Fluid particle dynamics: a synthesis of dissipative particle dynamics and smoothed particle dynamics

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We present a generalization of dissipative particle dynamics that includes shear forces between particles. The new algorithm has the same structure as the (isothermal) smoothed particle dynamics algorithm, except that it conserves angular momentum and includes thermal fluctuations consistently with the principles of equilibrium statistical mechanics. This clarifies the connection of dissipative particle dynamics with numerical resolution algorithms of the macroscopic Navier-Stokes equations.

Dissipative particle dynamics (DPD) is an off-lattice simulation technique that has been introduced by Hoogerbrugge and Koelman in order to address hydrodynamic problems in complex fluids [1,2]. The technique has received substantial theoretical support [3,4] and it has been successfully applied in a large variety of systems including flow in porous media [2], colloidal suspension [2,5], dilute polymeric suspensions [6], and immiscible binary fluids [7].

The idea behind DPD is to simulate a Newtonian fluid (as, for example, the Newtonian solvent in colloidal or polymeric suspensions) in terms of mesoscopic “lumps” or “droplets” of fluid, named dissipative particles [1,8]. It is postulated that these dissipative particles interact with each other with a pair-wise conservative potential, with dissipative forces that depend on the relative approaching velocity of the particles, and with random forces that satisfy a fluctuation-dissipation theorem [3]. Newton’s third law is satisfied and the total momentum of the system is conserved, although energy is not [1]. This implies that there are local conservation equations for mass and momentum, i.e. the system behaves hydrodynamically at long times and distances [4]. The advantage of DPD over conventional molecular dynamics relies on the fact that DPD is a coarse-grained technique which captures the gross features of mesoscopic portions of fluid. The microscopic details, which are computationally expensive and not even interesting, are averaged out in DPD.

The spirit of DPD turns out to be quite similar to that of smoothed particle dynamics SPD [9]. This technique was originally intended to simulate astrophysical non-viscous flows and has been recently been applied in a variety of non-viscous [10,11] and viscous problems [12,13]. SPD consists on a discretization of the Navier-Stokes equations in a Lagrangian moving grid with the aid of a weight function. In this way, the nodes of the grid can be identified as “smooth particles” interacting through prescribed laws of force, thus allowing to solve Navier-Stokes equations with molecular dynamics codes. The Lagrangian nature of the technique makes it very appropriate to study flows in complex geometries (like those appearing in colloidal suspensions) because there is no need of costly recalculations of the mesh as the boundary conditions evolve. Actually, the very dynamics takes care of it. Unfortunately, there is at present no implementation of the thermal fluctuations present in fluids at mesoscopic scales and which are the responsible for the Brownian motion of small suspended objects. It is not clear that the fluctuations that appear as a consequence of the discrete nature of the technique are compatible with the principles of statistical mechanics. In particular, that they obey a fluctuation-dissipation theorem. In other words, there is yet no implementation of SPD for fluctuating hydrodynamics [4].

In this letter we present a model of fluid particles that interact with dissipative forces that, besides the dissipative force of the original DPD algorithm, include shear forces between fluid particles. We regard this as a more realistic model in view of the fact that the proposed algorithm coincides in structure with the SPD algorithm. Therefore, it is expected that an even more reduced number of particles already reproduce the hydrodynamic behavior of the system. We also formulate the random forces between fluid particles in such a way that the distribution function of velocities is Gaussian, as predicted by equilibrium statistical mechanics. In this way, this work represents a generalization of SPD that includes thermal fluctuations. This opens up the possibility of applying a technique closely related to SPD to the study of complex fluids.

A shear force between particles $i,j$ is proportional to the relative velocities $v_{ij}$ of both particles, whereas the dissipative force in the original DPD algorithm is proportional to the approaching velocity $(e_{ij} \cdot v_{ij})e_{ij}$, where $e_{ij}$ is the unit vector in the joining line of both particles. The initial motivation for modifying the original algorithm of DPD by introducing shear forces was the identification of an elementary motion between dissipative particles that produces no force in that algorithm. If a dissipative particle is orbiting in a circumference around a reference particle, it will not exert any force on this particle. Nevertheless, on simple physical grounds one expect that the motion of...
the dissipative particle must drag in some way the reference particle. This is taken into account through the shear forces in the fluid particle model presented in this letter. We note, however that this relative motion might produce a drag even in the original DPD algorithm if many DPD particles are involved simultaneously. The same is true for a purely conservative molecular dynamics simulation. The point is, of course, that the effect is already captured with a much smaller number of particles in the fluid particle model.

