Angular-momentum conservative SPD for incompressible viscous flows

X. Y. Hu and N. A. Adams
Lehrstuhl für Aerodynamik, Technische Universität München
85748 Garching, Germany

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Current smoothed particle dynamics (SPD) discretizations for macro-scopic and meso-scopic viscous flows usually do not conserve angular momentum. Angular-momentum conservation, however, potentially stabilizes the solution for long-time simulations. We show that a simple angular-momentum conservative formulation of the viscous force, which was proposed previously based on empirical findings, can be derived theoretically under the condition of incompressible flow. The properties of this formulation are asserted by numerical simulations of two dimensional Taylor-Green flow.

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I. INTRODUCTION

The smoothed particle dynamics (SPD) is a fully Lagrangian, grid free method in which a smoothing kernel is introduced to approximate functions and their spatial derivatives from the interactions between neighboring particles. It is referred to as smoothed particle hydrodynamics (SPH) when simulating macro-scopic flows [10, 14, 16], and smoothed dissipative particle dynamics (SDPD) when simulating meso-scopic flows [7]. In SPD, the discretization of pressure usually conserves both linear and angular momentum locally. The discretization of the viscous force, however, usually does not strictly conserve angular momentum [3, 7, 9, 12]. Since the approximation of the random force (due to thermal-fluctuations) in SDPD is derived based on the viscous force, it usually does not conserve angular momentum either. We address angular-momentum conservation in the letter since it is potentially important to stabilize long-time simulations with SPD [17].

One approach is to correct SPH by a nested application of the gradient approximation to obtain global conservation of linear and angular momentum [1, 2, 15, 22]. Cleary et al. [4, 5] use artificial viscosity in inviscid SPH [17] to model real viscosity with a calibrated parameter. As the discretization is in compact and anti-symmetric form, linear and angular momentum are conserved both locally and globally. Since numerical experiments are ambiguous concerning the generality of this empirical parameter [4, 6, 19], it is difficulty to determine the conditions under which the particular parameter value is valid. In this letter we will derive a simple angular-momentum conservative formulation where the above mentioned parameter can be derived if the flow is incompressible. Subsequently, a random force for SDPD is derived by the fluctuation-dissipation theorem. The properties of this formulation are also asserted by numerical simulations of two dimensional Taylor-Green flow.

II. METHOD

We consider the isothermal incompressible Navier-Stokes equations on a moving Lagrangian frame

$$\frac{d\rho}{dt} = 0 \quad \text{or} \quad \nabla \cdot \mathbf{v} = 0 \tag{1}$$

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{v}, \tag{2}$$

where ρ, p, and $\mathbf{v}$ are material density, velocity and pressure, respectively, $\nu = \eta/\rho$ is the kinematic viscosity.

The smoothing function for particle i is given by

$$\chi_i(\mathbf{r}) = \frac{W(\mathbf{r}-\mathbf{r}_i, h)}{\sum_k W(\mathbf{r}-\mathbf{r}_k)} = \frac{W_i(\mathbf{r})}{\sigma(\mathbf{r})} \tag{3}$$

where $\mathbf{r}_i$ is the position of particle i, $k = 1, ..., N$, N is the total particle number, and h is the smoothing length [12]. $W_i(\mathbf{r})$ is a generic shape function known as the SPH smoothing kernel which is radially symmetric and has the properties $\int W(\mathbf{r}-\mathbf{r}', h)d\mathbf{r}' = 1$ and $\lim_{h\to 0} W(\mathbf{r}-\mathbf{r}', h) = \delta(\mathbf{r}-\mathbf{r}')$. $\sigma(\mathbf{r})$ is a measure of the particle number density which has a larger value in a dense particle region than in a dilute particle region. The volume of a particle is obtained through the following integral over the entire domain

$$\mathcal{V}_i = \int \chi_i(\mathbf{r})d\mathbf{r} \approx \frac{1}{\sigma_i}, \tag{4}$$

