Dissipative forces for Lagrangian models in computational fluid dynamics and application to smoothed-particle hydrodynamics

D. Violeau*

Saint-Venant Laboratory for Hydraulics, Université Paris-Est, Joint Research Unit EDF R&D, CETMEF, Ecole des Ponts, 6 quai Watier, 78400 Chatou, France

(Received 21 October 2008; revised manuscript received 25 March 2009; published 25 September 2009)

An investigation of dissipative forces for Lagrangian computational fluid dynamics is conducted from Hamiltonian considerations including energy dissipation for macroscopic systems. It is shown that discrete forces must fulfill particular rules to be in agreement with the fundamentals of Physics. Those rules are specified in the case of the smoothed particle hydrodynamics (SPH) numerical approach, leading to a clear treatment of friction forces in connection with energy dissipation. In particular, it is proved that the kernel function, which is at the heart of interpolation in SPH, must satisfy some constraints in order to be consistent with the dissipative properties of a real fluid. A numerical example is given to illustrate the abovementioned considerations.

DOI: 10.1103/PhysRevE.80.036705 PACS number(s): 47.11.St, 47.10.Df

I. INTRODUCTION

Lagrangian methods in computational fluid dynamics (CFD) are used more and more in the fields of confined and free-surface flows. All these methods, such as smoothed particle hydrodynamics (SPH) [1], dissipative particle dynamics (DPD) [2], or moving particle semi-implicit method (MPS) [3] are based on the idea that a flow can be seen as a collection a macroscopic particles exchanging momentum, energy, etc. In this context, the question of the discrete form of forces is crucial, and can be investigated from Lagrangian and Hamiltonian viewpoints. A key element is how to treat macroscopic systems such as fluid particles, for which the laws of thermodynamics predict a behavior, which is different than the behavior of individual molecules, leading to the concept of energy dissipation. Hence, the correct treatment of dissipative forces in Lagrangian methods, in connection to the principles of Hamiltonian and statistical mechanics, yields some rules that developers must obey when writing the discrete equations of a Lagrangian numerical method consistently with variational ideas.

In Sec. II, we will briefly review the backgrounds of the Hamiltonian theory, before focusing on dissipative (or friction) forces, first in a general context, and then applied to a system of macroscopic particles. We will show that, regardless of the considered numerical approach, the discrete particle friction forces should fulfill some requirements deduced from the conservation laws, but also from considerations of volume shrinkage in the phase space. In Sec. III, we will apply these considerations to find the constraints that the dissipative forces must satisfy in the context of the SPH method. This work will be based on a rigorous treatment of discrete viscous forces in the context of this method. The simulation of a steady flow in a periodic hill channel will illustrate our conclusions in Sec. III C.

*damien.violeau@edf.fr

II. CONSERVATIVE AND DISSIPATIVE SYSTEMS

A. General considerations on mechanical forces

In the present section, we remind a few statements regarding Lagrangian and Hamiltonian mechanics for dissipative systems. Since the pioneering work from Lagrange [4], it is generally considered that a classical mechanical system may be fully described by a Lagrangian L, playing the role of a state function depending on its N generalized coordinates q_i and their time derivative, or generalized velocities $\dot{q}_i$,

$$L = L(\{q_i\},\{\dot{q}_i\},t) = E_K(\{q_i\},\{\dot{q}_i\}) - U(\{q_i\},t), \tag{1}$$

where E_K and U are the kinetic and potential energies, respectively (here and in the following, we use the notation $\{q_i\}$ to denote the collection of all q_i's). Then, the Lagrange equations give the behavior of the system $\{q_i\}$ as

$$\forall i, \quad p_i \doteqdot \frac{dp_i}{dt} = \frac{\partial L}{\partial q_i} = -\frac{\partial U}{\partial q_i} = F_i^{cons}, \tag{2}$$

where the generalized momenta are defined by

$$p_i \doteqdot \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial E_K}{\partial \dot{q}_i}. \tag{3}$$

Equation (2) also appears the notion of conservative forces F_i^{cons}. The name and notation suggest that they conserve energy, as it is well known, since they can be written as the derivatives of some state function (potential energy) with respect to the coordinates q_i, i.e., as spatial gradients of a potential. The above equations are perfectly valid, for example, for a gas of interacting (colliding) molecules, and the total energy is indeed conserved at the microscopic scale. However, the behavior of such a system involving a very large number of degrees of freedom is better understood through a statistical viewpoint. This can be achieved through the Boltzmann equation, leading to the H theorem, which states that entropy (disorder) increases with time while collisions between molecules spread their velocities on a broader range [5]. This process transfers energy from the macroscopic to the microscopic (thermal) scale and thus

yields energy dissipation at macroscopic scales. It also tends to make the macroscopic (Boltzmann averaged) velocities more and more uniform as time goes on. At the macroscopic scale viewpoint, where the velocities are smooth, one must then admit that some forces F_i^{diss} exist, which can be qualified as dissipative, for they no longer conserve the macroscopic energy. As a consequence, those "friction" forces cannot be written as spatial gradients of any potential, but must depend on the macroscopic velocities $\{\dot{q}_j\}$. A Taylor expansion up to order 1 gives

$$F_i^{diss} = -\sum_j \alpha_{ij}(\{q_k\})\dot{q}_j, \tag{4}$$

where the α_{ij}'s are $N \times N$ unknown friction (or "kinetic") coefficients depending on the $\{q_k\}$ coordinates only. Next, Onsager's principle [6] states that these coefficients satisfy the following symmetry condition:

$$\alpha_{ji} = \alpha_{ij}. \tag{5}$$

This statement allows us to rewrite Eq. (4) in the following form

$$F_i^{diss} = -\frac{\partial F}{\partial \dot{q}_i}, \tag{6}$$

where we have defined the following quadratic form:

$$F = \frac{1}{2}\sum_{i,j} \alpha_{ij}(\{q_k\})\dot{q}_i\dot{q}_j. \tag{7}$$

The Lagrange momentum [Eq. (2)] can now be reformulated, for macroscopic systems, as

$$\forall i, \quad \dot{p}_i = -\frac{\partial U}{\partial q_i} - \frac{\partial F}{\partial \dot{q}_i} = F_i^{cons} + F_i^{diss}. \tag{8}$$

The system is totally defined at each time by the set of variables $(\{q_i\},\{\dot{q}_i\})$. However, Eq. (3) shows that the choice $(\{p_i\},\{q_i\})$ is also possible; the energy (or Hamiltonian) H is then defined by

$$H(\{p_i\},\{q_i\},t) = \sum_i p_i\dot{q}_i - L. \tag{9}$$

From considerations related to Galileo's relativity principle, it is also known [7] that the kinetic energy is a quadratic function of velocities, with coefficients depending on the generalized coordinates as

$$E_K = \frac{1}{2}\sum_{i,j} \Lambda_{ij}(\{q_k\})\dot{q}_i\dot{q}_j. \tag{10}$$

The positivity of E_K shows that the $\{\Lambda_{ij}\}$ are $N \times N$ coefficients of a positive definite quadratic form, and by definition they are symmetric; thus the matrix $\mathbf{\Lambda}$ of coefficients $\{\Lambda_{ij}\}$ has an inverse, hereafter denoted by $\mathbf{\Gamma} = \mathbf{\Lambda}^{-1}$. From Eqs. (3) and (10), we then obtain linear relations between the generalized momenta and velocities as

$$p_i = \sum_j \Lambda_{ij}(\{q_k\})\dot{q}_j. \tag{11}$$

Combining Eqs. (9) and (11) now gives the Hamiltonian as the sum or kinetic and potential energy, the former being a quadratic function of generalized momenta,

$$\begin{aligned} H(\{p_i\},\{q_i\},t) &= E_K(\{q_i\},\{\dot{q}_i\}) + U(\{q_i\},t) \\ &= \frac{1}{2}\sum_{i,j} \Gamma_{ij}(\{q_k\})p_ip_j + U(\{q_i\},t), \end{aligned} \tag{12}$$

where the $\{\Gamma_{ij}\}$ are the coefficients of the matrix $\mathbf{\Gamma}$. Using Eqs. (3) and (8), the differential of H can be written as

$$\begin{aligned} dH &= \sum_i (\dot{q}_i dp_i + p_i d\dot{q}_i) - \frac{\partial L}{\partial t}dt - \sum_i \left(\frac{\partial L}{\partial q_i}dq_i + \frac{\partial L}{\partial \dot{q}_i}d\dot{q}_i\right) \\ &= -\frac{\partial L}{\partial t}dt + \sum_i \left[\dot{q}_i dp_i - \left(\dot{p}_i + \frac{\partial F}{\partial \dot{q}_i}\right)dq_i\right], \end{aligned} \tag{13}$$

from which the set of Hamiltonian (macroscopic) dissipative equations immediately follows:

$$\begin{aligned} \frac{\partial H}{\partial t} &= -\frac{\partial L}{\partial t}, \\ \frac{\partial H}{\partial p_i} &= \dot{q}_i, \\ \frac{\partial H}{\partial q_i} &= -\dot{p}_i - \frac{\partial F}{\partial \dot{q}_i}. \end{aligned} \tag{14}$$

From Eq. (13) the time behavior of energy also follows:

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t} - \sum_i \frac{\partial F}{\partial \dot{q}_i}\dot{q}_i. \tag{15}$$

When the system is isolated from any external influence, the Lagrangian is independent of time ($\partial L/\partial t = 0$). Moreover, the quadratic form [Eq. (7)] of the function F finally yields the following relation:

$$\frac{dH}{dt} = -2F. \tag{16}$$

For this reason, F is usually called the dissipation function. The fact that the macroscopic energy decreases with time immediately implies the positiveness of F, meaning that the quadratic form defined by the $\{\alpha_{ij}\}$ is positive definite. The dissipation of energy has an important geometrical consequence. Let us consider a small ensemble $\tilde{\Omega}$ of initial conditions $(\{p_i\},\{q_i\})$ for the system in the phase space, and let us call $\tilde{V}$ the volume of this ensemble. Let us look at the evolution of the system along time for all these possible initial values. In the phase space, the subsequent values of $(\{p_i\},\{q_i\})$ will draw an ensemble of curves following the "velocity field" $(\{\dot{p}_i\},\{\dot{q}_i\})$ according to the set of Eq. (14). We can now affect to each point $(\{p_i\},\{q_i\})$ a probability Φ, considered as a "density" in the phase space. The conservation of total probability (which equals unity) is then formally equivalent to the conservation of mass of a virtual fluid in the

phase space [6]. With volume $\tilde{V}$, density Φ, positions $(\{p_i\},\{q_i\})$ and velocities $(\{\dot{p}_i\},\{\dot{q}_i\})$, and using Eqs. (4) and (14), the continuity equation reads

$$-\frac{1}{\Phi}\frac{d\Phi}{dt} = \sum_i \left(\frac{\partial \dot{p}_i}{\partial p_i} + \frac{\partial \dot{q}_i}{\partial q_i}\right) = \sum_i \left(-\frac{\partial^2 H}{\partial p_i \partial q_i} - \frac{\partial^2 F}{\partial p_i \partial \dot{q}_i} + \frac{\partial^2 H}{\partial q_i \partial p_i}\right) = -\sum_{i,j} \frac{\partial \alpha_{ij}\dot{q}_j}{\partial p_i}. \quad (17)$$

We mentioned earlier that the α_{ij}'s are functions of the q_i's only. Thus, with Eqs. (14) and (12), we obtain

$$\frac{1}{\tilde{V}}\frac{d\tilde{V}}{dt} = -\sum_{i,j} \alpha_{ij}\frac{\partial^2 H}{\partial p_i \partial p_j} = -\sum_{i,j} \alpha_{ij}\Gamma_{ij} = -\mathrm{tr}(\boldsymbol{\alpha}\boldsymbol{\Gamma}), \quad (18)$$

where $\boldsymbol{\alpha}$ is the $N\times N$ matrix of coefficients α_{ij}. Eq. (18) gives the time evolution of the volume $\tilde{V}$ of $\tilde{\Omega}$ in the phase space. Now, reminding that the trace of the product of two positive definite matrices is positive, one comes to the conclusion that the volume $\tilde{V}$ in the (macroscopic) phase space decreases under the effect of dissipative forces. In the absence of dissipative forces, Eq. (18) turns back to Liouville's theorem, stating that the volumes are preserved in the (microscopic) phase space. On the other hand, at the macroscopic scale, the larger the friction forces, the more the volumes decrease in the phase space (volume shrinkage). This means that the paths $(\{p_i\},\{q_i\})$ of the mechanical system get closer and closer, tending to an attractor, which is a known feature of dissipative systems. This deserves an interpretation: while disorder increases at the microscopic scale, the resulting friction at large scales, making the macroscopic velocities more and more homogeneous, increases macroscopic order, so that the qualitative behavior of the system in the phase space depends on the scale at which we investigate it. In other terms, the measure of the volume in the phase space depends on the spatial scale of observation, as it is for a fractal object.

