], Monaghan [11], Violeau [14] and Colagrossi et al. [13] are considered. These foregoing analyses have been combined together to show how inter-particle dissipative forces can be formulated when a liquid is modeled as a macroscopic system of fluid particles. The framework of the Smoothed Particle Hydrodynamics (SPH) model is used in order to get a closed system of ODEs for the dynamics of

the particles. Within the SPH framework a consistent approximation to the Newtonian viscous term has been derived that incorporates both inter-particle radial and non-radial terms [33]. However, in order to derive a formulation that is invariant under Galilean transformations and that preserves the angular momentum of the overall particle system, the non-radial terms must be null. We show that this constraint implies that first and second viscosities are equal or, conversely, that the bulk and shear viscosities are not independent from each other. Moreover, we have also shown that, even in the simplest SPH model consistent with the aforementioned physical requirements, bulk and shear viscosities are of the same order of magnitude. Therefore a finite positive value for the bulk viscosity, as given in eq. (II.42), needs to be set in SPH models for fluid dynamics, in contradiction with the referred Stokes' hypothesis, and closer to values of this coefficient referred in the literature for monatomic gases and common liquids such as water.

APPENDIX A: CONSIDERATIONS ON THE VISCOUS DISSIPATION

Multiplying the governing equation of particles' motion (II.6) by $\boldsymbol{u}_i$, it is possible to write the mechanical energy variation of the particle system as:

$$\dot{\mathcal{E}}_k + \dot{\mathcal{E}}_p + \sum_i m_i\, p_i\, \frac{d(^1\!/_{\rho_i})}{dt} = \sum_i \left(\boldsymbol{Q}_i \cdot \boldsymbol{u}_i + \boldsymbol{Q}_i^V \cdot \boldsymbol{u}_i \right), \qquad (A.1)$$

where the sum $\mathcal{E}_k + \mathcal{E}_p$ is the mechanical energy (i.e. kinetic plus potential energy). The last term in the left-hand side represents the power exerted by the pressure force, referred in what follows as the time variation of the elastic energy $\dot{\mathcal{E}}_c$.

If we consider that the generic non-conservative forces, $\boldsymbol{Q}_i = 0$, are null, equation (A.1)

becomes:

$$\frac{d}{dt}\left[\mathcal{E}_k + \mathcal{E}_p + \mathcal{E}_c\right] = -\Phi_D < 0, \tag{A.2}$$

where, on the right-hand side, the relation $\Phi_D = -\sum_i \boldsymbol{u}_i \cdot Q_i^V$ has been used. This relation follows from the fact that, on the one hand Φ_D is, by definition, quadratic in the velocities and, on the other, that Q_i^V can be written as $\sum_j Q_{ij}^V$, with $Q_{ij}^V = -Q_{ji}^V$ (action-reaction), in view of eq. (II.23).

Eq. (A.2) expresses the thermodynamic consistency of the formulation of the problem. In particular, Φ_D ought to be interpreted as the *entropy production* of the system, which should be positive definite to comply with the second principle [32]. Hence, the conservative energy of the system is a monotonously decreasing function, owing to the increase of the entropy of the system through dissipative forces.

The power dissipated by the viscous term of the macroscopic Navier-Stokes equation during the flow evolution is

$$\Phi_D = -\int_\Omega \boldsymbol{f}^V \cdot \boldsymbol{u}\, dV. \tag{A.3}$$

Using $\boldsymbol{f}^V$ definition (III.51), eq. (A.3) can be rewritten as (see [55] for details):

$$\Phi_D = 2\mu \int_\Omega \mathbb{D} : \mathbb{D}\, dV + \lambda \int_\Omega (\nabla \cdot \boldsymbol{u})^2\, dV. \tag{A.4}$$

Defining the Deviatoric tensor $\mathbb{S}$ as

$$\mathbb{S} := \mathbb{D} - \frac{1}{n} \nabla \cdot \boldsymbol{u}\, \boldsymbol{I}, \tag{A.5}$$

and introducing the bulk viscosity κ (see eq. (II.41)), eq. (A.4) becomes:

$$\Phi_D = 2\mu \int_\Omega \mathbb{S} : \mathbb{S}\, dV + \kappa \int_\Omega (\nabla \cdot \boldsymbol{u})^2\, dV \tag{A.6}$$

In order to satisfy the second law of thermodynamics, both these the two terms in the right-hand side of the above relation must always be positive separately, as stressed by Landau and Lifshitz [5] and, therefore, both μ an κ need to be strictly positive. This is in accordance with the results presented in this article, while the "Stokes' Hypothesis" $\kappa = 0$ violates this condition.

Regarding the equation (II.43) for the dissipation forces adopted in the Monaghan-Cleary-Gingold's formulation of the SPH model, the function Φ_D reads

$$\Phi_D = \mu\, (n+2) \sum_i \sum_j F(r_{ij})\, (\boldsymbol{u}_{ij} \cdot \boldsymbol{e}_{ij})^2\, V_i\, V_j$$

which, thanks to the positiveness of function F, also satisfies the second law of thermodynamics for the particle system. More details on the application of such a formula when simulating viscous

flows are given in *e.g.* [15], [43] and [56]; in the latter the generalization to multi-phase flows is considered.

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