which shows that $\sigma_i = \sigma(\mathbf{r_i})$ is approximately the inverse of the particle volume, i.e. the specific volume. For a smooth variable $\psi(\mathbf{r})$, two forms of discretizations for the spatial derivatives are given in Ref. [12]. The second of these forms is

$$\nabla\psi_i = -\frac{1}{\mathcal{V}_i}\int \psi(\mathbf{r})\nabla\chi_i(\mathbf{r})d\mathbf{r} \tag{5a}$$

$$\approx -\frac{1}{\mathcal{V}_i}\sum_j \overline{\psi}_{ij}\int \frac{1}{\sigma(\mathbf{r})^2}\left[W_j(\mathbf{r})\nabla W_i(\mathbf{r}) - W_i(\mathbf{r})\nabla W_j(\mathbf{r})\right]d\mathbf{r} \tag{5b}$$

$$\approx \sigma_i\sum_j\left(\frac{1}{\sigma_i^2}+\frac{1}{\sigma_j^2}\right)\overline{\psi}_{ij}\frac{\partial W}{\partial r_{ij}}\mathbf{e}_{ij} \tag{5c}$$

$$= \sigma_i\sum_j A_{ij}\overline{\psi}_{ij}\mathbf{e}_{ij}. \tag{5d}$$

Here $\frac{\partial W}{\partial r_{ij}}\mathbf{e}_{ij} = \nabla W(\mathbf{r}_i - \mathbf{r}_j)$, and $\frac{\partial W}{\partial r_{ij}} \le 0$, $\mathbf{r}_i - \mathbf{r}_j = \mathbf{r}_{ij} = r_{ij}\mathbf{e}_{ij}$, and $\mathbf{e}_{ij}$ is the normalized vector from particle i to j. $A_{ij} = \left(\frac{1}{\sigma_i^2}+\frac{1}{\sigma_j^2}\right)\frac{\partial W}{\partial r_{ij}} < 0$. Note that A_{ij} depends on the particular choice of the SPH smoothing kernels $W_i(\mathbf{r})$ in Eq. (3). $\overline{\psi}_{ij} = \overline{\psi}(\psi(\mathbf{r}_i), \psi(\mathbf{r}_j))$ is an inter-particle-averaged value. A simple inter-particle average is, e.g.,

$$\overline{\psi}_{ij} = \frac{1}{2}[\psi(\mathbf{r}_i) + \psi(\mathbf{r}_j)], \tag{6}$$

which will be used in the following. Note that Eq. (5) gives a particle approximation of the gradient of $\psi(\mathbf{r})$. If $\psi(\mathbf{r})$ is a vector, the particle approximation of the divergence of $\psi(\mathbf{r})$ is obtained by taking the trace of Eq. (5), that is

$$\nabla\cdot\psi_i = -\int \psi(\mathbf{r})\cdot\nabla\mathcal{W}_i(\mathbf{r})d\mathbf{r} \approx \sigma_i\sum_j A_{ij}\overline{\psi}_{ij}\cdot\mathbf{e}_{ij}. \tag{7}$$

A. Viscous force in incompressible SPH

According to Hu and Adams [12], the equation of motion Eq. (2) can be discretized by

$$\frac{d\mathbf{v}_i}{dt} = -\frac{1}{m_i}\sum_j A_{ij}\overline{p}_{ij}\mathbf{e}_{ij} + \frac{\eta}{m_i}\sum_j A_{ij}\frac{\mathbf{v}_{ij}}{r_{ij}} \tag{8}$$

where m_i is the mass of particle i, $\overline{p}_{ij} = \frac{1}{2}(p_i + p_j)$ and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$. While the viscous-force term (the third term) conserves linear momentum, it does not strictly conserve angular momentum. Cleary et al. [4, 5] discretize the viscous-force term in a fashion similar to artificial viscosity in inviscid SPH [17]

$$\mathbf{F}_i = \zeta\frac{\eta}{m_i}\sum_j A_{ij}\frac{\mathbf{e}_{ij}\cdot\mathbf{v}_{ij},}{r_{ij}}\mathbf{e}_{ij}, \tag{9}$$

with an arbitrary positive parameter ζ. This formulation conserves linear and angular momentum locally and globally. Cleary [4] found empirically that $\zeta \approx 4.963$ by calibrating with incompressible flows using a weakly compressible SPH [18]. Cummins and Rudman [6] find $\zeta \approx 4.17$ for incompressible SPH simulation of two-dimensional flows employing a pressure projection.