It is also known that the total linear and angular momenta of a closed system are both conserved, with or without dissipative forces. These conservation laws, according to Noether's theorem, are directly connected to the Hamiltonian form of the equations of motion [4].

B. Systems of particles

Extending the above considerations to the case of a system of N_p macroscopic particles labeled by the letters a, b, etc. is straightforward, the number of degrees of freedom being now $N=nN_p$, where n is the dimension of the physical space (generally equal to 2 or 3). Knowing the particle masses $\{m_a\}$, their respective positions $\{\mathbf{r}_a\}$ and velocities $\{\mathbf{u}_a=\dot{\mathbf{r}}_a\}$ (now playing the role of the $\{q_i\}$ and $\{\dot{q}_i\}$, respectively) and internal energies $\{E_{\mathrm{int},a}\}$, the Lagrangian [Eq. (1)] reads

$$L = \sum_a \frac{1}{2}m_a u_a^2 - \sum_a E_{\mathrm{int},a} - U_{ext}(\{\mathbf{r}_a\}), \quad (19)$$

where u_a is the norm of $\mathbf{u}_a$, the kinetic and potential energies being defined by

$$E_K = \sum_a \frac{1}{2}m_a u_a^2 = \frac{1}{2}\sum_{a,b} \mathbf{u}_a^T \boldsymbol{\Lambda}_{ab}\mathbf{u}_b,$$

$$U = \sum_a E_{\mathrm{int},a} + U_{ext}(\{\mathbf{r}_a\}). \quad (20)$$

Note that the kinetic energy is indeed in the form [Eq. (10)] with a $N\times N$ matrix $\boldsymbol{\Lambda}$ which coefficients are given by

$$\Lambda_{ij} = m_a\delta_{kl}\delta_{ab},$$

$$i = n(a-1)+k,$$

$$j = n(b-1)+l, \quad (21)$$

where k and l here denote spatial directions (from 1 to n), so that i and j go from 1 to $N=nN_p$, as required. As pointed out by Eq. (20), we may also write the kinetic energy using N_p^2 matrices of dimension $n\times n$ attached to each pair of particles and denoted by $\boldsymbol{\Lambda}_{ab}$,

$$\boldsymbol{\Lambda}_{ab} = m_a\boldsymbol{\delta}_{ab}, \quad (22)$$

with $\boldsymbol{\delta}_{ab}$ being a Kronecker matrix of dimension $n\times n$, i.e., $\boldsymbol{\delta}_{ab}=\mathbf{I}_n$ (the $n\times n$ identity matrix) if $a=b$, otherwise $\boldsymbol{\delta}_{ab}=\mathbf{0}_n$ (the $n\times n$ null matrix). One must insist on the fact that in Eq. (22), the labels a and b do not represent matrix subscripts but particle labels. Note that here, the coefficients Λ_{ij}'s do not depend on $\{q_k\}$ (in other words, the matrices $\boldsymbol{\Lambda}_{ab}$ are independent on the particle positions $\{\mathbf{r}_c\}$). The equations of motion without friction forces [Eq. (2)] may be written in a vector form for each particle as

$$\forall a, \quad \frac{d\mathbf{p}_a}{dt} = \frac{\partial L}{\partial \mathbf{r}_a} = -\frac{\partial E_{\mathrm{int},a}}{\partial \mathbf{r}_a} - \frac{\partial U_{ext}}{\partial \mathbf{r}_a} = \mathbf{F}_a^{\mathrm{int}} + \mathbf{F}_a^{ext}, \quad (23)$$

where the momenta are defined, according to Eqs. (3) and (19), by

$$\mathbf{p}_a = \frac{\partial L}{\partial \mathbf{u}_a} = m_a\mathbf{u}_a. \quad (24)$$

The conservative force is, thus, now made of two parts, namely, internal and external forces,

$$\mathbf{F}_a^{cons} = \mathbf{F}_a^{\mathrm{int}} + \mathbf{F}_a^{ext}. \quad (25)$$

For a system of particles representing a fluid, the internal forces $\mathbf{F}_a^{\mathrm{int}}$ correspond to pressure forces, as we will see later (Sec. III A), while the external force $\mathbf{F}_a^{ext}$ is generally restricted to gravity,

$$U_{ext}(\{\mathbf{r}_a\}) = -\sum_a m_a\mathbf{g}\cdot\mathbf{r}_a = \sum_a m_a g z_a, \quad (26)$$

where $\mathbf{g}$ is the gravity acceleration (with norm g) and $\{z_a\}$ the particle elevations above an arbitrary reference level. The

above two forces are conservative ($\mathbf{F}_a^{\text{int}}+\mathbf{F}_a^{ext}=\mathbf{F}_a^{cons}$), since they are written in a gradient form. On the other hand, particle dissipative forces may now be taken into account, generalizing the Taylor expansion [Eq. (4)] and the definition Eq. (6) to write

$$\mathbf{F}_a^{diss}=-\sum_b \boldsymbol{\alpha}_{ab}(\{\mathbf{r}_c\})\mathbf{u}_{ab}, \tag{27}$$

where

$$\mathbf{u}_{ab}=\mathbf{u}_a-\mathbf{u}_b=-\mathbf{u}_{ba}, \tag{28}$$

and $\boldsymbol{\alpha}_{ab}$'s are N_p^2 matrices of order n attached to each pair of particles (like with the matrices $\boldsymbol{\Lambda}_{ab}$ defined above, a and b do not represent matrix indices put particle labels), depending on the collection of particle positions $\{\mathbf{r}_c\}$ and satisfying

$$\boldsymbol{\alpha}_{ba}=\boldsymbol{\alpha}_{ab} \tag{29}$$

according to Onsager's principle [Eq. (5)] regarding kinetic coefficients. The main difference with Eq. (4) is that now the dissipative forces depend on the velocity *differences*. The reason is that a set of particles moving with a uniform velocity does not experience any friction (in a continuous media viewpoint, the latter proposition states that shear forces depend on velocity *gradients*, see Sec. III B). The friction force [Eq. (27)] can be separated into individual forces due to each particle b, namely, $\mathbf{F}_{b\to a}^{diss}=-\boldsymbol{\alpha}_{ab}(\{\mathbf{r}_c\})\mathbf{u}_{ab}$. Since such a force can only involve the positions of the particles a and b, only $\mathbf{r}_a$ and $\mathbf{r}_b$ must appear in $\boldsymbol{\alpha}_{ab}$ among the list $\{\mathbf{r}_c\}$. Besides, the friction force vanishes when $a=b$, so that $\boldsymbol{\alpha}_{ab}$ must be a function of $\mathbf{r}_{ab}$, defined by

$$\mathbf{r}_{ab}=\mathbf{r}_a-\mathbf{r}_b=-\mathbf{r}_{ba}. \tag{30}$$

Lastly, for isotropy reasons the shear forces $\mathbf{F}_{b\to a}^{diss}$ do not depend on the orientation $\mathbf{r}_{ab}$. Hence, we must have

$$\boldsymbol{\alpha}_{ab}=\boldsymbol{\alpha}_{ab}(r_{ab}) \tag{31}$$

where $r_{ab}=|\mathbf{r}_{ab}|$, which is consistent with Eq. (29). The latter symmetry, as in Eq. (6), allows to write the friction force experienced by particle a as

$$\mathbf{F}_a^{diss}=-\frac{\partial F}{\partial \mathbf{u}_a}, \tag{32}$$

where

$$F=\frac{1}{2}\sum_{a,b}\mathbf{u}_{ab}^T\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab} \tag{33}$$

(we will sometimes drop the explicit dependency of $\boldsymbol{\alpha}_{ab}$ in r_{ab}, for simplicity). With these premises, the dissipative particle momentum equation appears in a form analogous to Eq. (8):

$$\forall a,\quad \frac{d\mathbf{p}_a}{dt}=\frac{\partial E_{\text{int},a}}{\partial \mathbf{r}_a}-\frac{\partial F}{\partial \mathbf{u}_a}-\frac{\partial U_{ext}}{\partial \mathbf{r}_a}=\mathbf{F}_a^{\text{int}}+\mathbf{F}_a^{diss}+\mathbf{F}_a^{ext}. \tag{34}$$

The conservation of the total linear momentum of a closed ensemble of interacting particles directly stems from the fact that the sum of all forces is equal to zero. In particular, from Eqs. (28) and (29) it immediately follows that the action-reaction law is fulfilled by particle friction forces:

$$\mathbf{F}_{b\to a}^{diss}=-\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab}=-\mathbf{F}_{a\to b}^{diss}. \tag{35}$$

Similarly to Eq. (3), and using Eqs. (19), (20), and (22), one defines the particles momentum vectors by

$$\mathbf{p}_a=\frac{\partial L}{\partial \mathbf{u}_a}=\sum_b \boldsymbol{\Lambda}_{ab}\mathbf{u}_b=m\mathbf{u}_a. \tag{36}$$

The Hamiltonian now becomes

$$H(\mathbf{r}_a,\mathbf{p}_a)=\frac{1}{2}\sum_{a,b}\mathbf{p}_a^T\boldsymbol{\Gamma}_{ab}\mathbf{p}_b+\sum_a E_{\text{int},a}+U(\{\mathbf{r}_a\}), \tag{37}$$

where the $\boldsymbol{\Gamma}_{ab}$'s are N_p^2 matrices of order n defined by

$$\boldsymbol{\Gamma}_{ab}=\boldsymbol{\Lambda}_{ab}^{-1}=\frac{1}{m_a}\boldsymbol{\delta}_{ab}, \tag{38}$$

Equation (37) is the macroscopic-particle analogue of Eq. (12). The law of energy dissipation [Eq. (15)], for a closed set of particles, now reads

$$\frac{dH}{dt}=-\sum_a \frac{\partial F}{\partial \mathbf{u}_a}\cdot\mathbf{u}_a. \tag{39}$$

However, rearranging Eq. (39) to give energy losses as a function of F now gives a slightly different result in comparison to Eq. (16). Indeed, using Eq. (27) and swapping the dummy labels a and b, we get

$$\frac{dH}{dt}=-\sum_{a,b}(\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab})\cdot\mathbf{u}_a=\sum_{a,b}(\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab})\cdot\mathbf{u}_b \tag{40}$$

[we used the symmetry laws Eqs. (28) and (29)]. Then, taking the average of the former two expressions, one comes to

$$\frac{dH}{dt}=-\frac{1}{2}\sum_{a,b}\mathbf{u}_{ab}^T\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab}=-F. \tag{41}$$

Comparing the last relation to Eq. (16), we see that the dissipation rate is now assumed by F (instead of $2F$); this is due to the fact that the friction forces are linear functions of the velocity *differences*, as mentioned above. The energy decrease then requires each matrix $\boldsymbol{\alpha}_{ab}$ to be positive definite. Obviously, the energy lost by the "coarse-grained" velocities $\mathbf{u}_a$ is converted into heat (molecular motion), so that the total energy is still preserved at the molecular scale.

