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# Fluid particle model

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We present a mechanistic model for a Newtonian fluid called fluid particle hydrodynamics. By analyzing the concept of ''fluid particle'' from the point of view of a Voronoi tessellation of a molecular fluid, we propose a heuristic derivation of a dissipative particle dynamics algorithm that incorporates shear forces between dissipative particles. The inclusion of these noncentral shear forces requires the consideration of angular velocities of the dissipative particles in order to comply with the conservation of angular momentum. It is shown that the equilibrium statistical mechanics requirement that the linear and angular velocity fields are Gaussian is sufficient to construct the random thermal forces between dissipative particles. The proposed algorithm is very similar in structure to the (isothermal) smoothed particle hydrodynamics algorithm. In this way, this work represents a generalization of smoothed particle hydrodynamics that incorporates consistently thermal fluctuations and exact angular momentum conservation. It contains also the dissipative particle dynamics algorithm as a special case. Finally, the kinetic theory of the dissipative particles is derived and explicit expressions for the transport coefficients of the fluid in terms of model parameters are obtained. This allows us to discuss resolution issues for the model. [S1063-651X(98)07803-9]

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## I. INTRODUCTION

Complex fluid systems such as colloidal or polymeric suspensions, micelles, immiscible mixtures, etc., represent a challenge for conventional methods of simulation due to the presence of disparate time scales in their dynamics. There is presently a great effort in developing new techniques of simulation that overcome some of the difficulties of microscopic (molecular dynamics) and macroscopic (numerical solution of continuum equations) conventional techniques.

On one hand, molecular dynamics captures all the detailed dynamics from times scales of the order of atomic collision times to macroscopic hydrodynamic times. However, in order to explore these large macroscopic times the number of particles required is enormous. Although large scale molecular dynamics simulations with millions of particles are currently performed one realizes that not all the information generated is actually required or even relevant at the time scales at which rheological processes in complex fluids take place.

On the other hand, from a continuum point of view the conventional solution of partial differential equations like the Navier-Stokes equation encounters difficulties due to the cumbersome treatment of moving boundary conditions to be imposed in a system as, for example, a colloidal suspension. These problems can be alleviated by the use of Lagrangian descriptions in which the discretizing grid moves according to the flow. A particularly exciting development has been the technique of smoothed particle hydrodynamics (SPH), which is essentially a discretization by weight functions that transforms the partial differential equations of continuum mechanics into ordinary differential equations [1,2]. These equations can be further interpreted as the equations of motion for a set of particles interacting with prescribed laws of force. The technique thus allows one to solve partial differential equation (PDE's) with molecular dynamics codes. Another advantage of a Lagrangian description relies on the fact that no expensive recalculations of the mesh are required as the dynamics takes care of it. Smoothed particle hydrodynamics has been used for simulating astrophysical flows with nonviscous terms (this was the original aim of the technique at the early 1970's [2]), and very recently in the study of viscous [3,4] and thermal flows [5,6] in simple geometries. It has not been applied to the study of complex fluids and this may be due, in part, to the fact that there is no easy implementation of Lagrangian *fluctuating* hydrodynamics [7] with SPH. Such implementation would be highly desirable in order to study the Brownian realm in which many of the processes in complex fluids take place. It must be noted that the particulate nature of the algorithm in SPH produces fluctuations that, from a computational point of view, are regarded as *numerical noise*. It is not clear that in the presence of viscous terms this noise satisfies the appropriate fluctuation-dissipation theorem. A second problem with SPH is that for viscous problems the noncentral nature of the viscous shear force breaks the conservation of angular momentum, even though the initial continuum equations are perfectly isotropic and conserve angular momentum.

In between microscopic and macroscopic descriptions, mesoscopic levels of description are gaining attention in order to address flow problems in complex fluids and/or geometries [8]. Lattice gas automata [9,10], lattice Boltzmann automata [11] or the direct simulation Monte Carlo method for dilute gases [12] have been useful tools in studying hydrodynamic problems in complex geometries. For the case of colloidal suspensions, lattice Boltzmann techniques represent a serious competitor to Brownian dynamics [13] or Stokesian dynamics [14] in that the computational cost scales linearly with the number of colloidal particles whereas, as a consequence of the long ranged hydrodynamic interactions, it increases with the cube of the number of particles in the latter

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techniques [11]. A drawback of the lattice approaches is that the dynamics is constrained by the lattice. This makes the consideration of boundary conditions on shaped bodies cumbersome.

In the same spirit of looking at mesoscopic descriptions, a very appealing idea was introduced by Hoogerbrugge and Koelman [15,16] in which a coarse grained description of the solvent fluid in terms of dissipative particles was devised. The technique was coined dissipative particle dynamics (DPD) and it is an off-lattice technique that does not suffer from the above mentioned drawbacks of lattice gas and lattice Boltzmann simulations. DPD consists essentially on a molecular dynamics simulation in which the force between particles has, in addition to a conservative part, a dissipative part represented as a Brownian dashpot. This Brownian dashpot damps out the *relative approaching velocity* between particles and introduces a noise term that keeps the system in thermal agitation. The dissipative particles are understood as ‘‘droplets’’ or cluster of molecules that interact with each other conserving the total momentum of the system [15,17]. This global conservation law has its local counterpart in the form of a balance equation for the momentum density, and the dissipative particles behave hydrodynamically in the low wave number and frequency regime.

DPD has received substantial theoretical support. It has been shown that the original DPD algorithm of Ref. [15] has associated, under a slight modification, a Fokker-Planck equation with Gibbs equilibrium states [18]. The extension to multicomponent systems has also been considered [19]. A first principles derivation of DPD for a harmonic chain has been presented in [20]. The macroscopic hydrodynamic equations have been obtained with projection operator techniques [21]. A very important further step has been the formulation of the kinetic theory for DPD by Marsh, Backx, and Ernst [22], which allows one to relate the transport coefficients in the hydrodynamic equations with the DPD model parameters. Finally, the effect of finite time steps on the equilibrium state of the system has been considered in [23]. DPD has been since applied to the study of colloidal suspensions [16,24,25], porous flow [15], polymer suspensions [26], and multicomponent flows [27].

In this work we provide a more precise meaning to the concept of ‘‘droplet’’ or ‘‘fluid particle’’ from a Voronoi tessellation of physical space. This conceptual framework allows one to model the different processes that intervene in the interaction between fluid particles or mesoscopic clusters of atoms of the fluid. The outcome is a generalization of the algorithm of DPD that includes shearing forces between the fluid particles. These forces are noncentral and do not conserve total angular momentum. This enforces the inclusion in the model of a spin variable with a well-defined physical meaning for the fluid particles. In this way angular momentum conservation is restored. We also investigate the structure of the random forces that must be included in order to recover a Gaussian distribution of linear and angular velocities for the fluid particles (note that the equilibrium fluctuations of the hydrodynamic velocity *field* are Gaussian). The structure of the random forces is postulated after analogy with the structure of the random stress tensor in terms of the Wiener process in the fluctuating hydrodynamics theory [29].

We show that the form of the equations of this fluid particle model at zero temperature (when fluctuations are absent) and with no angular variables is identical to the form of the equations obtained in a simple version of smoothed particle hydrodynamics as applied to fluid systems. In this sense, this work can be regarded as a generalization of SPH that includes fluctuations consistent with the principles of statistical mechanics and that conserves exactly the total angular momentum of the system. In other words, the obtained fluid particle algorithm may be viewed as a Lagrangian discretization of the equations of (isothermal) fluctuating hydrodynamics.

The paper is structured as follows. Section II considers the definition of a fluid particle in terms of the Voronoi tessellation and this serves to motivate the type of forces and torques between fluid particles introduced in Sec. III. Section IV presents the equivalent Fokker-Planck equation to the equations of motion. This allows one to establish requirements on the model parameters in order to have a proper equilibrium distribution. A summary of the model is presented in Sec. V. Section VI contains the kinetic theory of the model in the simple case when conservative forces are absent. The transport coefficients are computed and this permits us to discuss its dependence on the number density of fluid particles in Sec. VII. A final discussion and conclusions are presented in the last section.

## II. FLUID PARTICLES THROUGH VORONOI TESSELLATION

In an attempt to better understand the physical meaning of DPD, we have devised a coarse graining procedure for a molecular dynamics simulation of point particles (atoms) interacting through continuous potentials [17]. The coarsening is performed through the Voronoi tessellation, which allows one to divide physical space into a set of nonoverlapping cells that cover all the space in a well-defined manner. Given a discrete set of points (that can be distributed at random) the Voronoi tessellation assigns to each point (called ‘‘cell center’’) that region of space that surrounds it and that is nearer to this point than to any other point of the set. With this tessellation the atoms of the molecular dynamics simulation are distributed into clusters around the centers of the Voronoi cells. The practical way to perform the Voronoi tessellation in the simulation is by computing the distance of a given atom to all the center cells and assign that atom to the nearest center. Subsequently, the Voronoi cells are set in motion according to the velocity and acceleration of the center of mass of the particles that are within the cell. In this way, the cells capture the motion of the fluid at mesoscopic scales.