We present here a theoretical argument for $\zeta = d + 2$ in Eq. (9) where d is the spatial dimension. Español & Revenga [7] and Monaghan [19] propose an approximation for second derivatives at the locus of particle i based on the following identity which is valid for an arbitrary smooth function $\phi(\mathbf{r})$

$$(\nabla\nabla\phi)_i = \int \frac{\phi_i - \phi(\mathbf{r})}{r_i(\mathbf{r})}\left[(d+2)\nabla\mathcal{W}_i(\mathbf{r})\mathbf{e}_i(\mathbf{r}) - \mathbf{I}\nabla\mathcal{W}_i(\mathbf{r})\cdot\mathbf{e}_i(\mathbf{r}))\right]d\mathbf{r} + \mathcal{O}(h^2), \tag{10}$$

where $\mathbf{e}_i(\mathbf{r})$ and $r_i(\mathbf{r})$ are the unit vector and distance from particle i to a coordinate $\mathbf{r}$, respectively. Comparing Eq. (10) to Eqs.(5) and (7) by setting $\psi(\mathbf{r})$ to

$$\frac{\phi_i - \phi(\mathbf{r})}{r_i(\mathbf{r})}(d+2)\mathbf{e}_i(\mathbf{r}) \quad \text{and} \quad \frac{\phi_i - \phi(\mathbf{r})}{r_i(\mathbf{r})}\mathbf{e}_i(\mathbf{r})$$

respectively, and on using Eq. (6), one finds the relation

$$(\nabla\nabla\phi)_i \approx \frac{\sigma_i}{2}\sum_j A_{ij}\frac{\phi_{ij}}{r_{ij}}\left[(d+2)\mathbf{e}_{ij}\mathbf{e}_{ij} - \mathbf{I}\right]. \tag{11}$$

For $\phi(\mathbf{r}) = \mathbf{v}(\mathbf{r})$ as the velocity field, one obtains from

Eq. (11) by taking the trace of the tensor operator $\nabla\nabla$

$$(\nabla^2 \mathbf{v})_i \approx \sigma_i \sum_j A_{ij} \frac{\mathbf{v}_{ij}}{r_{ij}}, \tag{12}$$

which returns a second-order discretization of the viscous force term in Eq. (8). Similarly, taking the trace of the tensor $\nabla\mathbf{v}$ in the left-hand side of Eq. (11), one obtains

$$(\nabla\nabla \cdot \mathbf{v})_i \approx \frac{\sigma_i}{2} \sum_j A_{ij} \frac{1}{r_{ij}} \left[(d+2)\mathbf{v}_{ij} \cdot \mathbf{e}_{ij}\mathbf{e}_{ij} - \mathbf{v}_{ij}\right]. \tag{13}$$

When the left-hand-side of Eq. (13) vanishes due to a divergence-free velocity field, then follows from the right-hand side together with Eq. (12) that the discrete viscous force of Eq. (8) is approximately equivalent to Eq. (9) with the parameter $\zeta = d + 2$, which proves our result. The parameter $\zeta = d + 2$ is close to the empirical result of Cummins & Rudman [6] (in two dimensions). As Eq. (13) is contains no further implicit dependence on A_{ij}, the parameter ζ is also formally independent of the chosen smoothing kernels.