We will now investigate the appropriate form for the matrices $\boldsymbol{\alpha}_{ab}$. We already mentioned that shear forces satisfy the conservation of linear momentum [Eq. (35)]. This is a direct consequence of the fact that these forces take their origin in *additive* microscopic phenomena, which obey this conservation law. Similarly, the angular momentum having the same additive property at the microscopic scale, one must immediately deduce that shear forces should fulfill the condition of total-angular momentum conservation, which is achieved by imposing that the angular momenta of individual shear forces are antisymmetric with respect to particle labels,

$$\mathbf{r}_a \times (\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab}) = -\mathbf{r}_b \times (\boldsymbol{\alpha}_{ba}\mathbf{u}_{ba}) \tag{42}$$

or, using the symmetry properties,

$$\mathbf{r}_{ab} \times (\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab}) = \mathbf{0}. \tag{43}$$

The condition [Eq. (43)] is fulfilled only if the vector $\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab}$ is collinear to $\mathbf{r}_{ab}$; thus, there must exist a scalar quantity β_{ab} symmetric with respect to a and b, such that $\boldsymbol{\alpha}_{ab}\mathbf{u}_{ab}=\beta_{ab}\mathbf{r}_{ab}$. Besides, the latter relation shows that β_{ab} must be linearly depending on $\mathbf{u}_{ab}$, hence of the form $\beta_{ab}=\boldsymbol{\gamma}_{ab}\cdot\mathbf{u}_{ab}$, where $\boldsymbol{\gamma}_{ab}$ is an antisymmetric vector. This gives

$$\boldsymbol{\alpha}_{ab} = \mathbf{r}_{ab} \otimes \boldsymbol{\gamma}_{ab},$$

$$\boldsymbol{\gamma}_{ba} = -\boldsymbol{\gamma}_{ab}, \tag{44}$$

where the tensorial product of two tensors of $\mathbf{A}$ and $\mathbf{B}$ of respective orders of p and q is the tensor of order $p+q$ with components $A_{i_1\ldots i_p}\times B_{j_1\ldots j_q}$. The above condition is not sufficient to properly model shear forces in a particle formalism. In addition to the conservation of total-angular momentum, these forces should vanish for a set of particles moving according to a rigid body rotation, i.e., for a velocity distribution defined by $\mathbf{u}_a=\mathbf{u}+\mathbf{r}_a\times\boldsymbol{\omega}$ where $\mathbf{u}$ and $\boldsymbol{\omega}$ are arbitrary constant vectors, i.e., $\mathbf{u}_{ab}=\mathbf{r}_{ab}\times\boldsymbol{\omega}$. Coming back to the general form [Eq. (27)], the latter condition is satisfied if

$$\forall\,\boldsymbol{\omega},\quad \sum_b \boldsymbol{\alpha}_{ab}(\mathbf{r}_{ab}\times\boldsymbol{\omega}) = \mathbf{0}. \tag{45}$$

By similar arguments, it can easily be proved that this requires the existence of vectors $\boldsymbol{\gamma}'_{ab}=-\boldsymbol{\gamma}'_{ba}$ such that

$$\boldsymbol{\alpha}_{ab} = \boldsymbol{\gamma}'_{ab} \otimes \mathbf{r}_{ab}. \tag{46}$$

Conditions [Eqs. (44) and (46)] are simultaneously fulfilled if and only if there exist symmetric scalar coefficients γ_{ab} so that $\boldsymbol{\gamma}_{ab}=\gamma_{ab}\mathbf{r}_{ab}=\boldsymbol{\gamma}'_{ab}$. Finally, the matrices $\boldsymbol{\alpha}_{ab}$ can be written as

$$\boldsymbol{\alpha}_{ab} = \gamma_{ab}\mathbf{r}_{ab} \otimes \mathbf{r}_{ab},$$

$$\gamma_{ba} = \gamma_{ab}. \tag{47}$$

With this formula, the particle friction forces [Eq. (27)] take the form

$$\mathbf{F}_a^{diss} = -\sum_b \gamma_{ab}(r_{ab})(\mathbf{u}_{ab}\cdot\mathbf{r}_{ab})\mathbf{r}_{ab} \tag{48}$$

(we remind that the $\boldsymbol{\alpha}_{ab}$'s, and thus the γ_{ab}'s, are functions of the particle distance r_{ab}). The dissipation function [Eq. (33)] now reads

$$F = \frac{1}{2}\sum_{a,b} \gamma_{ab}(r_{ab})(\mathbf{u}_{ab}\cdot\mathbf{r}_{ab})^2. \tag{49}$$

As required, both the shear forces [Eq. (48)] and the energy dissipation [Eq. (49)] vanish for a rigid body motion ($\mathbf{u}_{ab}\cdot\mathbf{r}_{ab}=0$). One could be surprised that the friction force exerted on a by b takes the form $\mathbf{F}_{b\to a}^{diss}=\gamma_{ab}(\mathbf{u}_{ab}\cdot\mathbf{r}_{ab})\mathbf{r}_{ab}$, thus is collinear to $\mathbf{r}_{ab}$, contrary to what the theory of continuous viscous fluids suggests, i.e., a shear force collinear with $\mathbf{u}_{ab}$ (see Sec. III B). The latter case would involve matrices $\boldsymbol{\alpha}_{ab}$ proportional to the identity $\mathbf{I}_n$, but would violate the conservation of total angular momentum and the nondissipative character of rigid motions.

In order to ensure the definite positiveness of the $\boldsymbol{\alpha}_{ab}$'s, the γ_{ab}'s must be positive non zero quantities. It is apparently surprising to find that, for $b=a$, $\mathbf{r}_{aa}$ is simply the null vector 0, thus the $\boldsymbol{\alpha}_{aa}$'s seem to be null matrices, contrary to the what latter condition states. However, one should remember that the γ_{ab}'s are functions of the distances r_{ab}. From Eq. (47), it appears that the non-nullity of the matrices $\boldsymbol{\alpha}_{aa}$'s can be obtained provided $\gamma_{ab}\mathbf{r}_{ab}\otimes\mathbf{r}_{ab}$ tends to a nonzero constant while $\mathbf{r}_{ab}$ tends to zero, i.e., if γ_{ab} varies according to r_{ab}^{-2} when r_{ab} tends to zero. Thus, there must exist a function $g_{ab}(r_{ab})$ so that

$$\gamma_{ab} = \frac{g_{ab}(r_{ab})}{r_{ab}^2},$$

$$g_{ab}(r_{ab}) \underset{r_{ab}\to 0}{\to} g_a > 0, \tag{50}$$

where g_a's are positive quantities, constant with respect to the particle distance (however, g_a can depend on local thermodynamical properties of the particle a, like its temperature). Formulae (48) and (49) now read

$$\mathbf{F}_a^{diss} = -\sum_b g_{ab}(r_{ab})(\mathbf{u}_{ab}\cdot\mathbf{e}_{ab})\mathbf{e}_{ab},$$

$$F = \frac{1}{2}\sum_{a,b\neq a} \frac{g_{ab}(r_{ab})}{r_{ab}}(\mathbf{u}_{ab}\cdot\mathbf{e}_{ab})^2, \tag{51}$$

where we have used unit vectors

$$\mathbf{e}_{ab} = \frac{\mathbf{r}_{ab}}{r_{ab}} = -\mathbf{e}_{ba}. \tag{52}$$

To finish this section, let us examine how the particle friction forces influence the volume in the macroscopic phase space. According to Eqs. (18) and (38), one can write

$$\frac{1}{\tilde{V}}\frac{d\tilde{V}}{dt} = -\sum_{a,b} \mathrm{tr}(\boldsymbol{\alpha}_{ab}\boldsymbol{\Gamma}_{ab}) = -\sum_a \frac{\mathrm{tr}\,\boldsymbol{\alpha}_{aa}}{m_a}, \tag{53}$$

where the matrices are of order n (i.e., the space dimension), contrary to Eq. (18) where those were of order N (i.e., the number of mechanical parameters). With Eq. (53), it appears even more clearly than with Eq. (18) that the dissipative property of friction forces (or the positiveness of *all* the matrices $\boldsymbol{\alpha}_{ab}$) is responsible for a decrease of volumes in the phase space. If the matrices $\boldsymbol{\alpha}_{aa}$ were null, the decrease of volumes in the macroscopic phase space would not be fulfilled by the model. With Eq. (50), we finally get

$$\frac{1}{\tilde{V}}\frac{d\tilde{V}}{dt} = -\sum_a \frac{1}{m_a}\lim_{b\to a}[\gamma_{ab}(r_{ab})r_{ab}^2] = -\sum_a \frac{g_a}{m_a} < 0 \tag{54}$$

(keeping in mind the positiveness of masses).

III. APPLICATION TO THE SPH NUMERICAL METHOD

A. Brief overview of the SPH background

At the limit where the size of the particles tends to zero while their number tends to infinity, the above equations lead to the Lagrangian theory of continuous fluids [8]. However, a Lagrangian computational approach can be directly constructed from the discrete viewpoint developed in the previous section. We will now investigate how the above principles can serve to write the discrete equations of the SPH numerical method in relevant forms. SPH is today widely used in CFD (see Ref. [1] for a detailed review). It is not within the scope of this paper to repeat or summarize the numerous works already made on the accuracy of SPH interpolants and operators; we will first give a brief overview of these principles. SPH is based on the idea that a flow may be modeled using a collection of macroscopic particles $\{a\}$ following the ideas and notations of Sec. II. However, writing the equations of motion of a fluid requires further assumptions. Discrete approximations of continuous differential operators are performed through the following process. For any scalar field A, the ensemble of its values at the points occupied by the particles is denoted by $\{A_a\}$. First, Ω being the fluid domain, A_a is approximated by

$$\begin{aligned} A_a = A(\mathbf{r}_a) &= \int_\Omega A(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_a)d^n\mathbf{r} \\ &\approx \int_\Omega A(\mathbf{r})w_h(\mathbf{r}-\mathbf{r}_a)d^n\mathbf{r} \\ &\approx \sum_b V_b A(\mathbf{r}_b)w_h(\mathbf{r}_{ab}). \end{aligned} \tag{55}$$

The first line of Eq. (55) is exact. The Dirac distribution δ is then approximated by a kernel regular function w_h, and the integral is approximated by a discrete (Riemann) summation over the particles b, where $\{V_a\}$ are the volumes of the particles. The kernel is generally compactly supported, so that the discrete sum involves a limited number of neighbor particles. Besides, it is proved [9] that the approximation [Eq. (55)] is better if w_h only depends on the particle distance, i.e., $w_h(\mathbf{r})=w_h(r)$. We, thus, introduce a positive dimensionless kernel f such that

$$w_h(r) = \frac{\alpha_{w,n}}{h^n} f(q), \tag{56}$$

where $q=r/h$, h being the so-called smoothing length and $\alpha_{w,n}$ a dimensionless constant depending on the choice of the kernel and the space dimension n (usually equal to 2 or 3). Note that we restrict here are considerations to a constant smoothing length. The kernel is also usually required to be normalized, i.e., to satisfy

$$\int_\Omega w_h(r)d^n\mathbf{r} = 1. \tag{57}$$

Under this assumption, considerations of spatial symmetry easily show that all momenta of odd orders of $\dot{w}_h$ vanish, i.e., for all integers m:

$$\int_\Omega \dot{w}_h(r)\underbrace{\mathbf{r}\otimes\mathbf{r}\otimes\ \ldots\ \otimes\mathbf{r}}_{2m+1}d^n\mathbf{r} = \mathbf{0} \tag{58}$$