The shear forces are not central and therefore angular momentum is not conserved. We restore angular momentum conservation by including in the description a spin variable. If one thinks of the fluid particles as mesoscopic portions of fluid, this spin variable has a sounded physical interpretation: it describes the angular momentum of the molecules that constitute the fluid particle with respect to the center of mass of the fluid particle.

I. THE FLUID PARTICLE MODEL

The fluid particle model is defined by \( N \) identical particles of mass \( m \) and moment of inertia \( I \). The state of the system is characterized by the positions \( \mathbf{r}_i \), velocities \( \mathbf{v}_i \), and angular velocities \( \omega_i \) of each particle. We do not include here an internal energy variable and the resulting algorithm, like DPD, will not conserve energy locally. This may be a minor problem when one is interested only in rheological properties.

The equations of motion of the system are given by

\[
\begin{align*}
\dot{\mathbf{r}}_i &= \mathbf{v}_i \\
\dot{\mathbf{v}}_i &= \frac{1}{m} \sum_{j \neq i} \mathbf{F}_{ij} \\
\dot{\omega}_i &= \frac{1}{I} \sum_{j \neq i} \mathbf{N}_{ij}
\end{align*}
\]

where \( \mathbf{F}_{ij}, \mathbf{N}_{ij} \) are the force and torque that particle \( j \) exerts on particle \( i \). We require that the forces satisfy Newton’s third law, \( \mathbf{F}_{ij} = -\mathbf{F}_{ji} \), in such a way that the total linear momentum \( \mathbf{P} = \sum_i m \mathbf{v}_i \) is a dynamical invariant, \( \mathbf{P} = 0 \). In addition, we assume that the torques in \( \mathbf{N}_{ij} \) are given by \( \mathbf{N}_{ij} = -\mathbf{r}_{ij} \times \mathbf{F}_{ij}/2 \) and one checks immediately that the total angular momentum \( \mathbf{J} = \sum_i (\mathbf{r}_i \times \mathbf{p}_i + I \omega_i) \) is conserved exactly, \( \mathbf{J} = 0 \).

We model the force \( \mathbf{F}_{ij} \) between fluid particles according to \( \mathbf{F}_{ij} = \mathbf{F}^C_{ij} + \mathbf{F}^T_{ij} + \mathbf{F}^R_{ij} + \tilde{\mathbf{F}}_{ij} \) where the different contributions are given by

\[
\begin{align*}
\mathbf{F}^C_{ij} &= -V'(r_{ij})\mathbf{e}_{ij} \\
\mathbf{F}^T_{ij} &= -\gamma m \mathbf{M}^T(r_{ij}) \cdot \mathbf{v}_{ij} \\
\mathbf{F}^R_{ij} &= -\gamma m \mathbf{M}^R(r_{ij}) \cdot \left( \frac{\mathbf{F}_{ij}}{2} \times [\omega_i + \omega_j] \right) \\
\tilde{\mathbf{F}}_{ij} dt &= \sigma m \left( A(r_{ij})\mathbf{W}_{ij}^c + \mathbf{B}(r_{ij}) \right) \frac{1}{D} \left( \mathbf{r}[d\mathbf{W}_{ij}] + \mathbf{\dot{C}}(r_{ij}) d\mathbf{W}_{ij}^A \right) \cdot \mathbf{e}_{ij}
\end{align*}
\]