The Voronoi cells are a well defined realization of what is loosely regarded in fluid mechanics textbooks as ‘‘fluid particles.’’ We would like to know how these fluid particles move, that is, which explicit law of force between fluid particles would reproduce the actual motion of the Voronoi cells observed in the simulations. It is apparent that the number of cells is much smaller than the number of atoms in the molecular dynamics simulation, and therefore if one knows how the clusters move, one can try to simulate the clusters and capture the mesoscopic behavior of the underlying liquid with much less computational effort.

For sufficiently large clusters, that is, when the typical distance $\lambda_{\mathrm{mes}}$ between cell centers is much larger than the typical distance $\lambda_{\mathrm{mic}}$ between atoms we expect that the clusters move *hydrodynamically*. More precisely, we consider the conserved densities

$$\rho_{\mathbf{r}}=\frac{M_{\mathbf{r}}}{V_{\mathbf{r}}},$$
$$\mathbf{g}_{\mathbf{r}}=\frac{\mathbf{P}_{\mathbf{r}}}{V_{\mathbf{r}}}, \tag{1}$$
$$e_{\mathbf{r}}=\frac{E_{\mathbf{r}}}{V_{\mathbf{r}}},$$

where $M_{\mathbf{r}},\mathbf{P}_{\mathbf{r}},E_{\mathbf{r}}$ are the instantaneous total mass, momentum, and energy, respectively, of the system of particles that happen to be within the Voronoi cell centered at $\mathbf{r}$ and $V_{\mathbf{r}}$ is the volume of the cell. One also introduces

$$\mathbf{v}_{\mathbf{r}}\equiv\frac{\mathbf{g}_{\mathbf{r}}}{\rho_{\mathbf{r}}}, \tag{2}$$

which is the instantaneous velocity of the center of mass of the system of particles within the Voronoi cell at $\mathbf{r}$.

If (1) the cells are large enough for the system of particles that are within it to be considered as a thermodynamic system, and (2) the variations of the conserved quantities from neighbor cells are small, then the variables (1) obey the equations of fluctuating hydrodynamics [7] (see [29] for the nonlinear case). The conserved quantities (1) are subject to fluctuations because the atoms can enter and go out from the Voronoi cells due to their thermal agitation. The size of fluctuations, that is, the noise amplitude appearing in the equations of fluctuating hydrodynamics is proportional to the square root of the inverse of the volume of the cell, in accordance with the $1/\sqrt{N}$ dependence of fluctuations in equilibrium ensemble theory [29]. Therefore, depending on the ''resolution'' (the number of Voronoi cells per unit volume) used to describe the system, the amplitude of the noise term in the hydrodynamic equations that govern the instantaneous values of the conserved variables will be different.

Now, one is faced with two possible routes in order to simulate the dynamics of clusters. The first route is to consider the conserved discrete variables (1) as the state variables and update them according to some discretized version of the equations of hydrodynamics. This poses some subtle problems regarding the formulation of *fluctuating* hydrodynamics in a moving mesh, in particular with the treatment of the $1/\sqrt{V_{\mathbf{r}}}$ singularity. The second route, which is the one we follow in this paper, is to *postulate* the laws of force between cells. Despite the strong assumptions made to model these forces, the final expressions satisfy symmetry requirements that ensure that the behavior of the clusters will be, on average, that of real clusters.

A final word on the angular momentum is in order. We have not included in the above set of conserved variables (1) the angular momentum density defined by

$$\mathbf{J}_{\mathbf{r}}=\mathbf{r}\times\mathbf{g}_{\mathbf{r}}+\frac{\mathbf{S}_{\mathbf{r}}}{v_{\mathbf{r}}}, \tag{3}$$

where we have decomposed the angular momentum of the system of particles in cell $\mathbf{r}$ as the sum of the angular momentum of the center of mass with respect to the origin plus the intrinsic angular momentum $\mathbf{S}_{\mathbf{r}}$ of the particles of the cell with respect to the center of mass of the cell. We could, in principle, compute the inertia tensor $\mathbf{I}_{\mathbf{r}}$ for the system of particles in cell $\mathbf{r}$ and define the angular velocity $\boldsymbol{\omega}_{\mathbf{r}}$ through

$$\boldsymbol{\omega}_{\mathbf{r}}=\mathbf{I}_{\mathbf{r}}^{-1}\mathbf{S}_{\mathbf{r}}. \tag{4}$$

The reason the angular momentum density is usually not considered in the derivation of Newtonian hydrodynamics is that the second contribution in Eq. (3) vanishes in the ''continuum limit.'' This can be seen by noting that $\mathbf{S}_{\mathbf{r}}$ must scale as a typical size of the cell. In the continuum limit this typical distance goes to zero and there is no intrinsic angular momentum contribution. The situation here is different from the case of molecular fluids with spin [28], where the rotation of the molecules themselves originates an angular momentum that does not scale with the size of the cells and produces a finite value in the continuum limit.

## III. MODELING THE FORCES AND TORQUES BETWEEN FLUID PARTICLES

In this section we formulate the fluid particle model under a set of simplifying hypotheses. In the real clusters, the mass is a fluctuating quantity as particles can enter and go out from the Voronoi cell. Also, the shape of the cells changes as the cells move. However, the first assumption is that all clusters are identical, having a fixed mass $m$ and fixed isotropic inertia tensor of moment of inertia $I$. We assume that the state of the cluster system is completely characterized by the positions $\mathbf{r}_i$, the velocities of the center of mass $\mathbf{v}_i$ and the angular velocities $\boldsymbol{\omega}_i$. Note that we do not include any internal energy variable and therefore the resulting algorithm will not capture appropriately the thermal effects that occur in real fluids. This may be a minor problem when one is interested only in rheological properties. A generalization of the model including energy conservation has been recently proposed independently in Refs. [30,31].

The next step is to specify the forces and torques that are responsible for changing the values of the linear and angular velocities of the clusters. We model the forces between two clusters by considering several heuristic arguments about how one expects that the actual Voronoi clusters interact with each other. In this respect we make first a strong pairwise additivity assumption. In the real system one expects that the force between two clusters (that is between all the atoms of the first cluster that are interacting with the atoms of the second cluster) will depend in general not only on the state variables of these two clusters but also on the configuration of other neighboring clusters. For the sake of simplicity, though, we neglect this collective effect and assume that the force between two clusters depends only on the position and velocities of these two clusters.

The equations of motion are therefore

$$\dot{\mathbf{r}}_i=\mathbf{v}_i,$$

$$\dot{\mathbf{v}}_i=\frac{1}{m}\sum_{j\neq i}\mathbf{F}_{ij}, \tag{5}$$

$$\dot{\boldsymbol{\omega}}_i=\frac{1}{I}\sum_{j\neq i}\mathbf{N}_{ij},$$

where $\mathbf{F}_{ij},\mathbf{N}_{ij}$ are the force and torque that cluster $j$ exerts on cluster $i$. 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 $\mathbf{P}=\Sigma_i m\mathbf{v}_i$ is a dynamical invariant, $\dot{\mathbf{P}}=0$. In addition, we assume that the torques in Eq. (5) are given by

$$\mathbf{N}_{ij}=-\tfrac{1}{2}\mathbf{r}_{ij}\times\mathbf{F}_{ij} \tag{6}$$

and one checks immediately that the total angular momentum

$$\mathbf{J}=\sum_i \mathbf{r}_i\times\mathbf{p}_i+I\boldsymbol{\omega}_i \tag{7}$$

is exactly conserved, $\dot{\mathbf{J}}=\mathbf{0}$.

We will model the force between clusters according to

$$\mathbf{F}_{ij}=\mathbf{F}^C_{ij}+\mathbf{F}^T_{ij}+\mathbf{F}^R_{ij}+\tilde{\mathbf{F}}_{ij}. \tag{8}$$

The first three contributions are deterministic forces whereas the last one is random. We discuss them separately.

### A. Deterministic forces

The first contribution $\mathbf{F}^C_{ij}$ to the force is assumed to arise from a conservative potential $V(r)$ that depends on the separation distance between clusters. In Ref. [17] we have argued that a plausible definition of this potential is through the logarithm of the radial distribution function of cluster centers. The resulting soft potential has a bell-shaped form and has the virtue that when used as the potential between clusters in a molecular dynamics (MD) simulation, it reproduces consistently the radial distribution function of the real clusters (as has been checked through an actual MD simulation). It therefore captures the static or equilibrium properties of the system of clusters. The physical interpretation of this force is that it provides the excluded volume effect of each cluster. The center of the cluster (and its center of mass) is usually located ''in the middle'' of the cell and therefore it is not very probable that two cluster centers are closer to each other than the typical size of the cell.