(in our notations, for any set of m vectors $\mathbf{A},\mathbf{B},\ldots,\mathbf{Z}$, the quantity $\mathbf{A}\otimes\mathbf{B}\otimes\ldots\otimes\mathbf{Z}$ is a tensor of order m whose components are $A_{i_1}B_{i_2}\ldots Z_{i_m}$). The constant $\alpha_{w,n}$ is chosen such that the normalizing condition (57) is fulfilled, which gives

$$\alpha_{w,n} = \frac{1}{S_n\displaystyle\int_0^{R_f} f(q)q^{n-1}dq}, \tag{59}$$

where R_f is the radius of the support of f and S_n is the surface of the unit sphere in dimension n. We consider here the following example of kernel, namely, the spline of order 5 given by

$$f_5(q) = \begin{cases} (3-q)^5 - 6(2-q)^5 + 15(1-q)^5 & \text{if} \quad 0 \le q \le 1 \\ (3-q)^5 - 6(2-q)^5 & \text{if} \quad 1 \le q \le 2 \\ (3-q)^5 & \text{if} \quad 2 \le q \le 3 \\ 0 & \text{if} \quad 3 \le q, \end{cases} \tag{60}$$

with support of radius $R_f=3$, while (59) gives

$$\alpha_{w,2} = \frac{7}{478\pi},$$

$$\alpha_{w,3} = \frac{1}{120\pi}. \tag{61}$$

Let us now come back to the SPH interpolation. Denoting $w_{ab} \doteqdot w_h(r_{ab})$, Eq. (55) reads

$$A_a \approx \sum_b V_b A_b w_{ab}. \tag{62}$$

As an example, the density $\{\rho_a\}$ of the particles are defined by

$$\rho_a = \frac{m_a}{V_a} \tag{63}$$

and can be interpolated using Eq. (62) to give

$$\rho_a \approx \sum_b m_b w_{ab}. \tag{64}$$

The assumption regarding the kernel dependency on r_{ab} also yield the following rule:

$$\frac{\partial w_h(r_{ab})}{\partial \mathbf{r}_a} = \dot{w}_h(r_{ab})\mathbf{e}_{ab}, \tag{65}$$

where

$$\dot{w}_h = \frac{\alpha_{w,n}}{h^{n+1}}\dot{f}(q) \tag{66}$$

is the first derivative of w_h and $\mathbf{e}_{ab}$ is defined by Eq. (52). Introducing the notation $\dot{w}_{ab} \doteqdot \dot{w}_h(r_{ab})$, we can write

$$w_{ab} = w_{ba},$$

$$\dot{w}_{ab} = \dot{w}_{ba}. \tag{67}$$

Then, taking the gradient of Eq. (62) with respect to $\mathbf{r}_a$ and using Eq. (65) lead to a discrete approximation of the gradient of A:

$$(\text{grad } A)_a \approx \sum_b V_b A_b \dot{w}_{ab} \mathbf{e}_{ab}. \tag{68}$$

Such considerations can be applied to any kind of tensor. We will thus introduce discrete gradient ($\mathbf{G}$) and divergence (D) operators of scalar ($\{A_b\}$) and vector ($\{\mathbf{A}_b\}$) fields at the location of the particle a as

$$\mathbf{G}_a\{A_b\} \doteq \sum_b V_b A_b \dot{w}_{ab} \mathbf{e}_{ab} \approx (\text{grad } A)_a,$$

$$D_a\{\mathbf{A}_b\} \doteq \sum_b V_b \mathbf{A}_b \cdot \dot{w}_{ab} \mathbf{e}_{ab} \approx (\text{div } \mathbf{A})_a. \tag{69}$$

Formulas (69) are not the only possible ones allowing gradient and divergence discrete approximations. We may first observe that for every real number k, the following exact rules stand:

$$\text{grad } A = \rho^k \text{ grad} \frac{A}{\rho^k} + \frac{A}{\rho^k} \text{grad}(\rho^k),$$

$$\text{div } \mathbf{A} = \frac{1}{\rho^k} \text{div}(\rho^k \mathbf{A}) - \frac{\mathbf{A}}{\rho^k} \cdot \text{grad}(\rho^k). \tag{70}$$

Writing the above two expressions at the location of the particle a, and using $\mathbf{G}$ and D to approximate the continuous operators, then using the definitions [Eq. (69)], we find a family of discrete gradient ($\mathbf{G}^k$) and divergence (D^k) operators,

$$\mathbf{G}_a^k\{A_b\} \doteq \sum_b V_b \frac{\rho_b^{2k} A_a + \rho_a^{2k} A_b}{(\rho_a \rho_b)^k} \dot{w}_{ab} \mathbf{e}_{ab},$$

$$D_a^k\{\mathbf{A}_b\} \doteq -\frac{1}{\rho_a^{2k}} \sum_b V_b (\rho_a \rho_b)^k \mathbf{A}_{ab} \cdot \dot{w}_{ab} \mathbf{e}_{ab} \tag{71}$$

(see e.g. Refs. [9,10]). Under the assumptions of isotropy and normalization of the kernel [in particular, from the important consequence Eq. (58)], the various operators introduced above are accurate up to order 2 regarding h [9]. They have different properties, which make them more or less relevant to model the equations of motion in a discrete form. Let us remind the continuity and inviscid momentum equations for a compressible fluid:

$$\frac{d\rho}{dt} = -\rho \text{ div } \mathbf{u},$$

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \text{grad } p + \mathbf{g}. \tag{72}$$

Using the operators $\mathbf{G}^k$ and D^k [Eq. (71)] to approximate grad p and div $\mathbf{u}$, we immediately find the following discrete form giving the evolution of particle densities along time:

$$\forall a, \quad \frac{d\rho_a}{dt} = \frac{1}{\rho_a^{2k-1}} \sum_b V_b (\rho_a \rho_b)^k \mathbf{u}_{ab} \cdot \dot{w}_{ab} \mathbf{e}_{ab},$$

$$\frac{d\mathbf{u}_a}{dt} = -\sum_b m_b \frac{\rho_b^{2k} p_a + \rho_a^{2k} p_b}{(\rho_a \rho_b)^{k+1}} \dot{w}_{ab} \mathbf{e}_{ab} + \mathbf{g}. \tag{73}$$

Equation (73) can be used to compute the particle densities $\{\rho_a\}$ and velocities $\{\mathbf{u}_a\}$. The SPH equation of motion thus takes the form of a discrete particle momentum equation involving individual forces, just as in Sec. II. The choice of $\mathbf{G}^k$ as a gradient operator shows the advantage that the pressure (i.e., internal) forces are now written as

$$\mathbf{F}_{b\to a}^{\text{int}} = -m_a m_b \frac{\rho_b^{2k} p_a + \rho_a^{2k} p_b}{(\rho_a \rho_b)^{k+1}} \dot{w}_{ab} \mathbf{e}_{ab} = -\mathbf{F}_{a\to b}^{\text{int}}. \tag{74}$$

The last equality stems from the symmetry rules [Eqs. (52) and (67)]. Thus, the internal forces satisfy the conservation of total linear momentum of a closed set of particles, as required by the theory. Moreover, forces [Eq. (74)] are collinear with $\mathbf{e}_{ab}$ and hence satisfy the conservation of total-angular momentum [11]. As a matter of fact, the above discrete conservation law suggests that the SPH equation of motion [Eq. (73)] may be derived from an action principle, which has been known for a long time for some particular forms of this equation (Refs. [9,10]). This shows the relevance of the choice made in Eq. (73) for the discrete form of the divergence (D^k) and gradient ($\mathbf{G}^k$) operators, respectively. We may say that the discrete operators $\mathbf{G}^k$ and D^k are compatible in a variational acceptation. Ref. [12] shows how this compatibility stems from the nondissipative Hamiltonian principles, as stated in Sec. II B.

B. SPH dissipative forces

We now come to SPH approximations of dissipative forces, using the considerations developed in Sec. II B. We first remind the general continuous form of the momentum equation for viscous fluids. The extension of Euler's momentum Eq. (72) to friction forces, i.e., the Navier-Stokes momentum equation, can be written as

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \text{grad } p + \frac{1}{\rho} \text{div } \boldsymbol{\tau} + \mathbf{g}, \tag{75}$$

with

$$\boldsymbol{\tau} = \mu \mathbf{s}^D + \zeta (\text{div } \mathbf{u}) \mathbf{I},$$

$$\text{div } \boldsymbol{\tau} = \text{div}(\mu \mathbf{s}) + \text{grad}\left[\left(\zeta - \frac{2}{3}\mu\right) \text{div } \mathbf{u}\right],$$

$$\mathbf{s} = \frac{1}{2}[\text{grad } \mathbf{u} + (\text{grad } \mathbf{u})^T], \tag{76}$$

where μ and ζ are the fluid viscosities, $\mathbf{s}$ the rate-of-strain tensor and the superscript ^{D} denotes its deviatoric part [13]. We must then extend our SPH considerations to discrete op-

erators of order 2. It is known that using second-order derivatives of the kernel leads to unphysical diffusion properties [1] and to numerical instabilities. It is therefore recommended to find SPH interpolands of first order, through the following scheme. We first give an idea of the typical SPH form of such operators by focusing on the vector $[\mathrm{div}(K_A\ \mathrm{grad}\ \mathbf{A})]_a$, where K_A is a scalar diffusion coefficient relative to the vector field $\mathbf{A}$. Using a vectorial form of the operator D^k [Eq. (71)] to estimate grad $\mathbf{A}$ gives the following approximation:

$$\mathbf{D}_a^k\{(K_A\ \mathrm{grad}\ \mathbf{A})_b\} = \sum_b V_b \frac{\rho_b^{2k} K_{A,a}(\mathrm{grad}\ \mathbf{A})_a + \rho_a^{2k} K_{A,b}(\mathrm{grad}\ \mathbf{A})_b}{(\rho_a\rho_b)^k} \cdot \dot{w}_{ab}\mathbf{e}_{ab}. \tag{77}$$

The gradients appearing in Eq. (77) could be estimated with the operators $\mathbf{G}^k$ [12], but this method would lead to double discrete summations, resulting in a too demanding numerical algorithm. We will then approximate the gradients by Taylor-expanding $\mathbf{A}_b$ to the first order around $\mathbf{r}_a$,

$$\mathbf{A}_b = \mathbf{A}_a - (\mathrm{grad}\ \mathbf{A})_a \cdot \mathbf{r}_{ab} + \mathbf{O}(r_{ab}^2) \tag{78}$$

(the "minus" sign stems from the definition $\mathbf{r}_{ab}=\mathbf{r}_a-\mathbf{r}_b$). We thus obtain

$$(\mathrm{grad}\ \mathbf{A})_a \cdot \mathbf{e}_{ab} \approx \frac{\mathbf{A}_{ab}}{r_{ab}}. \tag{79}$$

Swapping indices in Eq. (79) also gives

$$(\mathrm{grad}\ \mathbf{A})_b \cdot \mathbf{e}_{ab} = -(\mathrm{grad}\ \mathbf{A})_b \cdot \mathbf{e}_{ba} \approx -\frac{\mathbf{A}_{ba}}{r_{ba}} = \frac{\mathbf{A}_{ab}}{r_{ab}}. \tag{80}$$