Note that Eq.(13) also implies an estimate for numerical errors committed by replacing the viscous term in Eq. (8) by Eq. (9). Eq. (10) is a second-order accurate approximation of second derivatives, and contains an integral which needs to be evaluated from a particle approximation. The accuracy of this particle approximation depends on the number particles used for evaluation. For an incompressible SPH simulation the number of neighboring particles within a kernel radius does not change (due to incompressibility) during time evolution and thus is essentially fixed by the initial choices for the ratio of smoothing length and the neighboring particle distance $\alpha = h/\Delta$ and for the kernel radius. Therefore, it can be expected that this particle-approximation error of Eq. (10) would not change much with the overall number of particles and with viscosity. This fact can explain discrepancies between the carefully calibrated and the theoretical value for the parameter [4, 6] as we will show below. If we consider the kernel radius of [6] which is 25% larger than that of [4], and $\alpha = 1.3$ is larger as well, the particle approximation of the integral is more accurate in [6] than in [4] so that the calibrated parameter is closer to the theoretical result for [6] than of [4]. Since the approximation error is determined by α and the kernel radius and not by resolution and viscosity, both calibrating simulations find that ζ is independent on resolution and viscosity since α and kernel radius remain unchanged.

B. Incompressible SDPD

With Eqs. (8) and (9) the equation of motion Eq. (2) can be discretized and written as an equation for particle momentum as

$$\dot{\mathbf{P}}_i = -\sum_j A_{ij}\overline{p_{ij}}\mathbf{e}_{ij} + \eta\zeta \sum_j A_{ij} \frac{\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}}{r_{ij}} \mathbf{e}_{ij}. \tag{14}$$

Note that the pressure term is reversible and conserves kinetic energy and that the viscous force reflects the irreversibility of the flow. In the original DPD method [11] the momentum equation for a particle is

$$\dot{\mathbf{P}}_i = \sum_{j \neq i} \left[F^C_{ij} + F^D_{ij} + F^R_{ij}\right] \mathbf{e}_{ij}, \tag{15}$$

where F^C_{ij}, F^D_{ij} and F^R_{ij} are the magnitudes of conservative force, dissipative force and random force, respectively. On can see that the pressure force and the viscous force in Eq. (14) can be written analogously to the conservative force and the dissipative force in Eq. (15), i.e.

$$F^C_{ij} = -A_{ij}\overline{p_{ij}} \quad \text{and} \quad \mathrm{F^D_{ij}} = -\eta \left(-\zeta \frac{\mathrm{A_{ij}}}{\mathrm{r_{ij}}}\right) (\mathbf{e}_{\mathrm{ij}} \cdot \mathbf{v}_{\mathrm{ij}}). \tag{16}$$

A random force for Eq. (14) can also be formulated by simply following the original DPD formulation. As the amplitude of dissipative force and random force are given according to the Fluctuation-Dissipation Theorem [8] the magnitude of the random force can be obtained as

$$F^R_{ij} = (2k_B T\eta)^{1/2} \left(-\zeta \frac{A_{ij}}{r_{ij}}\right)^{1/2} \xi_{ij}, \tag{17}$$

where ξ_{ij} is a Gaussian variable with zero mean and a variance equal to Δt^{-1}, Δt is the time step, which is defined by the underlying Wiener process, and $k_B T$ is the Boltzmann temperature of the system. Note that this random force also conserves both linear and angular momentum. The current expression is simpler than previous formulations as only one Wiener process per particle pair needs to evaluated unlike for previous SDPD formulations [7, 12].

Note that the pressure terms in the conservative force are obtained by enforcing a divergence-free condition on the velocity [6]. Consequently, the conservative force does not relate to an equation of state, and the incompressible SDPD has no intrinsic numerical viscosity due to artificial compressibility [21].