It is clear, though, that this conservative contribution cannot be the only contribution to the force because it does not capture friction effects between clusters. These friction effects will depend on the velocities between clusters and will give rise to dissipative processes. The second contribution in (8) is a friction force that depends on the relative translational velocities of the clusters $i,j$ with positions $\mathbf{r}_i,\mathbf{r}_j$ and velocities $\mathbf{v}_i,\mathbf{v}_j$ in the following way:

$$\mathbf{F}^T_{ij}=-\gamma m\mathbf{M}^T(\mathbf{r}_{ij})\cdot\mathbf{v}_{ij}, \tag{9}$$

where $\mathbf{v}_{ij}=\mathbf{v}_i-\mathbf{v}_j$ is the relative velocity and the dimensionless matrix $\mathbf{M}^T(\mathbf{r}_{ij})$ is the most general matrix that can be constructed out of the vector $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$, this is

$$\mathbf{M}^T(\mathbf{r}_{ij})\equiv A(r_{ij})\mathbf{1}+B(r_{ij})\mathbf{e}_{ij}\mathbf{e}_{ij}, \tag{10}$$

where $\mathbf{1}$ is the unit matrix, $\mathbf{e}_{ij}=\mathbf{r}_{ij}/r_{ij}$ is the unit vector joining the particles, $r_{ij}=|\mathbf{r}_{ij}|$ and the dimensionless 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. The first contribution to the dissipative force (9) is in the direction of the relative velocities and tends to damp out the difference between the velocities. *It is a shearing force, which is noncentral*. The second contribution is directed along the joining line of the particles and damps out the relative approaching motion of the particles. The dissipative force in the original algorithm of Hoogerbrugge and Koelman is obtained with $A(r)=0$ [15]. Note that the form of the force $\mathbf{F}^T_{ij}$ is the more general expression for a vector that depends on $\mathbf{r}_{ij}$ and is linear in the relative velocities.

We now discuss the effects of rotation in the dissipative force. Let us assume for a moment that the clusters $i$ and $j$ were spheres of radius $r_{ij}/2$ in contact and spinning with angular velocities $\boldsymbol{\omega}_i,\boldsymbol{\omega}_j$ with no translational velocities. We would have a relative velocity at the ''surface'' of the spheres equal to $\frac{1}{2}\mathbf{r}_{ij}\times(\boldsymbol{\omega}_i+\boldsymbol{\omega}_j)$ and it is plausible to associate a friction force between the spheres proportional (in matrix sense) to this relative velocity. Therefore, the rotational contribution to the dissipative force is of the form

$$\mathbf{F}^R_{ij}=-\gamma m\mathbf{M}^R(\mathbf{r}_{ij})\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times[\boldsymbol{\omega}_i+\boldsymbol{\omega}_j]\right). \tag{11}$$

Again, the dimensionless matrix $\mathbf{M}^R$ depends only on the vector $\mathbf{r}_{ij}$ and therefore it must have the form

$$\mathbf{M}^R(\mathbf{r}_{ij})=C(r_{ij})\mathbf{1}+D(r_{ij})\mathbf{e}_{ij}\mathbf{e}_{ij}, \tag{12}$$

where $C(r),D(r)$ are scalar functions. The first part of the matrix gives rise to a friction force proportional to the relative velocity at the ''surface'' of the spheres. The effect of this force is twofold. On one hand, the spinning of a particle causes translational motion onto the neighboring particles. On the other, it also causes rotational motion in such a way that two neighboring particles prefer to be with opposite angular velocities (in a sort of ''engaging'' effect). The presence of a third particle frustrates the spinning of both particles and, therefore, the global effect of this force is to damp out to zero the angular velocities of the particles. The second contribution to the force (12) is actually zero because the cross product is perpendicular to $\mathbf{e}_{ij}$. We retain this term just to maintain the analogy between both matrices $\mathbf{M}^R$ in Eq. (9) and $\mathbf{M}^T$ in Eq. (11). Finally, we use the same value for $\gamma$ in Eq. (9) and in Eq. (12) because any difference can be taken into account through the functions $A(r),B(r),C(r),D(r)$.

If we use, instead of the polar vector representation for the angular velocity, the antisymmetric tensor representation $\varpi_{xy}=-\varpi_{yx}=\omega_z$ (cyclic), we can write the force in the form

$$\mathbf{F}^R_{ij}=-\gamma m\mathbf{M}^R(\mathbf{r}_{ij})\cdot(\varpi_i+\varpi_j)\cdot\frac{\mathbf{r}_{ij}}{2} \tag{13}$$

which shows explicitly the vectorial nature of the force (that is, $\mathbf{F}_{ij}^{R}$ transforms under rotations as a vector).

### B. Random forces

The first three contributions $\mathbf{F}_{ij}^{C},\mathbf{F}_{ij}^{T},\mathbf{F}_{ij}^{R}$ to the force between clusters in Eq. (8) are deterministic while the last one is stochastic. The reason we introduce a random force is that it is well known that whenever a coarse graining procedure is performed, dissipation and noise arise and both are related through a fluctuation-dissipation theorem. After discussing the form of the dissipative forces we will now consider the form that the random force should have.

Inspired by the tensorial structure of the random forces that appear in the fluctuating hydrodynamics theory [29], we expect that the dissipation due to shear has associated a traceless symmetric random matrix and that the dissipation due to compressions has associated a diagonal trace matrix. By symmetry reasons, we expect that the noise associated to rotational dissipation will involve an antisymmetric matrix. Therefore, we *postulate* the following velocity independent random force:

$$\tilde{\mathbf{F}}_{ij}dt=\sigma m\left(\tilde{A}(r_{ij})\overline{d\mathbf{W}_{ij}^{S}}+\tilde{B}(r_{ij})\frac{1}{D}\mathrm{tr}[d\mathbf{W}_{ij}]\mathbf{1}+\tilde{C}(r_{ij})d\mathbf{W}_{ij}^{A}\right)\cdot\mathbf{e}_{ij}, \tag{14}$$

where $\tilde{A}(r),\tilde{B}(r),\tilde{C}(r)$ are scalar functions, $\sigma$ is a parameter governing the overall noise amplitude, and we introduce the following symmetric, antisymmetric and traceless symmetric random matrices

$$\begin{aligned} d\mathbf{W}_{ij}^{S\mu\nu}&=\frac{1}{2}[d\mathbf{W}_{ij}^{\mu\nu}+d\mathbf{W}_{ij}^{\nu\mu}],\\ d\mathbf{W}_{ij}^{A\mu\nu}&=\frac{1}{2}[d\mathbf{W}_{ij}^{\mu\nu}-d\mathbf{W}_{ij}^{\nu\mu}], \qquad (15)\\ \overline{d\mathbf{W}_{ij}^{S}}&=d\mathbf{W}_{ij}^{S}-\frac{1}{D}\mathrm{tr}[d\mathbf{W}_{ij}^{S}]\mathbf{1}. \end{aligned}$$

The overline in a matrix denotes its traceless part. Here, $D$ is the physical dimension of space and $d\mathbf{W}_{ij}^{\mu\nu}$ is a matrix of independent Wiener increments, which is assumed to be symmetric under particle interchange

$$d\mathbf{W}_{ij}^{\mu\nu}=d\mathbf{W}_{ji}^{\mu\nu}. \tag{16}$$

This symmetry will ensure momentum conservation because $\tilde{\mathbf{F}}_{ij}=-\tilde{\mathbf{F}}_{ji}$. The matrix $d\mathbf{W}_{ij}^{\mu\nu}$ is an infinitesimal of order 1/2, and this is summarized in the Ito mnemotechnical rule

$$d\mathbf{W}_{ii'}^{\mu\mu'}d\mathbf{W}_{jj'}^{\nu\nu'}=[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{ji'}]\delta_{\mu\nu}\delta_{\mu'\nu'}dt. \tag{17}$$

From this stochastic property, one derives straightforwardly the following rules from the different parts in Eq. (14):

$$\begin{aligned} &\mathrm{tr}[d\mathbf{W}_{ii'}]\mathrm{tr}[d\mathbf{W}_{jj'}]=[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{ji'}]D\,dt,\\ &\overline{d\mathbf{W}_{ii'}^{S}}^{\mu\mu'}\overline{d\mathbf{W}_{jj'}^{S}}^{\nu\nu'}\\ &\quad=[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{ji'}]\left[\frac{1}{2}(\delta_{\mu\nu}\delta_{\mu'\nu'}+\delta_{\mu\nu'}\delta_{\mu'\nu})\right.\\ &\qquad\left.-\frac{1}{D}\delta_{\mu\mu'}\delta_{\nu\nu'}\right]dt,\\ &d\mathbf{W}_{ii'}^{A\mu\mu'}d\mathbf{W}_{jj'}^{A\nu\nu'}=[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{ji'}]\\ &\qquad\times\frac{1}{2}(\delta_{\mu\nu}\delta_{\mu'\nu'}-\delta_{\mu\nu'}\delta_{\mu'\nu})dt, \qquad (18)\\ &\mathrm{tr}[d\mathbf{W}_{ii'}]d\overline{\mathbf{W}}_{jj'}^{S}=0,\\ &\mathrm{tr}[d\mathbf{W}_{ii'}]d\mathbf{W}_{jj'}^{A}=0,\\ &\overline{d\mathbf{W}_{ii'}^{S}}^{\mu\mu'}d\mathbf{W}_{jj'}^{A\nu\nu'}=0. \end{aligned}$$

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 (14) is required in order to be consistent with the tensor structure of the dissipative friction forces (9) and (11). This will become apparent when considering the associated Fokker-Planck equation in the next section and requiring that it has a proper equilibrium ensemble.