Introducing Eqs. (79) and (80) into Eq. (77) gives a new family of "Laplacian" operators:

$$\mathbf{L}_a^k[\{K_{A,b}\},\{\mathbf{A}_b\}] \doteq \sum_b V_b \frac{\rho_b^{2k} K_{A,a} + \rho_a^{2k} K_{A,b}}{(\rho_a\rho_b)^k} \frac{\mathbf{A}_{ab}}{r_{ab}} \dot{w}_{ab} \approx [\mathrm{div}(K_{\mathbf{A}}\ \mathrm{grad}\ \mathbf{A})]_a. \tag{81}$$

For $k=0$, we find

$$\mathbf{L}_a^0[\{K_{\mathbf{A},b}\},\{\mathbf{A}_b\}] \doteq 2\sum_b V_b \frac{\bar{K}_{\mathbf{A},ab}\mathbf{A}_{ab}}{r_{ab}} \dot{w}_{ab}, \tag{82}$$

with, for any arbitrary field B,

$$\bar{B}_{ab} = \frac{B_a + B_b}{2}. \tag{83}$$

However, this method can hardly be extended to arbitrary second derivatives. Following Ref. [1], we will use the following general discrete approximation of the ij component of the tensor $[\mathrm{grad}(K_{\mathbf{A}}\ \mathrm{grad}\ \mathbf{A})]_a$:

$$\left[\frac{\partial}{\partial x_i}\left(K_A \frac{\partial A}{\partial x_j}\right)\right]_a \approx \sum_b V_b \frac{\bar{K}_{A,ab} A_{ab}}{r_{ab}} [(n+2)e_{ab,i}e_{ab,j} - \delta_{ij}]\dot{w}_{ab}, \tag{84}$$

where $e_{ab,i}$ is the i-th component of the vector $\mathbf{e}_{ab}$ (n is still the dimension of the problem). This form was first suggested by [2] for a similar Lagrangian numerical method (smoothed dissipative particle dynamics) in the case $n=3$ and constant K_A, and extended to the cases $n=2$ and $n=3$ for SPH and arbitrary K_A in Ref. [1]. However, the latter paper does not provide any accurate proof of this result for nonconstant diffusion coefficients. We give an accurate demonstration of Eq. (84) for arbitrary dimensions and diffusion coefficients in the Appendix of the present paper. Note that the case of a nonconstant viscosity is important for modeling multiphase flows; it can also be required when considering turbulent flows modeled through Boussinesq's eddy viscosity assumption as a closure for the Reynolds stress tensor (see e.g., Ref. [14] or Ref. [15]. for its application to SPH).

All second order operators can be deduced by applying Eq. (84) to an arbitrary component A_l of a vector, and by multiplying the result by the unit vector corresponding to the mth axis,

$$\left[\frac{\partial}{\partial x_i}\left(K_A \frac{\partial A_l}{\partial x_j}\right)\right]_a \mathbf{e}_m \approx \sum_b V_b \frac{\bar{K}_{A,ab} A_{ab,l}}{r_{ab}} [(n+2)e_{ab,i}e_{ab,j} - \delta_{ij}]\dot{w}_{ab}\mathbf{e}_m. \tag{85}$$

Contracting indices $l=m$ and $i=j$ gives

$$[\mathrm{div}(K_A\ \mathrm{grad}\ \mathbf{A})]_a \approx 2\sum_b V_b \frac{\bar{K}_{A,ab}\mathbf{A}_{ab}}{r_{ab}} \dot{w}_{ab}, \tag{86}$$

which is identical to Eq. (82). Next, coming back to Eq. (85) and setting $l=i$ and $m=j$ yields

$$\{\mathrm{div}[K_A(\mathrm{grad}\ \mathbf{A})^T]\}_a \approx \sum_b V_b \frac{\bar{K}_{A,ab}}{r_{ab}} [(n+2)(\mathbf{A}_{ab}\cdot\mathbf{e}_{ab})\mathbf{e}_{ab} - \mathbf{A}_{ab}]\dot{w}_{ab}. \tag{87}$$

Then, setting $l=j$ and $m=i$ in Eq. (85) leads to

$$[\mathrm{grad}(K_A\ \mathrm{div}\ \mathbf{A})]_a \approx \sum_b V_b \frac{\bar{K}_{A,ab}}{r_{ab}} [(n+2)(\mathbf{A}_{ab}\cdot\mathbf{e}_{ab})\mathbf{e}_{ab} - \mathbf{A}_{ab}]\dot{w}_{ab} \tag{88}$$

[note that the discrete forms Eqs. (87) and (88) are identical, although the corresponding continuous operators are equal only if K_A is a constant]. The last three approximations allow to write an SPH form of shear forces [Eq. (76)] as

$$(\mathrm{div}\ \boldsymbol{\tau})_a \approx \sum_b \frac{V_b}{r_{ab}}\left[(n+2)\left(\frac{\bar{\mu}_{ab}}{3} + \bar{\zeta}_{ab}\right)(\mathbf{u}_{ab}\cdot\mathbf{e}_{ab})\mathbf{e}_{ab} + \left(\frac{5\bar{\mu}_{ab}}{3} - \bar{\zeta}_{ab}\right)\mathbf{u}_{ab}\right]\dot{w}_{ab}. \tag{89}$$

For $n=2$ and constant viscosities, the latter equation gives the viscous force proposed in Ref. [2]. The case of an incompressible flow [div $\mathbf{u}=0$, or $\zeta=\frac{2}{3}\mu$ according to Eq. (76)] simplifies it to

$$(\text{div } \boldsymbol{\tau})_a \approx \sum_b V_b \frac{\bar{\mu}_{ab}}{r_{ab}}[(n+2)(\mathbf{u}_{ab}\cdot\mathbf{e}_{ab})\mathbf{e}_{ab}+\mathbf{u}_{ab}]\dot{w}_{ab}. \tag{90}$$

If in addition to the incompressibility assumption, we state that the viscosity μ is constant in space, we observe that

$$\text{div}[(\text{grad } \mathbf{u})^T] = \text{grad div } \mathbf{u} = \mathbf{0}. \tag{91}$$

Thus, according to Eq. (86) we get

$$(\text{div } \boldsymbol{\tau})_a = \mu[\text{div}(\text{grad } \mathbf{u})]_a \approx 2\mu\sum_b V_b \frac{\mathbf{u}_{ab}}{r_{ab}}\dot{w}_{ab}. \tag{92}$$

This form of SPH viscous forces was proposed first in Ref. [16] with a nonconstant viscosity, similarly to Eq. (82). Finally, under the same assumptions we may invoke Eq. (91) to write

$$(\text{div } \boldsymbol{\tau})_a = \mu[\text{div}(\text{grad } \mathbf{u} + 2(\text{grad } \mathbf{u})^T)]_a \approx 2(n+2)\mu\sum_b V_b \frac{\mathbf{u}_{ab}\cdot\mathbf{e}_{ab}}{r_{ab}}\dot{w}_{ab}\mathbf{e}_{ab}, \tag{93}$$

which agrees with the standard SPH artificial viscous forces proposed in ref [10], as well as the molecular of turbulent viscous forces suggested on identical backgrounds in Ref. [15], although both papers incorrectly assumed this model to be valid for variable viscosities. We thus got four formulae [Eqs. (89), (90), (92), and (93) to estimate shear forces, the last three being applicable to incompressible flows and the last two to constant viscosities only. Referring to Sec. II B, we notice that all of them consist of individual friction forces $\mathbf{F}^{diss}_{b\to a}$ between pairs of particles, according to the general form [Eq. (27) and (31)]. Equation (89) corresponds to friction matrices defined by

$$\boldsymbol{\alpha}_{ab} = -\frac{V_a V_b}{r_{ab}}\dot{w}_{ab}\left[(n+2)\left(\frac{\bar{\mu}_{ab}}{3}+\bar{\zeta}_{ab}\right)\mathbf{e}_{ab}\otimes\mathbf{e}_{ab} + \left(\frac{5\bar{\mu}_{ab}}{3}-\bar{\zeta}_{ab}\right)\mathbf{I}_n\right], \tag{94}$$

while Eq. (90) gives

$$\boldsymbol{\alpha}_{ab} = -V_a V_b \frac{\bar{\mu}_{ab}}{r_{ab}}\dot{w}_{ab}[(n+2)\mathbf{e}_{ab}\otimes\mathbf{e}_{ab}+\mathbf{I}_n]. \tag{95}$$

Equation (92) gives

$$\boldsymbol{\alpha}_{ab} = -2\mu\frac{V_a V_b}{r_{ab}}\dot{w}_{ab}\mathbf{I}_n \tag{96}$$

and Eq. (93) yields

$$\boldsymbol{\alpha}_{ab} = -2(n+2)\mu\frac{V_a V_b}{r_{ab}}\dot{w}_{ab}\mathbf{e}_{ab}\otimes\mathbf{e}_{ab} \tag{97}$$

[note that, with a constant μ, Eq. (95) is the average of Eqs. (96) and (97)]. In formulae (94)–(97) the dependency of the $\boldsymbol{\alpha}_{ab}$'s on particle distance r_{ab} stands through the quantities $\dot{w}_{ab}=\dot{w}_h(r_{ab})$. The symmetry condition [Eq. (29)] of the matrices $\boldsymbol{\alpha}_{ab}$ [i.e., the action-reaction law, Eq. (35)] is satisfied by these four models, but not the definite positiveness. Indeed, the general form [Eq. (94)] yields the following dissipation function from [Eq. (33)], after some algebra,

$$F = -\frac{1}{2}\sum_{a,b}\frac{V_a V_b}{r_{ab}}\left\{\frac{\bar{\mu}_{ab}}{3}[(n+2)(\mathbf{e}_{ab}\cdot\mathbf{u}_{ab})^2+5u_{ab}^2] + \bar{\zeta}_{ab}[(n+2)(\mathbf{e}_{ab}\cdot\mathbf{u}_{ab})^2-u_{ab}^2]\right\}\dot{w}_{ab}, \tag{98}$$

which sign is not fixed, due to the factor $-u_{ab}^2$. In contrast, note that the original Navier-Stokes Eq. (75) gives the energy loss by dissipation (for a closed fluid, ideally without contact forces at its boundary) as

$$\frac{dH}{dt} = -\int_\Omega \boldsymbol{\tau}:\mathbf{s}d\Omega = -\int_\Omega [\mu\mathbf{s}^D:\mathbf{s}^D+\zeta(\text{div } \mathbf{u})^2]d\Omega. \tag{99}$$