The first contribution \( \mathbf{F}^C_{ij} \) is a repulsive conservative force derived from a soft potential \( V(r) \). If only this force is present we have the version of SPD for non-viscous flows studied extensively in Refs. \([10]\) (i.e. a MD simulation). The second contribution \( \mathbf{F}^T_{ij} \) is a friction force that depends on the relative translational velocities \( \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j \). The dimensionless matrix \( \mathbf{M}^T(r_{ij}) \) is the most general matrix that can be constructed out of the vector \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \), this is \( \mathbf{M}^T(r_{ij}) = A(r_{ij}) \mathbf{1} + B(r_{ij}) \mathbf{e}_{ij} \) where \( \mathbf{1} \) is the unit matrix, \( \mathbf{e}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}| \) is the unit vector joining the particles, \( \mathbf{r}_{ij} = |\mathbf{r}_{ij}| \) and the functions \( A(r) \) and \( B(r) \) provide the range of the force. The friction coefficient \( \gamma \) has been introduced as an overall factor for convenience and has dimensions of inverse of time. \( \mathbf{F}^T_{ij} \) is the sum of a shear force \( -\gamma m A(r) \mathbf{v}_{ij} \) and a central force \( -\gamma m B(r) (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{e}_{ij} \). The rotational contribution \( \mathbf{F}^R_{ij} \) in \( (2) \) is given also in terms of a dimensionless matrix \( \mathbf{M}^R = \mathbf{M}^R(r_{ij}) = C(r_{ij}) \mathbf{1} + D(r_{ij}) \mathbf{e}_{ij} \mathbf{e}_{ij} \) where \( C(r) \), \( D(r) \) are scalar functions (even though the \( D(r) \) contribution to \( \mathbf{F}^R_{ij} \) is zero we maintain this term to keep the analogy between \( \mathbf{M}^R \) and \( \mathbf{M}^T \)). Note that if particles \( i \) and \( j \) were spheres of radius \( r_{ij}/2 \) in contact and spinning with angular velocities \( \omega_i, \omega_j \) the relative velocity at the “surface” of the spheres would be equal to \( \frac{1}{2} \mathbf{r}_{ij} \times (\omega_i + \omega_j) \). Then \( \mathbf{F}^R \) gives a friction force between the spheres proportional to this relative velocity. This force produces an “engaging” effect in which neighbour particles prefer to spin in opposite senses.

The last contribution in \( (2) \) is a velocity-independent stochastic force which is inspired by the tensorial structure of the random forces that appear in the fluctuating hydrodynamics theory \([14]\). \( \sigma \) is a parameter governing the overall
noise amplitude, the scalar functions \( \tilde{A}(r), \tilde{B}(r), \tilde{C}(r) \) define the range of the random force, and we have introduced the following symmetric, antisymmetric and traceless symmetric random matrices

\[
\begin{align*}
W_{ij}^{S\mu\nu} &= \frac{1}{2} [W_{ij}^{\mu\nu} + W_{ij}^{\nu\mu}] \\
W_{ij}^{A\mu\nu} &= \frac{1}{2} [W_{ij}^{\mu\nu} - W_{ij}^{\nu\mu}] \\
\bar{W}_{ij} &= \frac{1}{D} tr[W_{ij}^S] \mathbf{1}
\end{align*}
\]

Here, \( D \) is the physical dimension of space and \( W_{ij}^{\mu\nu} \) is a matrix of independent Wiener increments which is assumed to be symmetric under particle interchange \( W_{ij}^{\mu\nu} = W_{ji}^{\mu\nu} \). This symmetry will ensure momentum conservation because \( \tilde{F}_{ij} = -\tilde{F}_{ji} \). The matrix \( W_{ij}^{\mu\nu} \) is an infinitesimal of order 1/2, and this is summarized in the Ito mnemotechnical rule

\[
W_{ij}^{\mu\nu} W_{ji}^{\rho\sigma} = \left[ \delta_{ij} \delta_{\nu\rho} + \delta_{ij} \delta_{\nu\sigma} + \delta_{ij} \delta_{\mu\rho} - \delta_{ij} \delta_{\mu\sigma} \right] \delta_{\mu\nu} \delta_{\rho\sigma} dt.
\]