Despite the heuristic arguments and strong assumptions made in order to model the force $\mathbf{F}_{ij}$ between clusters, we note that this force is the most general force that can be constructed out of the vectors $\mathbf{r}_i,\mathbf{r}_j,\mathbf{v}_i,\mathbf{v}_j,\boldsymbol{\omega}_i,\boldsymbol{\omega}_j$ and that satisfies the following properties: (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 will be a conserved quantity of the system.

## IV. FOKKER-PLANCK EQUATION AND EQUILIBRIUM STATE

The equations of motion (5) are Langevin equations, which in the form of proper stochastic differential equations (SDE) become

$$\begin{aligned} d\mathbf{r}_i&=\mathbf{v}_i dt,\\ d\mathbf{v}_i&=\frac{1}{m}\sum_{i'}[\mathbf{F}_{ii'}^{C}+\mathbf{F}_{ii'}^{T}+\mathbf{F}_{ii'}^{R}]dt+\sum_{i'}d\tilde{\mathbf{v}}_{ii'}, \qquad (19)\\ d\boldsymbol{\omega}_i&=-\frac{1}{I}\sum_{i'}\frac{\mathbf{r}_{ii'}}{2}\times[\mathbf{F}_{ii'}^{T}+\mathbf{F}_{ii'}^{R}]dt-\frac{m}{I}\sum_{i'}\frac{\mathbf{r}_{ii'}}{2}\times d\tilde{\mathbf{v}}_{ii'}, \end{aligned}$$

where we have introduced

$$d\tilde{\mathbf{v}}_{ii'} \equiv \frac{1}{m}\tilde{\mathbf{F}}_{ii'}dt = \sigma\Bigg(\tilde{A}(r_{ii'})\overline{d\mathbf{W}^S_{ii'}} + \tilde{B}(r_{ii'}) \times \frac{1}{D}\mathrm{tr}[d\mathbf{W}_{ii'}]\mathbf{1} + \tilde{C}(r_{ii'})d\mathbf{W}^A_{ii'}\Bigg)\cdot\mathbf{e}_{ii'}. \tag{20}$$

In principle, one should specify which stochastic interpretation (Itô or Stratonovich) must be used in these equations [32]. Nevertheless, both interpretations produce the same answers because the random forces are velocity independent.

Associated to the SDE (19) there exists a mathematically equivalent Fokker-Planck equation (FPE). The FPE governs the distribution function $\rho(r,v,\omega;t)$ that gives the probability density that the $N$ clusters of the system have specified values for the positions, velocities, and angular velocities. We show in the Appendix that the FPE is given by

$$\partial_t\rho(r,v,\omega;t) = [L^C + L^T + L^R]\rho(r,v,\omega;t). \tag{21}$$

The operator $L^C$ is the usual Liouville operator of a Hamiltonian system interacting with conservative forces $\mathbf{F}^C$, this is,

$$L^C = -\left[\sum_i \mathbf{v}_i\frac{\partial}{\partial\mathbf{r}_i} + \sum_{i,j\neq i}\frac{1}{m}\mathbf{F}^C_{ij}\frac{\partial}{\partial\mathbf{v}_i}\right]. \tag{22}$$

The operators $L^T, L^R$ are given by

$$\begin{aligned} L^T &= \sum_{i,j\neq i}\frac{\partial}{\partial\mathbf{v}_i}\cdot[\mathbf{L}^T_{ij} + \mathbf{L}^R_{ij}], \\ L^R &= -\frac{m}{I}\sum_{i,j\neq i}\frac{\partial}{\partial\boldsymbol{\omega}_i}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times[\mathbf{L}^T_{ij} + \mathbf{L}^R_{ij}]\right), \end{aligned} \tag{23}$$

with

$$\begin{aligned} \mathbf{L}^T_{ij} &\equiv -\frac{1}{m}\mathbf{F}^T_{ij} + \frac{\sigma^2}{2}\mathbf{T}_{ij}\cdot\left[\frac{\partial}{\partial\mathbf{v}_i} - \frac{\partial}{\partial\mathbf{v}_j}\right], \\ \mathbf{L}^R_{ij} &\equiv -\frac{1}{m}\mathbf{F}^R_{ij} + \frac{m}{I}\frac{\sigma^2}{2}\mathbf{T}_{ij}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times\left[\frac{\partial}{\partial\boldsymbol{\omega}_i} + \frac{\partial}{\partial\boldsymbol{\omega}_j}\right]\right). \end{aligned} \tag{24}$$

Here, the matrix $\mathbf{T}_{ij}$ is given by

$$\mathbf{T}_{ij} = \frac{1}{2}[\tilde{A}^2(r_{ij}) + \tilde{C}^2(r_{ij})]\mathbf{1} + \left[\left(\frac{1}{2} - \frac{1}{D}\right)\tilde{A}^2(r_{ij}) + \frac{1}{D}\tilde{B}^2(r_{ij}) - \frac{1}{2}\tilde{C}^2(r_{ij})\right]\mathbf{e}_{ij}\mathbf{e}_{ij}. \tag{25}$$

The steady state solution of Eq. (21), $\partial_t\rho = 0$, gives the equilibrium distribution $\rho^{\mathrm{eq}}$. We now consider the conditions under which the steady state solution is the Gibbs canonical ensemble:

$$\begin{aligned} \rho^{\mathrm{eq}}(r,v,\omega) &= \frac{1}{Z}\exp\{-H(r,v,\omega)/k_BT\} \\ &= \frac{1}{Z}\exp\left\{-\left(\sum_i\frac{m}{2}v_i^2 + \frac{I}{2}\omega_i^2 + V(r)\right)\Big/ k_BT\right\}, \end{aligned} \tag{26}$$

where $H$ is the Hamiltonian of the system, $V$ is the potential function that gives rise to the conservative forces $\mathbf{F}^C$, $k_B$ is Boltzmann's constant, $T$ is the equilibrium temperature, and $Z$ is the normalizing partition function. We note that the velocity and angular velocity *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., $L^C\rho^{\mathrm{eq}} = 0$. If in addition the following equations are satisfied

$$\begin{aligned} \mathbf{L}^T_{ij}\rho^{\mathrm{eq}} &= 0, \\ \mathbf{L}^R_{ij}\rho^{\mathrm{eq}} &= 0, \end{aligned} \tag{27}$$

then we will have $L\rho^{\mathrm{eq}} = 0$ and the Gibbs equilibrium ensemble will be the unique stationary solution of the dynamics. Equations (27) will be satisfied if

$$\gamma = \frac{\sigma^2 m}{2k_BT}, \tag{28}$$

which is a detailed balance condition, and also

$$\mathbf{M}^R(\mathbf{r}_{ij}) = \mathbf{M}^T(\mathbf{r}_{ij}) = \mathbf{T}_{ij}. \tag{29}$$

This is the fluctuation-dissipation theorem for the fluid particle model. We observe, therefore, that the initial hypothesis for the tensorial structure of the dissipative (9), (13), and random (14) forces was correct and consistent with equilibrium statistical mechanics.

A final word about an H-theorem is in order. It has been shown in Ref. [22] that the original DPD algorithm has an H-theorem that ensures that the equilibrium ensemble is the final solution for whatever initial condition selected. In the model presented in this paper there is also a functional of $\rho(z)$ that is a Lyapunov functional. It is not necessary to prove again that an H-theorem exists for the fluid particle model, because a *general* H-theorem exists for *any* Fokker-Planck equation [33]. The only condition is that the diffusion matrix accompanying the second derivative terms of the FPE is positive (semi) definite. However, in the model presented in this paper the diffusion matrix is positive semidefinite by construction, because the FPE has been obtained from a SDE. The diffusion matrix is obtained from the product of two identical matrices. Therefore, its eigenvalues are the square of the eigenvalues of these matrices and are necessarily positive (or zero).