Equation (99) gives the energy dissipation from a positive form (provided μ and ζ are positive, see Ref. [13]), which can be seen as an extension of Eq. (41) to continuous fluids. Equation (98) is, thus, a discrete approximation of (99), and its nonpositiveness points out a weakness of the proposed model [Eq. (84)] for the SPH second-order derivatives. However, for incompressible flows, the specific forms Eq. (95) and (97), respectively, read

$$F = -\frac{1}{2}\sum_{a,b} V_a V_b \frac{\bar{\mu}_{ab}}{r_{ab}}[(n+2)(\mathbf{e}_{ab}\cdot\mathbf{u}_{ab})^2+u_{ab}^2]\dot{w}_{ab} \tag{100}$$

for Eq. (95); then

$$F = -\mu\sum_{a,b}\frac{V_a V_b}{r_{ab}}u_{ab}^2\dot{w}_{ab} \tag{101}$$

for Eq. (96), and finally

$$F = -(n+2)\mu\sum_{a,b}\frac{V_a V_b}{r_{ab}}(\mathbf{e}_{ab}\cdot\mathbf{u}_{ab})^2\dot{w}_{ab} \tag{102}$$

for Eq. (97). Their positiveness is ensured provided $\dot{w}_{ab}<0$ for $b\neq a$, i.e., if the following condition is satisfied:

$$r>0:\dot{w}_h(r)<0. \tag{103}$$

Thus the kernel derivative must be negative for all nonzero particle distances, a condition satisfied by the kernel [Eq. (60)] introduced above (the behavior of $\dot{w}_h(r)$ in the vicinity of the origin will be stated below). On similar (thermodynamical) ideas, it has been noticed in Ref. [1] that this condition is necessary to model scalar (e.g., temperature) fluxes consistent with their gradients. The definite positive-

ness of energy dissipation through dissipative matrices Eq. (95) to Eq. (97) are then ensured; however, they possess different properties in view of the considerations made in Sec. II B. The proposition [Eq. (92)] presents the advantage to give shear forces collinear to the velocity difference $\mathbf{u}_{ab}$, in accordance to what the theory of continuous incompressible fluids suggests with $\boldsymbol{\tau}=\mu\mathbf{s}$. Nevertheless, our considerations regarding discrete dissipative forces show that the forces given by this model do not conserve angular momentum nor vanish for a rigid body motion. The latter two conditions require $\boldsymbol{\alpha}_{ab}=\gamma_{ab}\mathbf{r}_{ab}\otimes\mathbf{r}_{ab}$ [Eq. (47)], which is only satisfied by Eq. (97) [i.e., Eq. (93)] with

$$\gamma_{ab}=-2(n+2)\mu\frac{V_aV_b}{r_{ab}^3}\dot{w}_{ab}>0, \tag{104}$$

which thus seems to be the best of the three proposed formulae, but again, only experimental tests will drive us to firm conclusions about that point. In this case, the dissipation function [Eq. (102)] can be recovered from Eq. (49). Moreover, Eq. (50) tells us that $\gamma_{ab}(r_{ab})r_{ab}^2$ must tend to a positive, nonzero quantity g_a when r_{ab} tends to zero. With Eq. (104), we can conclude that $\dot{w}_h(r)$ must be equivalent to r when r tends to zero, in other words, using the dimensionless kernel Eq. (56), one must have

$$\dot{f}(q)\underset{q\to 0}{\sim}-C_wq, \tag{105}$$

where C_w is a positive, nonzero constant depending on the kernel. As a consequence, at the origin ($r=0$) the kernel first derivative must be null and its second derivative nonzero, negative:

$$\dot{f}(0)=0,$$

$$\ddot{f}(0)<0. \tag{106}$$

The kernel Eq. (60) satisfies these conditions with $C_w=120$. Dimensionally speaking, with Eq. (66), Eq. (105) reads

$$\dot{w}(r)\underset{r\to 0}{\sim}-\frac{C_w\alpha_{w,n}}{h^{n+2}}r. \tag{107}$$

A kernel which would not satisfy the conditions Eq. (106) would yield a wrong estimation of volumes in the phase space, and thus an incorrect behavior of the particle motion, as we will see later.

As an example, with model Eq. (93) for discrete viscous forces, the momentum Eq. (73) now takes the form

$$\forall a,\quad \frac{d\mathbf{u}_a}{dt}=\frac{1}{\rho_a}\sum_b V_b\left[-\frac{\rho_b^{2k}p_a+\rho_a^{2k}p_b}{(\rho_a\rho_b)^k}+2(n+2)\mu\frac{\mathbf{u}_{ab}\cdot\mathbf{e}_{ab}}{r_{ab}}\right]\dot{w}_{ab}\mathbf{e}_{ab}+\mathbf{g}. \tag{108}$$

As stated in Sec. II B, the (macroscopic) kinetic energy lost by the particles through the viscous forces is converted into heat. Modeling temperature raise in SPH does not present any additional difficulty, ensuring the exact conservation of total energy. A good review of these considerations is presented in Ref. [17].

Compared to more traditional approaches for modelling SPH viscous forces (see Refs. [10,16]), the present model does not increase computational time.

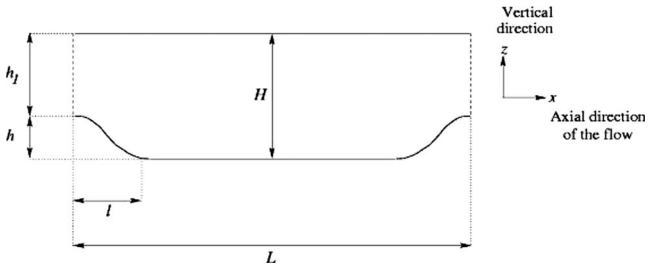

FIG. 1. Geometry of the periodic hill flow.

C. Application to a viscous steady flow

To illustrate the ability of the presented SPH interpolants to predict velocity fields, we now apply the model to a particular viscous flow. In order to compute the pressure, a state equation is used [18], based on a numerical speed of sound c_0 and a reference density ρ_0 (so that the flow keeps almost incompressible). The particles are initially placed on a regular Cartesian grid with initial particle spacing δr. We first use the kernel Eq. (60) with a smoothing length equal to 1.5 times the initial particle spacing. Wall conditions are specified through wall particles and fictitious particles, following the method, e.g., presented in Ref. [15]. These boundary particles are identical to fluid particles, i.e., they have the same mass and reference density, and are placed on a Cartesian grid, equally spaced with spacing δr. They prevent the fluid particles from crossing the walls, and thus ensure a total impermeability.

We successfully tested the present model on various configurations, including complex, rapidly moving free-surface flows. However, in order to present a clear quantitative validation in terms of velocity distribution, we focus here on a steady confined flow for which a comparison with a mesh-based method will be possible. We consider the test case of the two-dimensional (2D) periodic steady laminar hill flow [19] based on the geometry presented on Fig. 1 (the detailed geometry is available in Ref. [20]). The distances are $H=84.98$ mm, $L=252$ mm, $l=54$ mm, $h_H=28$ mm, and $h_I=56.98$ mm. About 20 000 water particles are driven by a horizontal propelling force with a constant mean velocity $U=1.785\times10^{-3}$ m/s. The Reynolds number, based on the hill height h_H and the mean velocity U, is equal to 50, and there is no free surface, the upper boundary being a solid wall (hence, gravity is not considered here). We set $\delta r=10^{-3}$ m and $c_0=0.06$ m/s. Consistently with the literature on weakly compressible SPH [16], the time step is determined by three conditions,

$$\delta t=\min\left(0.4\frac{h}{c_0};0.25\sqrt{\frac{h}{F_{\max}}};0.125\frac{h^2}{\nu}\right), \tag{109}$$

where h is the smoothing length, $\nu=10^{-6}$ m^2 s^{-1} the water molecular viscosity and $F_{\max}$ is the maximum force experi-

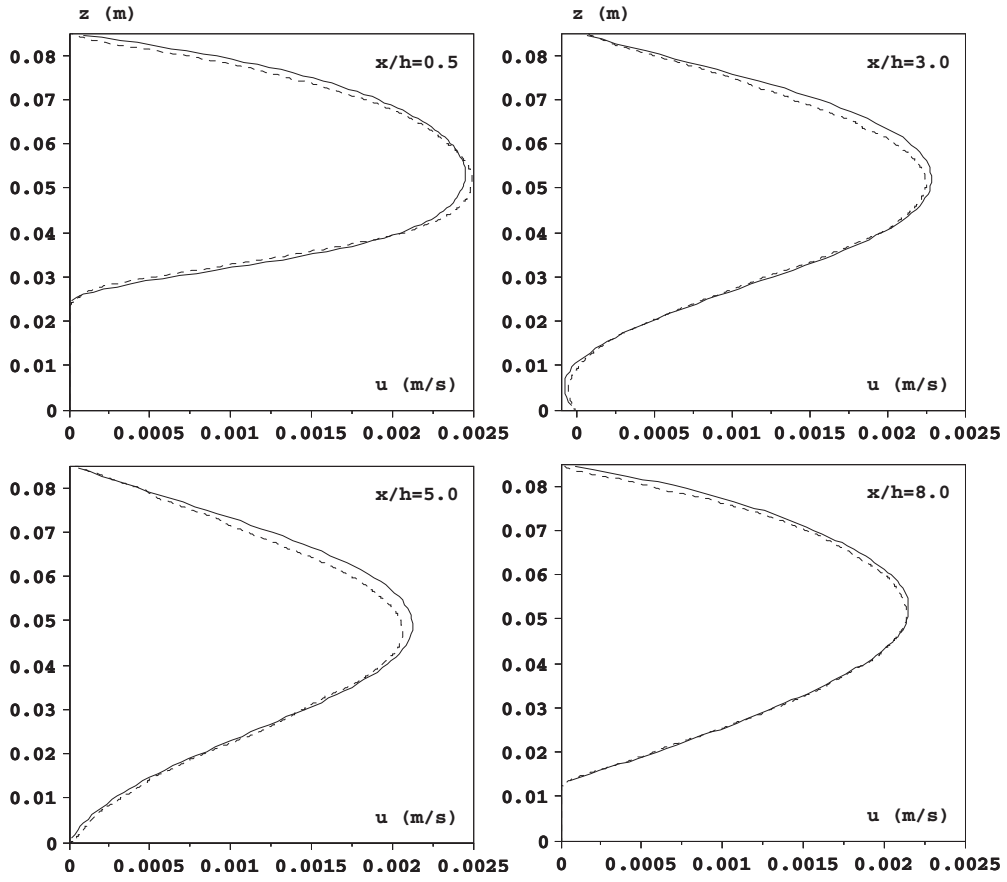

FIG. 2. Velocity profiles. Solid lines: Finite Volumes; dashed lines: SPH using Eq. (73) with $k=1$ (all choices for k give identical results) and model Eq. (93) for the dissipation, with the "standard' kernel" Eq. (60).

enced by a particle. In the present case, the Courant-Friedrich-Levy condition based on the speed of sound dominates and gives a constant time step $\delta t=10^{-2}$ s.

The results consist here of four vertical velocity profiles at $x/h=0.5$, 3.0, 5.0 and 8.0, respectively; they will be compared with the simulations presented in Ref. [20], made with the finite volume Eulerian method. Figure 2 shows that SPH presents a very good agreement to finite volumes. It may be emphasized that the Lagrangian nature of SPH yields small fluctuations that have been removed here using time averaging.