C. Numerical validation

A simulation of two-dimensional viscous Taylor-Green flow is provided to validate our viscous force formulation. The Taylor-Green flow is a periodic array of vortices with velocities

$$\begin{aligned} u(x,y,t) &= -Ue^{bt}\cos(2\pi x)\sin(2\pi y) \\ v(x,y,t) &= Ue^{bt}\sin(2\pi x)\cos(2\pi y) \end{aligned} \tag{18}$$

where $b = -\frac{8\pi^2}{\mathrm{Re}}$. The computation is performed in on a periodic domain $0 < x < 1$ and $0 < y < 1$. The initial particle velocity is assigned according to Eq. (18) with $t = 0$ and $U = 1$. A quintic spline kernel [20] is used for $W(\mathbf{r})$. Incompressibility is enforced by a projection

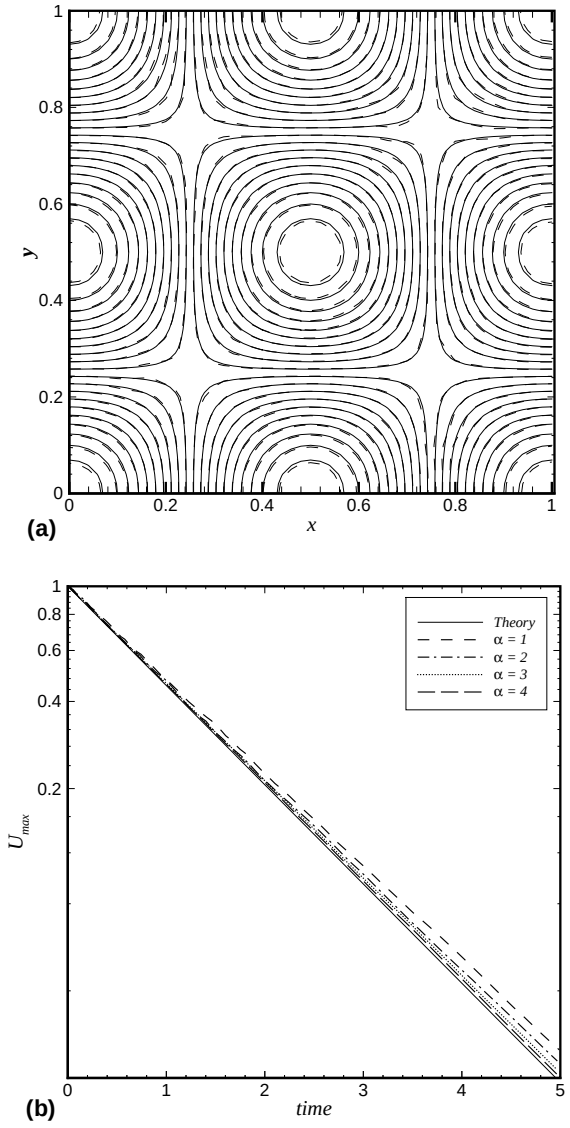

FIG. 1: Taylor-Green problem with Re = 100: (a) comparison between simulated vorticity profile (solid line) and analytical solution (dash line) at time $t = 1$, (b) simulated decay of the maximum velocity with different α.

SPH employing a diagonal conjugate gradient method for solving the Poisson equation [13].

In order to study the errors introduced by the approximation of integration in Eq. (13), first the parameter ζ is set to the theoretical value 4. Simulations are performed for Re = 100 with 900, 1600, 2500 and 3600 particles. The smoothing length is fixed at $h = \frac{1}{30}$ which gives for the ratio of smoothing length and neighboring particle distance with values $\alpha = 1$, 2, 3 and 4, respectively. Figure 1a shows the calculated vorticity at $t = 1$ with 2500 particles. It can be observed that the theoretical solution is quite well recovered with the maximum error arising near the vorticity peaks. Figure 1b shows the time evolution of the maximum velocity of the flow. It can be observed that the predicted Reynolds number is always slightly larger than the theoretical value. However, it can also be observed that the predicted Reynolds number converges to the theoretical value with increasing α, supporting our argument at the end of Section II A. For $\alpha = 4$ the relative error decreases to less than 1%.

In most of SPH simulations α is chosen between 1 and 2, so that the particle approximation of the integral in Eq. (13) is rather inaccurate. Since these errors for fixed α and smoothing length do not change with the overall particle number the parameter ζ can be calibrated to compensate these errors without inferring a strong dependence on resolution and viscosity.