## V. SUMMARY OF THE FLUID PARTICLE MODEL

In this section and for the sake of clarity we collect the results presented so far. 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 $\boldsymbol{\omega}_i$ of each particle. The forces and torques on the particles are given by

$$\mathbf{F}_i=\sum_j \mathbf{F}_{ij},$$
$$\mathbf{N}_i=-\sum_j \frac{\mathbf{r}_{ij}}{2}\times\mathbf{F}_{ij}, \tag{30}$$

where the force that particle $j$ exerts on particle $i$ is given by

$$\mathbf{F}_{ij}=\mathbf{F}^C_{ij}+\mathbf{F}^T_{ij}+\mathbf{F}^R_{ij}+\widetilde{\mathbf{F}}_{ij}. \tag{31}$$

The conservative ($C$), translational ($T$), rotational ($R$), and random (tildes) contributions are given by

$$\begin{aligned}
\mathbf{F}^C_{ij}&=-V'(r_{ij})\mathbf{e}_{ij},\\
\mathbf{F}^T_{ij}&=-\gamma m\mathbf{T}_{ij}\cdot\mathbf{v}_{ij},\\
\mathbf{F}^R_{ij}&=-\gamma m\mathbf{T}_{ij}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times(\boldsymbol{\omega}_i+\boldsymbol{\omega}_j)\right),\\
\widetilde{\mathbf{F}}_{ij}dt&=(2k_BT\gamma m)^{1/2}\bigg(\widetilde{A}(r_{ij})\overline{d\mathbf{W}^S_{ij}}+\widetilde{B}(r_{ij})\frac{1}{D}\mathrm{tr}[d\mathbf{W}_{ij}]\mathbf{1}\\
&\quad+\widetilde{C}(r_{ij})d\mathbf{W}^A_{ij}\bigg)\cdot\mathbf{e}_{ij}.
\end{aligned}\tag{32}$$

The random bits are defined in Eq. (15) and its stochastic properties are given in Eq. (18). Here, the matrix $\mathbf{T}$ is given by

$$\mathbf{T}_{ij}=A(r_{ij})\mathbf{1}+B(r_{ij})\mathbf{e}_{ij}\mathbf{e}_{ij}, \tag{33}$$

where

$$\begin{aligned}
A(r)&=\frac{1}{2}[\widetilde{A}^2(r)+\widetilde{C}^2(r)],\\
B(r)&=\frac{1}{2}[\widetilde{A}^2(r)-\widetilde{C}^2(r)]+\frac{1}{D}[\widetilde{B}^2(r)-\widetilde{A}^2(r)].
\end{aligned}\tag{34}$$

The model is thus specified by providing the scalar functions $V(r),\widetilde{A}(r),\widetilde{B}(r),\widetilde{C}(r)$. We note that the case $\widetilde{A}(r)=\widetilde{C}(r)=0$ corresponds to the original DPD algorithm of Hoogerbrugge and Koelman [15,18]. In this case, the random force is given in terms of a single random number (the trace), the forces are central and the torques vanish, rendering the spin variables unnecessary. Note that there is some freedom in selecting the functions $\widetilde{A}(r),\widetilde{B}(r),\widetilde{C}(r)$ and it might be convenient to take $\widetilde{A}(r)$ or $\widetilde{C}(r)$ equal to zero in order to compute only four of seven random numbers in each step of a simulation.

The model presented in the language of SDE is more appropriate for its direct use in simulations. For theoretical analysis it is more convenient to use the corresponding FPE, which is given by

$$\partial_t\rho(r,v,\omega;t)=[L^C+L^T+L^R]\rho(r,v,\omega;t), \tag{35}$$

where

$$\begin{aligned}
L^C&=-\sum_i \mathbf{v}_i\cdot\frac{\partial}{\partial\mathbf{r}_i}+\frac{\mathbf{F}^C_i}{m}\cdot\frac{\partial}{\partial\mathbf{v}_i},\\
L^T&=\sum_{i,j\neq i}\frac{\partial}{\partial\mathbf{v}_i}\cdot[\mathbf{L}^T_{ij}+\mathbf{L}^R_{ij}],\\
L^R&=-\frac{m}{I}\sum_{i,j\neq i}\frac{\partial}{\partial\boldsymbol{\omega}_i}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times[\mathbf{L}^T_{ij}+\mathbf{L}^R_{ij}]\right).
\end{aligned}\tag{36}$$

Here, the vector operators are given by

$$\begin{aligned}
\mathbf{L}^T_{ij}&\equiv\gamma\mathbf{T}_{ij}\cdot\left\{\mathbf{v}_{ij}+\frac{k_BT}{m}\left[\frac{\partial}{\partial\mathbf{v}_i}-\frac{\partial}{\partial\mathbf{v}_j}\right]\right\}\equiv\gamma\mathbf{T}_{ij}\cdot\boldsymbol{\mathcal{V}}_{ij},\\
\mathbf{L}^R_{ij}&\equiv\gamma\mathbf{T}_{ij}\cdot\left\{\left(\frac{\mathbf{r}_{ij}}{2}\times[\boldsymbol{\omega}_i+\boldsymbol{\omega}_j]\right)+\frac{k_BT}{I}\left(\frac{\mathbf{r}_{ij}}{2}\times\left[\frac{\partial}{\partial\boldsymbol{\omega}_i}+\frac{\partial}{\partial\boldsymbol{\omega}_j}\right]\right)\right\}\\
&\equiv\gamma\mathbf{T}_{ij}\cdot\boldsymbol{\mathcal{W}}_{ij}
\end{aligned}\tag{37}$$

where the last equality defines the two vector operators $\boldsymbol{\mathcal{V}}_{ij},\boldsymbol{\mathcal{W}}_{ij}$.

## VI. KINETIC THEORY

One would like to predict the macroscopic behavior of the fluid particle model and, in particular, check that this behavior conforms to the laws of hydrodynamics (as expected from symmetry considerations) and predict the value of the transport coefficients in terms of model parameters. The global conservation laws of mass and linear and angular momentum in the fluid particle model have a local counterpart in the form of balance equations. Our aim is to formulate these equations of transport within a kinetic theory approach, as has been done by Marsh, Backx, and Ernst recently for the case of the original DPD model in Ref. [22]. A derivation of the hydrodynamic equations with a projection operator technique for the original DPD algorithm was presented in Ref. [21]. The projector used was the Mori projector [34] and the resulting equations were the linearized equations of hydrodynamics. By using a *time-dependent* projector one can obtain the *nonlinear* equations of hydrodynamics with the transport coefficients expressed in terms of Green-Kubo formulas [35]. Although explicit calculations can be performed of these Green-Kubo formulas under certain approximations [36], we adopt in this paper the approach of kinetic theory, allowing for a straightforward comparison with the results of Ref. [22].

### A. General rate of change equation

The starting point is the formulation of the general rate of change equation for an arbitrary function $G(z)$ where $z$ is a shorthand for the set of all positions, velocities, and angular velocities of the $N$ particles of the fluid. By using the Fokker-Planck equation (35), we can write

$$\begin{aligned}\partial_t\langle G\rangle &= \int dz\, G(z)\partial_t\rho(z;t)\\ &= \int dz\, G(z)[L^C+L^T+L^R]\rho(z;t)\\ &= \int dz\, \rho(z;t)[L^{C+}+L^{T+}+L^{R+}]G(z),\end{aligned} \tag{38}$$

where an integration by parts is performed and the adjoint operators are defined by

$$\begin{aligned}L^{C+} &= \sum_i \mathbf{v}_i\cdot\frac{\partial}{\partial\mathbf{r}_i}+\frac{\mathbf{F}_i^C}{m}\cdot\frac{\partial}{\partial\mathbf{v}_i},\\ L^{T+} &= \gamma\sum_{i,j\neq i}(\bar{\boldsymbol{\mathcal{V}}}_{ij}+\bar{\boldsymbol{\mathcal{W}}}_{ij})\cdot\mathbf{T}_{ij}\cdot\frac{\partial}{\partial\mathbf{v}_i},\\ L^{R+} &= -\frac{m}{I}\gamma\sum_{i,j\neq i}\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot(\bar{\boldsymbol{\mathcal{V}}}_{ij}+\bar{\boldsymbol{\mathcal{W}}}_{ij})\right)\cdot\frac{\partial}{\partial\boldsymbol{\omega}_i}.\end{aligned} \tag{39}$$

Here, the vector operators are given by

$$\begin{aligned}\boldsymbol{\mathcal{V}}_{ij}^{+} &\equiv -\mathbf{v}_{ij}+\frac{k_BT}{m}\left[\frac{\partial}{\partial\mathbf{v}_i}-\frac{\partial}{\partial\mathbf{v}_j}\right],\\ \boldsymbol{\mathcal{W}}_{ij}^{+} &\equiv -\left(\frac{\mathbf{r}_{ij}}{2}\times[\boldsymbol{\omega}_i+\boldsymbol{\omega}_j]\right)+\frac{k_BT}{I}\left(\frac{\mathbf{r}_{ij}}{2}\times\left[\frac{\partial}{\partial\boldsymbol{\omega}_i}+\frac{\partial}{\partial\boldsymbol{\omega}_j}\right]\right)\end{aligned} \tag{40}$$

to be compared with Eq. (37).