From this stochastic property, one derives straightforwardly the following rules from the different parts

\[
\begin{align*}
\text{tr}[dW_{ij}^S] \text{tr}[dW_{j'i'}^S] &= [\delta_{ij} \delta_{j'i'} + \delta_{ij} \delta_{j'i'}] D dt \\
\text{tr}[dW_{ij}^S] \text{tr}[dW_{j'j'}^{A\mu\nu}] &= \left[ \frac{1}{2} \left( \delta_{\mu\nu} \delta_{\nu\sigma} + \delta_{\mu\sigma} \delta_{\nu\rho} \right) - \frac{1}{D} \delta_{\mu\nu} \delta_{\rho\sigma} \right] dt \\
\text{tr}[dW_{ij}^A] dW_{j'j'}^{S\mu\nu} &= \left[ \delta_{ij} \delta_{j'i'} + \delta_{ij} \delta_{j'i'} \right] \left[ \frac{1}{2} \left( \delta_{\mu\nu} \delta_{\nu\sigma} - \delta_{\mu\sigma} \delta_{\nu\rho} \right) \right] dt \\
\text{tr}[dW_{ij}^S] dW_{j'j'}^A &= \text{tr}[dW_{ij}^S] dW_{j'j'}^{A\mu\nu} = 0
\end{align*}
\]

These expressions show that the traceless symmetric, the trace and the antisymmetric parts are independent stochastic processes. The apparently complex structure of the random force is required in order to be consistent with the tensor structure of the dissipative friction forces. This will become apparent when considering the associated Fokker-Planck equation and requiring that it has a proper equilibrium ensemble.

The force \( \mathbf{F}_{ij} \) is the most general force that can be constructed out of the vectors \( \mathbf{r}_i, \mathbf{r}_j, \mathbf{v}_i, \mathbf{v}_j, \omega_i, \omega_j \) and satisfies that: 1) it is invariant under translational and Galilean transformations and transforms as a vector under rotations; 2) it is linear in the linear and angular velocities. This linearity is required in order to be consistent with the Gaussian distribution of velocities at equilibrium, as we will show later; 3) it satisfies Newton’s third law \( \mathbf{F}_{ij} = -\mathbf{F}_{ji} \) and, therefore, the total linear momentum is a conserved quantity of the system.

II. FOKKER-PLANCK EQUATION AND EQUILIBRIUM STATE

The equations of motion (1) are Langevin equations which have associated a mathematically equivalent Fokker-Planck equation (13). The FPE governs the distribution function \( \rho(r, v, \omega; t) \) that gives the probability density that the \( N \) particles of the system have specified values for the positions, velocities and angular velocities. Following standard (15) although quite tedious procedures, the FPE is given by

\[
\frac{\partial}{\partial t} \rho(r, v, \omega; t) = \left[ L^C + L^T + L^R \right] \rho(r, v, \omega; t)
\]

where

\[
\begin{align*}
L^C &= - \left[ \sum_i \mathbf{v}_i \frac{\partial}{\partial \mathbf{v}_i} + \sum_{i,j \neq i} \frac{1}{m} \mathbf{F}_{ij} \frac{\partial}{\partial \mathbf{v}_i} \right] \\
L^T &= \sum_{i,j \neq i} \frac{\partial}{\partial \mathbf{v}_i} \left[ L^T_{ij} + L^R_{ij} \right] \\
L^R &= - \frac{m}{T} \sum_{i,j \neq i} \frac{\partial}{\partial \omega_i} \left( \frac{r_{ij}}{2} \times \left[ L^T_{ij} + L^R_{ij} \right] \right) \\
L^T_{ij} &= - \frac{1}{m} \mathbf{F}_{ij} + \frac{\sigma^2}{2} T_{ij} \left[ \frac{\partial}{\partial \mathbf{v}_i} - \frac{\partial}{\partial \mathbf{v}_j} \right] \\
L^R_{ij} &= - \frac{1}{m} \mathbf{F}_{ij} + \frac{m \sigma^2}{2} T_{ij} \left( \frac{r_{ij}}{2} \times \left[ \frac{\partial}{\partial \omega_i} + \frac{\partial}{\partial \omega_j} \right] \right)
\end{align*}
\]
Here, the matrix $T_{ij}$ is given by

$$T_{ij} = \frac{1}{2} \left[ \tilde{A}^2(r_{ij}) + \tilde{C}^2(r_{ij}) \right] 1 + \left[ \left( \frac{1}{2} - \frac{1}{D} \right) \tilde{A}^2(r_{ij}) + \frac{1}{D} \tilde{B}^2(r_{ij}) - \frac{1}{2} \tilde{C}^2(r_{ij}) \right] \mathbf{e}_i \mathbf{e}_j \tag{7}$$