In order to study the convergence properties for calibrated ζ the same case as above is simulated with 900, 3600 and 14400 particles, respectively. By using a fixed $\alpha = 1$, the smoothing lengths are given as $h = \frac{1}{30}$, $\frac{1}{60}$ and $\frac{1}{120}$ with increasing resolution. The parameter $\zeta = 4.28$ is calibrated with a simulation at the lowest resolution. Note that this value is just in between those of [4] and [6] because for our setup the number of particles within a kernel radius is less than that in [4] but more than that in [6]. We measured the overall accuracy by L_1 errors

$$L_1 = \frac{\sum_{i=1}^{N} \left| U^{ex} - U^{SPH} \right|}{\sum_{i=1}^{N} \left| U^{ex} \right|} \tag{19}$$

where U and U^{ex} are the simulated and theoretical velocities, respectively, N is the number of particles. The convergence of the solution with increasing resolution (overall number of particles) is shown in Fig. 2a.

In order to study the influence of viscosity, we simulated the cases for Re = 10, 50, 150 and 200 with 3600 particles by using the above calibrated parameter $\zeta = 4.28$. Figure 2b shows a comparison between the predicted and the theoretical temporal evolution of the maximum velocity. The maximum relative error is less than 5%, which suggests only a weak dependence of ζ on viscosity. Also, we observe that for Reynolds numbers larger than the calibration Reynolds number the predicted Reynolds number is smaller than the theoretical value, and vice versa for Reynolds numbers smaller that the calibration value.

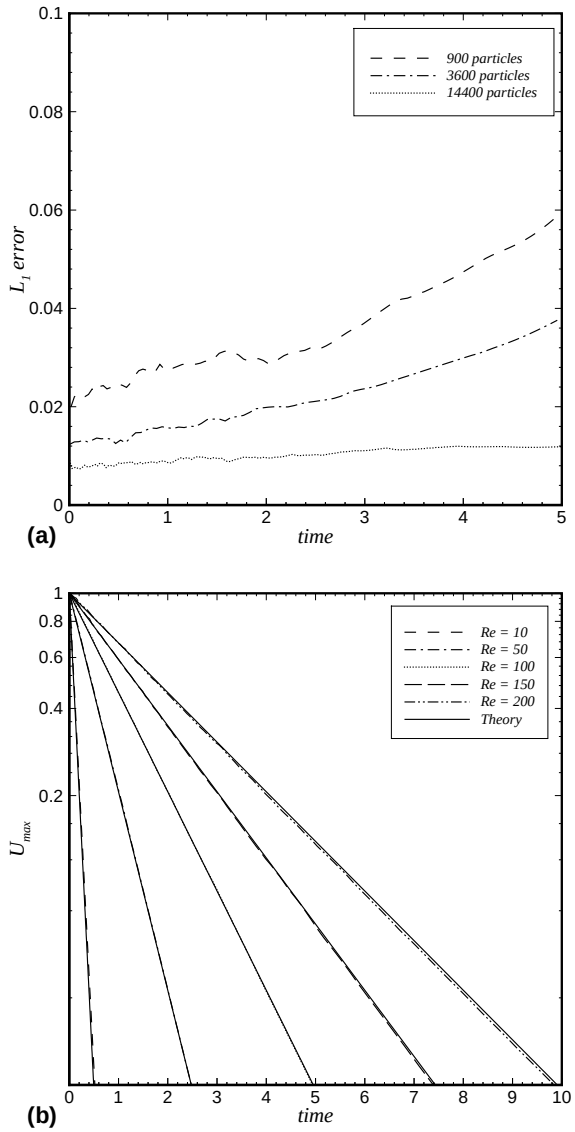

FIG. 2: Taylor-Green problem with different resolutions and Reynolds numbers: (a) history of L_1 errors, (b) decay of the maximum velocities.

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