### B. Balance equations

The conserved density fields are expected to behave hydrodynamically. The conserved density fields are the mass density $\rho(\mathbf{r},t)=mn(\mathbf{r},t)$, where $n(\mathbf{r},t)$ is the number density field; the momentum density $\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)$, where $\mathbf{u}(\mathbf{r},t)$ is the velocity field; and the total angular momentum density field $\mathbf{J}(\mathbf{r},t)=\mathbf{L}(\mathbf{r},t)+\mathbf{S}(\mathbf{r},t)$ where $\mathbf{L}(\mathbf{r},t)=\mathbf{r}\times\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)$ is the macroscopic angular momentum density and $\mathbf{S}(\mathbf{r},t)=In(\mathbf{r},t)\boldsymbol{\Omega}(\mathbf{r},t)$ is the intrinsic angular momentum density or spin density. Here $\boldsymbol{\Omega}(\mathbf{r},t)$ is the angular velocity field. The number density and the velocity and angular velocity fields are defined by

$$\begin{aligned}n(\mathbf{r},t) &= \left\langle\sum_i \delta(\mathbf{r}-\mathbf{r}_i)\right\rangle,\\ n(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) &= \left\langle\sum_i \mathbf{v}_i\delta(\mathbf{r}-\mathbf{r}_i)\right\rangle,\\ n(\mathbf{r},t)\boldsymbol{\Omega}(\mathbf{r},t) &= \left\langle\sum_i \boldsymbol{\omega}_i\delta(\mathbf{r}-\mathbf{r}_i)\right\rangle.\end{aligned} \tag{41}$$

By applying Eq. (38) to the mass and momentum densities (41) we obtain the set of balance equations

$$\begin{aligned}\partial_t\rho &= -\nabla\cdot\rho\mathbf{u},\\ \partial_t\rho\mathbf{u} &= -\nabla\cdot[\rho\mathbf{u}\mathbf{u}+\boldsymbol{\Pi}],\end{aligned} \tag{42}$$

where the total stress tensor $\boldsymbol{\Pi}=\boldsymbol{\Pi}^K+\boldsymbol{\Pi}^C+\boldsymbol{\Pi}^D$ and the kinetic, conservative, and dissipative contributions to the stress tensor are

$$\begin{aligned}\boldsymbol{\Pi}^K &= \left\langle m\sum_i[\mathbf{v}_i-\mathbf{u}(\mathbf{r},t)][\mathbf{v}_i-\mathbf{u}(\mathbf{r},t)]\,\delta(\mathbf{r}-\mathbf{r}_i)\right\rangle,\\ \boldsymbol{\Pi}^C &= \left\langle\frac{1}{2}\sum_{i,j\neq i}\mathbf{F}_{ij}^C\mathbf{r}_{ij}\int_0^1 d\lambda\,\delta(\mathbf{r}-\mathbf{r}_i-\lambda\mathbf{r}_{ij})\right\rangle,\\ \boldsymbol{\Pi}^D &= -\gamma m\left\langle\frac{1}{2}\sum_{i,j\neq i}\mathbf{r}_{ij}\mathbf{T}_{ij}\cdot\mathbf{g}_{ij}\int_0^1 d\lambda\,\delta(\mathbf{r}-\mathbf{r}_i-\lambda\mathbf{r}_{ij})\right\rangle.\end{aligned} \tag{43}$$

Here, $\mathbf{g}_{ij}=\mathbf{v}_{ij}+\mathbf{r}_{ij}\times[\boldsymbol{\omega}_i+\boldsymbol{\omega}_j]/2$ is the relative velocity at the ''surface of contact'' of two identical spheres separated a distance $r_{ij}$. We note that the kinetic and conservative parts to the stress tensor are symmetric tensors but the dissipative part is not and therefore we must be careful with the ordering of the indices. In Cartesian components we understand the momentum balance equation (42) as follows (summation over repeated indices is implied):

$$\partial_t\rho\mathbf{u}^\nu=\partial_\mu[\rho\mathbf{u}^\mu\mathbf{u}^\nu+\boldsymbol{\Pi}_{\mu\nu}] \tag{44}$$

and the dissipative stress tensor has the form

$$\boldsymbol{\Pi}_{\mu\nu}^D=-\gamma m\left\langle\frac{1}{2}\sum_{i,j\neq i}\mathbf{r}_{ij}^\mu\mathbf{T}_{ij}^{\nu\alpha}\mathbf{g}_{ij}^\alpha\int_0^1 d\lambda\,\delta(\mathbf{r}-\mathbf{r}_i-\lambda\mathbf{r}_{ij})\right\rangle. \tag{45}$$

Concerning the angular velocity field, by using again Eq. (38) on the definition (41) we obtain

$$\partial_t n\boldsymbol{\Omega}=-\nabla\cdot\left\langle\sum_i \mathbf{v}_i\boldsymbol{\omega}_i\cdot\delta(\mathbf{r}-\mathbf{r}_i)\right\rangle+\frac{m}{I}\gamma\left\langle\sum_{i,j\neq i}\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\mathbf{g}_{ij}\right)\delta(\mathbf{r}-\mathbf{r}_i)\right\rangle. \tag{46}$$

Note that the rate of change of the spin $\mathbf{S}=In\boldsymbol{\Omega}$ cannot be expressed entirely as the gradient of a flux. This is a reflection of the fact that the intrinsic angular momentum $\mathbf{S}$ is not a conserved quantity. In the same way, the macroscopic angular momentum $\mathbf{L}=\mathbf{r}\times\rho\mathbf{u}$ is not conserved either, as can be appreciated by taking the cross product of the momentum balance equation (42) with the position vector $\mathbf{r}$, that is,

$$\begin{aligned}\partial_t\mathbf{L} &= -\mathbf{r}\times\nabla\cdot(\rho\mathbf{u}\mathbf{u}+\boldsymbol{\Pi})\\ &= -\nabla\cdot(\mathbf{L}\mathbf{u}+\mathbf{r}\times\boldsymbol{\Pi})+2\boldsymbol{\Pi}^A,\end{aligned} \tag{47}$$

where $\boldsymbol{\Pi}^A$ is the antisymmetric part of the stress tensor (expressed here as an axial vector, that is, $\boldsymbol{\Pi}^{A\alpha}=\frac{1}{2}\boldsymbol{\epsilon}^{\alpha\mu\nu}\boldsymbol{\Pi}^{\mu\nu}$, where $\boldsymbol{\epsilon}^{\alpha\mu\nu}$ is the Levi-Civita symbol). If the stress tensor is symmetric (i.e., its antisymmetric part is zero), the macroscopic angular momentum is conserved. In the fluid particle model the noncentral nature of the forces implies that the antisymmetric part of the stress tensor is not zero. Actually, it is given by (as an axial vector)

$$2\boldsymbol{\Pi}^{A}=-\gamma m\left\langle \sum_{i,j\neq i}\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\mathbf{g}_{ij}\right)\int_{0}^{1}d\lambda\ \delta(\mathbf{r}-\mathbf{r}_{i}+\lambda\mathbf{r}_{ij})\right\rangle. \tag{48}$$

If we add the last term of Eq. (46) with the last term of Eq. (47), which is (48), we obtain

$$\begin{aligned}2\boldsymbol{\Pi}^{A}+\gamma m\left\langle \sum_{i,j\neq i}\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\mathbf{g}_{ij}\right)\delta(\mathbf{r}-\mathbf{r}_{i})\right\rangle &=\gamma m\left\langle \sum_{i,j\neq i}\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\mathbf{g}_{ij}\right)\left[\delta(\mathbf{r}-\mathbf{r}_{i})-\int_{0}^{1}d\lambda\ \delta(\mathbf{r}-\mathbf{r}_{i}+\lambda\mathbf{r}_{ij})\right]\right\rangle\\ &=\gamma m\nabla\left\langle \sum_{i,j\neq i}\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\mathbf{g}_{ij}\right)\mathbf{r}_{ij}\int_{0}^{1}d\lambda\int_{0}^{1}d\lambda'\,\delta(\mathbf{r}-\mathbf{r}_{i}+\lambda\lambda'\mathbf{r}_{ij})\right\rangle.\end{aligned} \tag{49}$$