The steady state solution of equation (7), $\partial_t \rho = 0$, gives the (unique) equilibrium distribution $\rho^{eq}$. We now consider the conditions under which the steady state solution is the Gibbs canonical ensemble

$$\rho^{eq}(r, v, \omega) = \frac{1}{Z} \exp\left\{ - \left( \sum \frac{m}{2} v_i^2 + \frac{1}{2} \omega_i^2 + V(r) \right) / k_B T \right\} \tag{8}$$

where $V$ is the potential function that gives rise to the conservative forces $F^C$, $k_B$ is Boltzmann’s constant, $T$ is the equilibrium temperature and $Z$ is the normalizing partition function. We note that the velocity and angular velocity hydrodynamic fields are Gaussian variables at equilibrium and, therefore, one expects that the distribution function of the discrete values of these fields is also Gaussian.

The canonical ensemble is the equilibrium solution for the conservative system, i.e. $L^C \rho^{eq} = 0$. If, in addition, the following equations are satisfied $L^R_{ij} \rho^{eq} = L^B_{ij} \rho^{eq} = 0$ then we will have $L \rho^{eq} = 0$ and the Gibbs equilibrium ensemble will be the unique stationary solution of the dynamics. These equations will be satisfied if the detailed balance condition $\gamma = \frac{\sigma^{eq}_{ij}}{2k_BT}$ is satisfied and also $M^R(r_{ij}) = M^T(r_{ij}) = T_{ij}$. This implies

$$A(r) = \frac{1}{2} \left[ \tilde{A}^2(r) + \tilde{C}^2(r) \right]$$

$$B(r) = \frac{1}{2} \left[ \tilde{A}^2(r) - \tilde{C}^2(r) \right] + \frac{1}{D} \left[ \tilde{B}^2(r) - \tilde{A}^2(r) \right] \tag{9}$$

We observe, therefore, that the initial hypothesis for the tensorial structure of the dissipative and random forces was correct and consistent with equilibrium statistical mechanics.

The structure of the dissipative forces postulated in the fluid particle model (disregarding angular variables) is essentially the same as the structure of the viscous forces in the (isothermal) SPD algorithm. By using the discretization of Takeáda et al. [12] the correspondence is

$$V(r) = 2 \frac{p_0}{m n_0^2} W(r)$$

$$\gamma m A(r) = \frac{1}{m n_0^2} \left[ \eta W''(r) + \left( \frac{\eta}{3} + \zeta \right) \frac{W'(r)}{r} \right]$$

$$\gamma m B(r) = \frac{1}{m n_0^2} \left[ \zeta + \frac{\eta}{3} \right] \left[ W''(r) - \frac{W'(r)}{r} \right] \tag{10}$$

where $p_0, n_0$ are the equilibrium pressure and number density, and $W(r)$ is the bell-shaped weight function used in the discretization of the Navier-Stokes equation (the assumption that the density of all particles is almost constant has been taken). The SPD algorithm does not conserve angular momentum and does not incorporate thermal fluctuations. The first issue can be reduced at the cost of increasing the resolution (i.e. by increasing the computational cost of the simulations [12]). Regarding the second issue, we have formulated in this letter how to introduce consistently the thermal noise (i.e. by selecting $A(r), B(r), C(r)$ satisfying (9)). However, we note a serious problem in the expression for the scalar function $A(r)$ in terms of the weight function $W(r)$ in (10). The left hand side of the second equation in (10) is negative for some values of $r$ for a bell-shaped weight function $W(r)$. This is unacceptable in view of Eqn. (9). The smoothed particle dynamics algorithm does not allow, then, for a consistent introduction of thermal noise, at least in the form presented in Ref. [12].

In summary, we have proposed a fluid particle model by introducing shear forces and spin into the original DPD algorithm. The model has the correct equilibrium state and has a structure similar to SPD, but with angular momentum conservation and correct thermal fluctuations. In this way, the connection between DPD and SPD is clarified.

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