The three viscous models Eqs. (90), (92), and (93) were tested together with model Eq. (73) for density estimation and conservative forces with the choice $k=1$ (other choices give identical results). It appears that, due to the incompressibility of the flow and the constantness of the viscosity μ, they all give identical velocity profiles (see Fig. 2, where only model Eq. (93) were plotted since the three viscous models give almost superimposed curves). Hence, despite the fact that the first two models do not conserve angular momentum, the velocity distributions are not affected here. So far, we used in all our computations the kernel Eq. (60), which satisfies the conditions Eq. (106). In a second step, we tested two kernels violating those rules. First, we considered the following kernel:

$$f(q) = -\frac{1}{2}q^2 + 2q - 2,$$

$$\dot{f}(q) = -q + 2, \tag{110}$$

having a nonzero first derivative at the origin. Its radius is $R_f=2$, while Eq. (59) gives

$$\alpha_{w,2} = \frac{3}{28\pi} \tag{111}$$

in two dimensions. Figure 3 shows that the velocity profiles, even time averaged, are very scattered and underestimated. The kernel used here does not fulfill the rule Eq. (50), so that Eq. (54) shows that it preserves the volumes $\tilde{V}$ in the phase space instead of reducing them, which is the reason of the observed instability. In other words, the kernel does not allow energy to be dissipated up to the exact amount; the resulting scattered velocities induce artificial energy dissipation to remove the remaining energy. Next, we considered the following kernel:

$$f(q) = \frac{1}{4}q^4 - \frac{4}{3}q^3 + \frac{3}{2}q^2 + \frac{9}{4},$$

$$\dot{f}(q) = q(q-1)(q-3), \tag{112}$$

which has a zero first-order derivative at the origin, but a positive second-order derivative for small q's. Its radius is $R_f=3$, while Eq. (59) gives, in two dimensions:

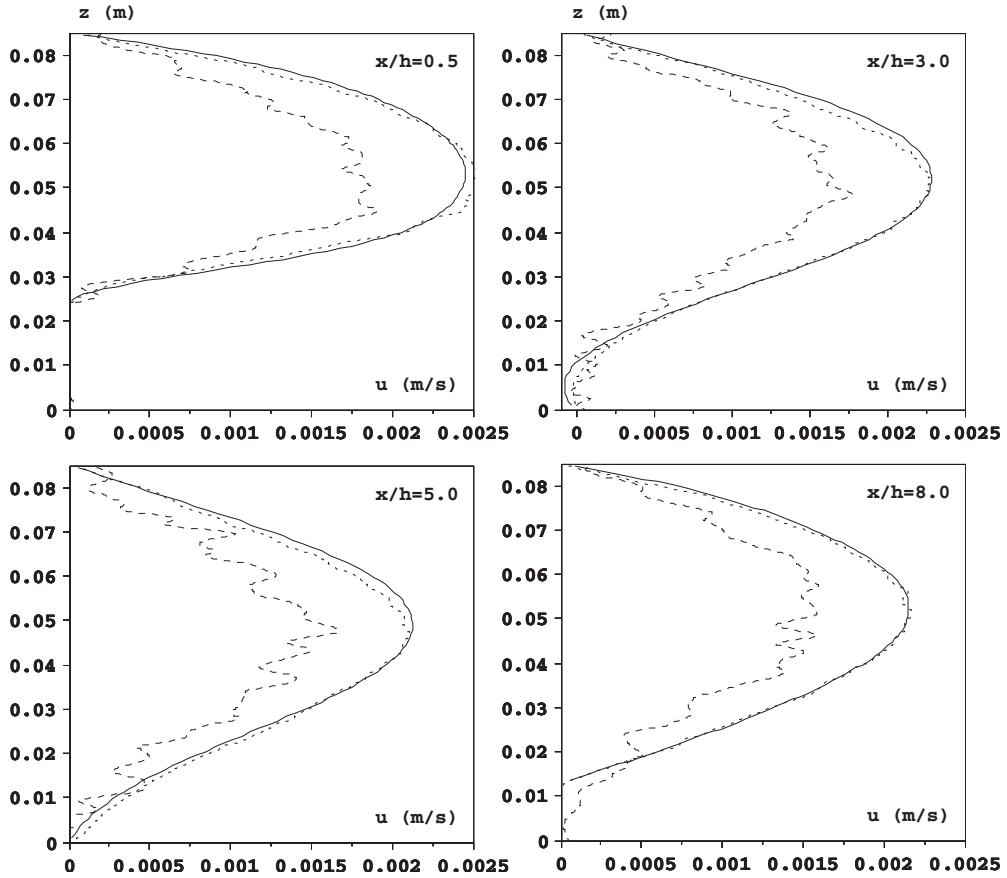

FIG. 3. Velocity profiles. Solid lines: Finite Volumes; dotted lines: SPH using the kernel Eq. (60); dashed lines: SPH using the kernel Eq. (110).

$$\alpha_{w,2} = \frac{20}{243\pi}. \tag{113}$$

This kernel gives better results than Eq. (110) in our test case when looking at time-averaged velocities (not plotted here), but Fig. 4 reveals that the instantaneous velocity profiles are again scattered, while with the kernel given by Eq. (60) they keep rather smooth and stable while time runs.

To finish, note that from Eq. (104), one can find the quantities g_a introduced at the end of Sec. II B,

$$g_a = \lim_{r_{ab}\to 0} (\gamma_{ab} r_{ab}^2) = \frac{2(n+2)C_w \alpha_{w,n}}{h^{n+2}} \mu V_a^2. \tag{114}$$

Thus, according to Eq. (54), the relative decrease in phase space volumes is given by

$$\frac{1}{\tilde{V}} \frac{d\tilde{V}}{dt} = -\frac{2(n+2)C_w \alpha_{w,n}}{h^{n+2}} \mu \sum_a \frac{V_a}{\rho_a}. \tag{115}$$

As expected, it is proportional to the fluid viscosity. One should not be surprised of the fact that Eq. (115) depends on the smoothing length h (i.e. on the spatial discretization) and on the choice of the kernel (through C_w and $\alpha_{w,n}$). The considerations at the end of Sec. II B show that the process of volume decrease in the phase space is strongly dependent on the scale at which the system is observed. As a matter of fact, dimensional considerations show that there cannot exist any formula giving the phase volume decrease in the continuous formalism of fluids, such as Eq. (99) for the energy dissipation.

IV. CONCLUSIONS

We have seen that Hamiltonian considerations can be extended to dissipative forces applied to a discrete system of particles, with consequences regarding the form of the discrete friction forces in order to satisfy the conservation properties as well as the volume shrinkage in the macroscopic phase space. Furthermore, we have given a solid demonstration of the general forms of second-order derivatives in SPH. Among those forms, our investigations on discrete particle dissipative forces reveal that only a limited number are consistent with the laws of Mechanics, in particular with the conservation of angular momentum. As for volume shrinkage and energy dissipation, a major requirement is that at the origin, the kernel $w_h(r)$ must have a first-order derivative which vanishes at the origin while its second-order derivative must be nonzero, negative in order to ensure stability. These constraints were found to be closely linked to the theoretical behavior of a dissipative mechanical system in the phase space. In the past, other conditions have been found to be necessary to keep SPH simulations stable in various acceptations: for example, it is known that the second-order

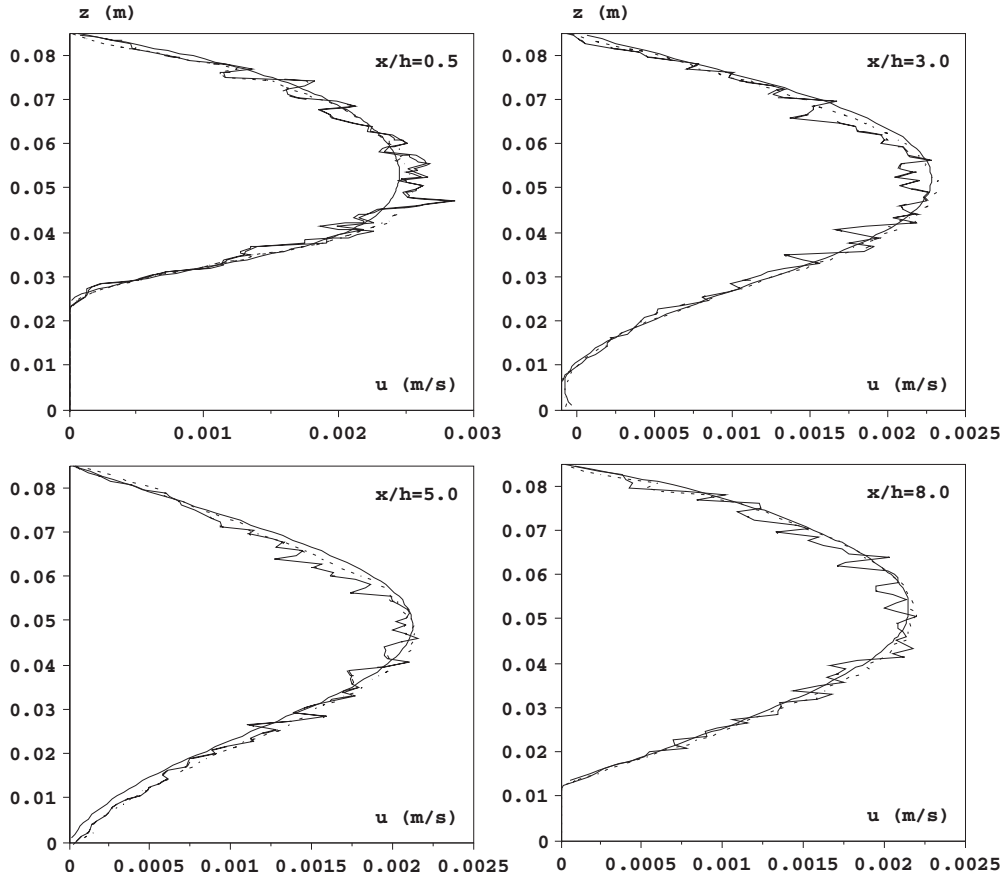

FIG. 4. Velocity profiles (here not time averaged). Solid lines: Finite Volumes; dotted lines: SPH using the kernel Eq. (60); dashed lines: SPH using the kernel Eq. (112).

derivative of the kernel must be nonzero, positive for all nonzero r_{ab}'s in order to avoid particle clustering [21]. The latter condition, together with our conditions, is obviously not easily satisfied. These considerations should be carefully considered by SPH developers, who often use arbitrary kernels. Besides, similar considerations could be extended, *mutatis mutandis*, to other particle methods such as DPD and MPS.

ACKNOWLEDGMENT

The author thanks Dr. Juan Uribe (University of Manchester, UK) for the laminar simulation over the periodic hill flow made with the Finite Volume software Code_Saturne (EDF R&D).

APPENDIX

We give here a demonstration of formula (84),

$$\left[\frac{\partial}{\partial x_i}\left(K_A\frac{\partial A}{\partial x_j}\right)\right]_a \approx \sum_b V_b \frac{\bar{K}_{A,ab}A_{ab}}{r_{ab}}[(n+2)e_{ab,i}e_{ab,j}-\delta_{ij}]\dot{w}_{ab}, \tag{A1}$$

which can be rewritten in a tensorial form as

$$\mathbf{G}_a \approx \sum_b V_b \frac{\bar{K}_{A,ab}A_{ab}}{r_{ab}}\left[(n+2)\frac{\mathbf{r}_{ab}\otimes\mathbf{r}_{ab}}{r_{ab}^2}-\mathbf{I}_n\right]\dot{w}_h(r_{ab}) \tag{A2}$$

where $\mathbf{G}$ is the following second order tensor:

$$\mathbf{G}=\mathrm{grad}[K_A(\mathrm{grad}\,A)]=\frac{\partial}{\partial x_i}\left(K_A\frac{\partial A}{\partial x_j}\right)\mathbf{e}_i\otimes\mathbf{e}_j \tag{A3}$$

(in which the $\mathbf{e}_i$'s are the unit vectors of a Cartesian basis). We first write an integral approximation of Eq. (A2), according to the SPH interpolation [Eq. (55)],

$$\mathbf{J}=\int_\Omega \frac{(\bar{K}_{A,ab}A_{ab})(\mathbf{r})}{r}\left[(n+2)\frac{\mathbf{r}\otimes\mathbf{r}}{r^2}-\mathbf{I}_n\right]\dot{w}_h(r)d^n\mathbf{r} \tag{A4}$$