Therefore, the *total* angular momentum density $\mathbf{J}=\mathbf{L}+\mathbf{S}$ satisfies a balance equation

$$\partial_{t}\mathbf{J}=-\nabla\cdot[\mathbf{J}\mathbf{v}+\mathbf{r}\times\boldsymbol{\Pi}+\boldsymbol{\Phi}], \tag{50}$$

where

$$\boldsymbol{\Phi}=\gamma m\left\langle \sum_{i,j\neq i}\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\mathbf{g}_{ij}\right)\mathbf{r}_{ij}\int_{0}^{1}d\lambda\int_{0}^{1}d\lambda'\,\delta(\mathbf{r}-\mathbf{r}_{i}+\lambda\lambda'\mathbf{r}_{ij})\right\rangle. \tag{51}$$

### C. Balance equations in terms of distribution functions

It is convenient to express the quantities appearing in the balance equations in terms of the single particle and pair distribution functions, defined as

$$\begin{aligned}f(\mathbf{x},t)&=f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)=\left\langle \sum_{i}\ \delta(\mathbf{x}-\mathbf{x}_{i})\right\rangle,\\ f^{(2)}(\mathbf{x},\mathbf{x}',t)&=\left\langle \sum_{i,j\neq i}\ \delta(\mathbf{x}-\mathbf{x}_{i})\,\delta(\mathbf{x}'-\mathbf{x}_{j})\right\rangle.\end{aligned} \tag{52}$$

The number density, the velocity, and angular velocities in Eq. (41) are the first moments of the single particle distribution function,

$$\begin{aligned}n(\mathbf{r},t)&=\int d\mathbf{v}\,d\boldsymbol{\omega}\,f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t),\\ n(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)&=\int d\mathbf{v}\,d\boldsymbol{\omega}\,\mathbf{v}f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t),\\ n(\mathbf{r},t)\boldsymbol{\Omega}(\mathbf{r},t)&=\int d\mathbf{v}\,d\boldsymbol{\omega}\ \boldsymbol{\omega}f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t).\end{aligned} \tag{53}$$

Next, by using that for an arbitrary function $G$

$$\left\langle \sum_{i,j\neq i}G(\mathbf{r}_{ij},\mathbf{v}_{i},\mathbf{v}_{j},\boldsymbol{\omega}_{i},\boldsymbol{\omega}_{j})\,\delta(\mathbf{r}-\mathbf{r}_{i}+\lambda\mathbf{r}_{ij})\right\rangle=\int d\mathbf{v}\,d\mathbf{v}'\,d\boldsymbol{\omega}\,d\boldsymbol{\omega}'\,d\mathbf{R}\,G(\mathbf{R},\mathbf{v},\mathbf{v}',\boldsymbol{\omega},\boldsymbol{\omega}')\,f^{(2)}(\mathbf{r}+\lambda\mathbf{R},\mathbf{v},\boldsymbol{\omega},\mathbf{r}+(\lambda-1)\mathbf{R},\mathbf{v}',\boldsymbol{\omega}'), \tag{54}$$

which, for $\lambda=0$ becomes

$$\left\langle \sum_{i,j\neq i}G(\mathbf{r}_{ij},\mathbf{v}_{i},\mathbf{v}_{j},\boldsymbol{\omega}_{i},\boldsymbol{\omega}_{j})\,\delta(\mathbf{r}-\mathbf{r}_{i})\right\rangle=\int d\mathbf{v}\,d\mathbf{v}'\,d\boldsymbol{\omega}\,d\boldsymbol{\omega}'\,d\mathbf{R}\,G(\mathbf{R},\mathbf{v},\mathbf{v}',\boldsymbol{\omega},\boldsymbol{\omega}')\,f^{(2)}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}-\mathbf{R},\mathbf{v}',\boldsymbol{\omega}') \tag{55}$$

we can write the different contributions (43) to the stress tensor in terms of the distribution functions

$$\mathbf{\Pi}^K = \int d\mathbf{v}\, d\boldsymbol{\omega}\, m(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u}) f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t),$$

$$\mathbf{\Pi}^C = \int d\mathbf{v}\, d\boldsymbol{\omega}\, d\mathbf{v}'\, d\boldsymbol{\omega}' \int d\mathbf{R} \frac{\mathbf{R}}{2} \mathbf{F}^C(\mathbf{R})\, \overline{f^{(2)}}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}',\mathbf{v}',\boldsymbol{\omega}'), \tag{56}$$

$$\mathbf{\Pi}^D = -\gamma m \int d\mathbf{v}\, d\boldsymbol{\omega}\, d\mathbf{v}'\, d\boldsymbol{\omega}' \int d\mathbf{R} \frac{\mathbf{R}}{2} \mathbf{T}(\mathbf{R}) \cdot \mathbf{g}\, \overline{f^{(2)}}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}',\mathbf{v}',\boldsymbol{\omega}'),$$

where $\mathbf{g} \equiv [\mathbf{v}-\mathbf{v}' + \mathbf{R}/2 \times [\boldsymbol{\omega}+\boldsymbol{\omega}']]$. We have introduced in these expressions the spatially averaged pair distribution function

$$\overline{f^{(2)}}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}',\mathbf{v}',\boldsymbol{\omega}') = \int_0^1 d\lambda\, f^{(2)}(\mathbf{r}+\lambda\mathbf{R},\mathbf{v},\boldsymbol{\omega},\mathbf{r}+(\lambda-1)\mathbf{R},\mathbf{v}',\boldsymbol{\omega}'). \tag{57}$$

In terms of the distribution functions the terms of the right-hand side of Eq. (46) can be written as

$$\left\langle \sum_{i,j\neq i} \mathbf{v}_i \boldsymbol{\omega}_i \delta(\mathbf{r}-\mathbf{r}_i) \right\rangle = \int d\mathbf{v}\, d\boldsymbol{\omega}\, \mathbf{v}\boldsymbol{\omega} f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$$

$$= \int d\mathbf{v}\, d\boldsymbol{\omega} (\mathbf{v}-\mathbf{u})(\boldsymbol{\omega}-\mathbf{\Omega}) f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) - n\mathbf{\Omega}\mathbf{u} + \mathbf{u} \int d\mathbf{v}\, d\boldsymbol{\omega}\, \boldsymbol{\omega} f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) + \mathbf{\Omega} \int d\mathbf{v}\, d\boldsymbol{\omega}\, \mathbf{v} f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t),$$

$$\left\langle \sum_{i,j\neq i} \left( \frac{\mathbf{r}_{ij}}{2} \mathbf{T}_{ij} \cdot \mathbf{g}_{ij} \right) \delta(\mathbf{r}-\mathbf{r}_i) \right\rangle = \int d\mathbf{v}\, d\boldsymbol{\omega}\, d\mathbf{v}'\, d\boldsymbol{\omega}' \int d\mathbf{R} \left( \frac{\mathbf{R}}{2} \times \mathbf{T}(\mathbf{R}) \cdot \mathbf{g} \right) f^{(2)}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}-\mathbf{R},\mathbf{v}',\boldsymbol{\omega}'). \tag{58}$$

Finally,

$$\mathbf{\Phi} = \gamma m \int d\mathbf{v}\, d\boldsymbol{\omega}\, d\mathbf{v}'\, d\boldsymbol{\omega}' \int d\mathbf{R} \left( \frac{\mathbf{R}}{2} \times \mathbf{T}(\mathbf{R}) \cdot \mathbf{g} \right) \mathbf{R}\, \overline{\overline{f^{(2)}}}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}',\mathbf{v}',\boldsymbol{\omega}'), \tag{59}$$

where

$$\overline{\overline{f^{(2)}}}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}',\mathbf{v}',\boldsymbol{\omega}') = \int_0^1 d\lambda \int_0^1 d\lambda'\, f^{(2)}(\mathbf{r}+\lambda\lambda'\mathbf{R},\mathbf{v},\boldsymbol{\omega},\mathbf{r}+(\lambda\lambda'-1)\mathbf{R},\mathbf{v}',\boldsymbol{\omega}'). \tag{60}$$