Next, we use a Taylor expansion of K_AA in the vicinity of the particle a, similarly to Eq. (78) but up to the second order,

$$\begin{aligned}K_{A,b}A_b = {} & K_{A,a}A_a - K_{A,a}(\mathrm{grad}\,A)_a\cdot\mathbf{r}_{ab} - A_a(\mathrm{grad}\,K_A)_a\cdot\mathbf{r}_{ab}\\ & +\frac{1}{2}\mathbf{G}_a{:}(\mathbf{r}_{ab}\otimes\mathbf{r}_{ab})+\frac{1}{2}[(\mathrm{grad}\,K_A)_a\cdot\mathbf{r}_{ab}]\\ & \times[(\mathrm{grad}\,A)_a\cdot\mathbf{r}_{ab}]+O(r_{ab}^3),\end{aligned} \tag{A5}$$

where the double contraction of two tensors $\mathbf{A}$ and $\mathbf{B}$ of

respective orders p and q is defined by $\mathbf{A}:\mathbf{B}=A_{i_1 i_2 \cdots i_{p-1} i_p} B_{i_p i_{p-1} i_3 \cdots i_{q-1} i_q}$, with Einstein's summation convention regarding the dummy indices i_{p-1} and i_p. We then use first order developments of K_A and A analogous to Eq. (79):

$$(\text{grad } A)_a \cdot \mathbf{r}_{ab} = A_{ab} + O(r_{ab}^2)$$

$$(\text{grad } K_A)_a \cdot \mathbf{r}_{ab} = K_{A,ab} + O(r_{ab}^2). \tag{A6}$$

Combining Eqs. (A5) and (A6) gives

$$\bar{K}_{A,ab} A_{ab} \approx (K_A \text{ grad } A)_a \cdot \mathbf{r}_{ab} - \frac{1}{2}\mathbf{G}_a:(\mathbf{r}_{ab} \otimes \mathbf{r}_{ab}) + O(r_{ab}^3). \tag{A7}$$

On this basis, the integral Eq. (A4) can be developed as

$$\mathbf{J} = \left[\mathbf{J}_1 (K_A \text{ grad } A)_a + \frac{1}{2}\mathbf{J}_2:\mathbf{G}_a + \mathbf{J}_3 \right]. \tag{A8}$$

The integrals $\mathbf{J}_1$, $\mathbf{J}_2$, and $\mathbf{J}_3$ are tensors of respective orders 3, 4, and 2, defined by

$$\mathbf{J}_1 = \int_\Omega \frac{1}{r^2}\left[(n+2)\frac{1}{r}(\mathbf{r} \otimes \mathbf{r} \otimes \mathbf{r}) - \mathbf{I}_n \otimes \mathbf{r} \right] \dot{w}_h(r) d^n\mathbf{r},$$

$$\mathbf{J}_2 = -\int_\Omega \frac{1}{r^2}\left[(n+2)\frac{1}{r}(\mathbf{r} \otimes \mathbf{r} \otimes \mathbf{r} \otimes \mathbf{r}) - \mathbf{I}_n \otimes \mathbf{r} \otimes \mathbf{r} \right] \dot{w}_h(r) d^n\mathbf{r},$$

$$\mathbf{J}_3 = \int_\Omega \frac{1}{r^2} O(r^3)\left[(n+2)\frac{1}{r}\mathbf{r} \otimes \mathbf{r} - \mathbf{I}_n \right] \dot{w}_h(r) d^n\mathbf{r}. \tag{A9}$$

The property [Eq. (58)] shows that $\mathbf{J}_1$ and $\mathbf{J}_3$ are null; thus, Eq. (A8) gives

$$\mathbf{J} = \frac{1}{2}\mathbf{J}_2:\mathbf{G}_a + \mathbf{O}(h^4). \tag{A10}$$

To calculate $\mathbf{J}_2$, we write the volume of integration in dimension n as $d^n\mathbf{r}=r^{n-1}drd\omega$, where $d\omega$ is the infinitesimal angle of dimension n, which allows separating the variables:

$$\mathbf{J}_2 = -\int_0^{h_t} \dot{w}_h(r) r^n dr \left((n+2)\int_{\Sigma_n} \mathbf{e} \otimes \mathbf{e} \otimes \mathbf{e} \otimes \mathbf{e} d\omega - \mathbf{I}_n \otimes \int_{\Sigma_n} \mathbf{e} \otimes \mathbf{e} d\omega \right), \tag{A11}$$

where $\mathbf{e}$ is the local unit vector $\mathbf{r}/r$, running over the n-sphere Σ_n of radius unity and surface S_n. The first integral in Eq. (A11) is easily calculated from the kernel normalization condition (59),

$$\int_0^{h_t} \dot{w}_h(r) r^n dr = [w_h(r) r^n]_0^{h_t} - n\int_0^{h_t} w_h(r) r^{n-1} dr = -n\alpha_{w,n}\int_0^{R_f} f(q) q^{n-1} dq = -\frac{n}{S_n}. \tag{A12}$$

The last two integrals in Eq. (A11) can be calculated from symmetry conditions. We begin with the second one: the components of the second-order tensor $\mathbf{e}\otimes\mathbf{e}$ are $e_i e_j$, where $e_i = x_i/r$ denotes the i-th component of the unit vector $\mathbf{e}$ (not to be confused with the i-th unit vector of the basis $\mathbf{e}_i$, written in bold). Obviously, changing e_i into $-e_i$ keeps the integral unchanged, since the sphere is invariant through plane reflections. Thus, the only integrals of $e_i e_j$, which do not vanish are those with $i=j$. Besides, they are all equal to each other for reasons of isotropy, while their sum is the integral of $e_i e_i = 1$. From this it immediately follows that

$$\int_{\Sigma_n} \mathbf{e} \otimes \mathbf{e} d\omega = \frac{S_n}{n}\mathbf{I}_n \tag{A13}$$

For the integral of $\mathbf{e}\otimes\mathbf{e}\otimes\mathbf{e}\otimes\mathbf{e}$ in Eq. (A11), similar considerations show that the only nonzero components are of the form e_i^4 or $e_i^2 e_j^2$ with $i \neq j$. Observing that a rotation of angle $\pi/4$ around the origin in the (i,j)-plane keeps the sphere unchanged, we get

$$\int_{\Sigma_n} e_i^4 d\omega = \int_{\Sigma_n} \left(\frac{e_i + e_j}{\sqrt{2}} \right)^4 d\omega. \tag{A14}$$

Developing the last integral and using symmetry and isotropy, we obtain

$$\int_{\Sigma_n} e_i^4 d\omega = 3\int_{\Sigma_n} e_i^2 e_j^2 d\omega. \tag{A15}$$

On the other hand, we may also write

$$\int_{\Sigma_n} \left(\sum_i e_i^2 \right)^2 d\omega = \int_{\Sigma_n} \left(\sum_i e_i^4 + \sum_{i\neq j} e_i^2 e_j^2 \right) d\omega \tag{A16}$$

which gives

$$S_n = n\int_{\Sigma_n} e_i^4 d\omega + n(n-1)\int_{\Sigma_n} e_i^2 e_j^2 d\omega. \tag{A17}$$

Combining with Eq. (A15) yields

$$\int_{\Sigma_n} e_i^4 d\omega = \frac{3S_n}{n(n+2)}. \tag{A18}$$

The surface of the unit sphere being $S_n = 2\pi^{n/2}/\Gamma(\frac{n}{2})$ [22], for $n=2$ one obtains

$$S_n = 2\pi,$$

$$\int_{\Sigma_2} e_i^4 d\omega = \frac{3\pi}{4},$$

$$\int_{\Sigma_2} e_i^2 e_j^2 d\omega = \frac{\pi}{4} \tag{A19}$$

as found in Ref. [1]. For $n=3$,

$$S_n = 4\pi,$$

$$\int_{\Sigma_3} e_i^4 d\omega = \frac{4\pi}{5},$$

$$\int_{\Sigma_3} e_i^2 e_j^2 d\omega = \frac{4\pi}{15} \tag{A20}$$

consistently with Refs. [1,2]. The above results can be used to rewrite the expected integral in the very simple form

$$\int_{\Sigma_n} \mathbf{e}\otimes\mathbf{e}\otimes\mathbf{e}\otimes\mathbf{e} d\omega = \frac{S_n}{n(n+2)}(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\mathbf{e}_i\otimes\mathbf{e}_j \otimes \mathbf{e}_k\otimes\mathbf{e}_l \tag{A21}$$

(the terms involving the integral of e_i^4 are implicitly included into the other terms). Finally, Eqs. (A11), (A13), and (A21) lead to

$$\mathbf{J}_2 = (\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\mathbf{e}_i\otimes\mathbf{e}_j\otimes\mathbf{e}_k\otimes\mathbf{e}_l. \tag{A22}$$

Coming back to (A10), we now get the expected result:

$$\frac{1}{2}\mathbf{J}_2:\mathbf{G}_a = \frac{1}{2}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\left[\frac{\partial}{\partial x_m}\left(K_A\frac{\partial A}{\partial x_n}\right)\right]_a \mathbf{e}_i\otimes\mathbf{e}_j = \left[\frac{\partial}{\partial x_i}\left(K_A\frac{\partial A}{\partial x_j}\right)\right]_a \mathbf{e}_i\otimes\mathbf{e}_j = [\mathrm{grad}(K_A\ \mathrm{grad}\ A)]_a. \tag{A23}$$

[1] J. J. Monaghan, Rep. Prog. Phys. **68**, 1703 (2005).
[2] P. Espanol and M. Revenga, Phys. Rev. E **67**, 026705 (2003).
[3] H. Gotoh, H. Ikari, T. Memita, and T. Sakai, Coastal Eng. **47**, 157 (2005).
[4] L. Landau and E. Lifchitz, *Mechanics*, 3rd ed. (Pergamon, New York, 1976).
[5] F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, New York, 1965).
[6] L. Landau and E. Lifchitz, *Statistical Physics Part 1*, 3rd ed. (Pergamon, New York, 1980.
[7] H. Goldstein, C. Poole, and J. Safko, *Classical Mechanics*, 3rd ed., edited by A. Wesley (Addison Wesley, San Francisco, 2002).
[8] T. Kambe, Fluid Dyn. Res. **40**, 399 (2008).
[9] G. Oger, M. Doring, B. Alessandrini, and P. Ferrant, J. Comput. Phys. **225**, 1472 (2007).
[10] J. J. Monaghan, Annu. Rev. Astron. Astrophys. **30**, 543 (1992).
[11] J. Bonet and T.-S. L. Lok, Comput. Methods Appl. Mech. Eng. **180**, 97 (1999).
[12] J. Bonet and M. X. Rodriguez-Paz, J. Comput. Phys. **209**, 541 (2005).
[13] L. Landau and E. Lifchitz, *Fluid Mechanics*, 3rd ed. (Pergamon, New York, 1989).
[14] S. B. Pope, *Turbulent Flows* (Cambridge University Press, Cambridge, England, 2000).
[15] D. Violeau and R. Issa, Int. J. Numer. Methods Fluids **53**, 277 (2007).
[16] J. P. Morris, P. J. Fox, and Y. Zhu, J. Comput. Phys. **136**, 214 (1997).
[17] J. J. Monaghan, Mon. Not. R. Astron. Soc. **335**, 843 (2002).
[18] J. J. Monaghan, J. Comput. Phys. **110**, 399 (1994).
[19] Temmerman and M. Leschziner, *Large Eddy Simulation of Separated Flow in a Streamwise Periodic Channel Construction*, International Symposium on Turbulence and Shear Flow Phenomena, Stockholm, 2001 (unpublished).
[20] J. C. Uribe and D. Laurence, Tenth Ercoftac (SIG15)/IAHR/QNET-CFD Workshop on Refined Turbulence Modelling, The University of Manchester, 2002, (unpublished) (http://cfd.mace.manchester.ac.uk/CfdTm/TestCase014).
[21] J. W. Swegle, D. L. Hicks, and S. W. Attaway, J. Comput. Phys. **116**, 123 (1995).
[22] M. G. Kendall, *A Course in the Geometry of Dimensions* (Dover Publications, Dover, 2004).