### D. Fokker-Planck-Boltzmann equation

The Fokker-Planck-Boltzmann equation (FPBE) is an approximate kinetic equation for the single particle distribution function $f(\mathbf{x},t)$. The FPBE is obtained by applying the general rate of change equation (38) to $f(\mathbf{x},t)$. After some algebra one arrives at

$$\partial_t f + \mathbf{v} \cdot \nabla f = \int d\mathbf{R}\, d\mathbf{v}'\, d\boldsymbol{\omega}'\, \partial \cdot [\mathbf{F}^C(\mathbf{R}) + \gamma \mathbf{T}(\mathbf{R}) \cdot \mathbf{g}] f^{(2)}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}-\mathbf{R},\mathbf{v}',\boldsymbol{\omega}')$$

$$+ \frac{k_B T}{m} \gamma \int d\mathbf{R}\, d\mathbf{v}'\, d\boldsymbol{\omega}'\, \partial \cdot \mathbf{T}(\mathbf{R}) \cdot \partial f^{(2)}(\mathbf{r},\mathbf{v},\boldsymbol{\omega},\mathbf{r}-\mathbf{R},\mathbf{v}',\boldsymbol{\omega}'), \tag{61}$$

where we have defined the operator

$$\partial \equiv \frac{\partial}{\partial \mathbf{v}} + \frac{m}{I} \left( \frac{\mathbf{R}}{2} \times \frac{\partial}{\partial \boldsymbol{\omega}} \right). \tag{62}$$

In obtaining Eq. (61), we have inserted at some point the identity

$$1 = \int d\mathbf{R}\, d\mathbf{v}'\, d\boldsymbol{\omega}'\, \delta(\mathbf{r}-\mathbf{R}-\mathbf{r}_j) \delta(\mathbf{v}'-\mathbf{v}_j) \delta(\boldsymbol{\omega}'-\boldsymbol{\omega}_j). \tag{63}$$

Equation (61) is not a closed equation for $f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$ because the pair function $f^{(2)}(\mathbf{x},\mathbf{x}',t)$ appears. Nevertheless it can be closed approximately by using the molecular chaos assumption. In what follows we will assume that the friction $\gamma$ is so large to allow for a neglect of the conservative forces $\mathbf{F}^C$ [22]. This simplifies considerably the calculations in the next section. The molecular chaos assumption in the absence of conservative forces becomes

$$f^{(2)}(\mathbf{x},\mathbf{x}',t)\approx f(\mathbf{x},t)f(\mathbf{x}',t). \tag{64}$$

The final closed Fokker-Planck-Boltzmann equation for the distribution function is, after using the molecular chaos assumption (64),

$$\partial_t f+\mathbf{v}\cdot\nabla f=I[f]=\gamma\int d\mathbf{R}\,d\mathbf{v}'\,d\boldsymbol{\omega}'\,f(\mathbf{r}-\mathbf{R},\mathbf{v}',\boldsymbol{\omega}')\times\partial\cdot\mathbf{T}(\mathbf{R})\cdot\left[\mathbf{g}+\frac{k_BT}{m}\partial\right]f(\mathbf{r},\mathbf{v},\boldsymbol{\omega}), \tag{65}$$

which is an integrodifferential nonlinear equation.

### E. Chapman-Enskog solution of the FPBE

Our aim is to solve the nonlinear FPBE (65) by using the perturbative method of Chapman and Enskog. The method is valid for situations in which the macroscopic conserved fields are slowly varying in typical molecular length scales. In these situations, the distribution function decays in a very short kinetic time (short compared to typical times of evolution of the conserved field) towards the so-called *normal* solution where the distribution function $f(\mathbf{v},\boldsymbol{\omega}|a(\mathbf{r},t))$ depends on space and time only through the first few moments $a(\mathbf{r},t)$ [22]. During this last hydrodynamic stage, the solution can be obtained perturbatively as an expansion in gradients, that is, $f(\mathbf{v},\boldsymbol{\omega}|\mathbf{u},\boldsymbol{\Omega})=f_0+f_1+O(\nabla^2)$ where $f_0$ is of zeroth order in gradients and $f_1$ is of first order in gradients. By substitution of this expansion into the FPBE (65) one obtains

$$\partial_t f_0+\partial_t f_1+\mathbf{v}\cdot\nabla f_0=I[f_0]+\left(\frac{dI}{df}\right)_{f_0}f_1+O(\nabla^2). \tag{66}$$

By analogy with the conventional kinetic theory and also with the kinetic theory for DPD in Ref. [22], we expect that the lowest order contribution $f_0$ is given by the *local equilibrium* form for the distribution function. In the presence of spin variables it takes the form

$$f_0(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)=n(\mathbf{r},t)\left(\frac{m}{2\pi k_BT}\right)^{D/2}\exp\left\{-\frac{m}{2k_BT}(\mathbf{v}-\mathbf{u})^2\right\}\times\left(\frac{I}{2\pi k_BT}\right)^{D/2}\exp\left\{-\frac{I}{2k_BT}(\boldsymbol{\omega}-\boldsymbol{\Omega})^2\right\}. \tag{67}$$

This local equilibrium distribution provides the correct averages for the first moments of $f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$, that is,

$$\begin{aligned}n(\mathbf{r},t)&=\int d\mathbf{v}\,d\boldsymbol{\omega}\,f_0(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t),\\ n(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)&=\int d\mathbf{v}\,d\boldsymbol{\omega}\,\mathbf{v}f_0(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t),\\ n(\mathbf{r},t)\boldsymbol{\Omega}(\mathbf{r},t)&=\int d\mathbf{v}\,d\boldsymbol{\omega}\,\boldsymbol{\omega}f_0(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t).\end{aligned} \tag{68}$$

This, in turn, implies that the first moments of $f_1$ are of order $O(\nabla^2)$.

The procedure is now a bit different from the Chapman-Enskog method in Ref. [22], because the inclusion of the spin variables produces new terms with different orders in gradients. We write Eq. (66) as follows:

$$\left(\frac{dI}{df}\right)_{f_0}f_1-\partial_t f_1=\partial_t f_0+\mathbf{v}\cdot\nabla f_0-I[f_0], \tag{69}$$

where we have neglected terms that are quadratic in gradients. We will check in the following that both sides of this equation are explicitly of first order in gradients. This linear equation (69) will be solved for $f_1$ and therefore we will obtain the solution of the FPBE (65) as $f_0+f_1$, up to terms of order $\nabla^2$.

We now consider each term of Eq. (69) separately. The temporal and spatial derivatives of $f_0$ can be computed to first order in gradients with the use of the balance equations (42) and (46). Only terms of order $\nabla$ are to be retained, which amounts to using the balance equations with the averages of the quantities appearing in them evaluated with the local equilibrium ensemble. Therefore, we need to compute the local equilibrium average of the stress tensor $\boldsymbol{\Pi}$ in the momentum balance equation, and the local equilibrium average of the two contributions in Eq. (58) to the equation for the angular velocity field. After using the molecular chaos assumption one easily obtains the following results:

$$\begin{aligned}\boldsymbol{\Pi}^{K0}_{\mu\nu}&=nk_BT\delta_{\mu\nu},\\ \boldsymbol{\Pi}^{D0}_{\mu\nu}&=-\gamma mn^2\frac{1}{2}[A_2[\partial_\nu\mathbf{u}^\mu+\epsilon^{\mu\nu\sigma}\boldsymbol{\Omega}^\sigma]\\ &\quad+B_2[\nabla\cdot\mathbf{u}\delta_{\mu\nu}+\partial_\nu\mathbf{u}^\mu+\partial_\mu\mathbf{u}^\nu]]+O(\nabla^2),\end{aligned} \tag{70}$$

where we have defined

$$\begin{aligned}A_2&\equiv\frac{1}{D}\int d\mathbf{R}\,R^2A(R),\\ B_2&\equiv\frac{1}{D(D+2)}\int d\mathbf{R}\,R^2B(R).\end{aligned} \tag{71}$$

The first contribution $\boldsymbol{\Pi}^{K0}$ produces an isotropic pressure term. Consistently with our assumption that the conservative forces are negligible this pressure is given by the ideal gas expression. The second contribution $\boldsymbol{\Pi}^{D0}$ contains terms of first order in gradients. We arrange a bit this contribution by introducing the velocity gradient tensor $(\nabla\mathbf{u})_{\nu\mu}=\partial_\nu\mathbf{u}^\mu$ and its traceless symmetric and antisymmetric parts

$$\overline{\nabla\mathbf{u}^S}\equiv\frac{1}{2}[\nabla\mathbf{u}+\nabla\mathbf{u}^T]-\frac{1}{D}\nabla\cdot\mathbf{u}\mathbf{1},$$

$$\nabla\mathbf{u}^A\equiv\frac{1}{2}[\nabla\mathbf{u}-\nabla\mathbf{u}^T]. \tag{72}$$

We have

$$\mathbf{\Pi}^{D0}=-\gamma m n^2\frac{1}{2}\bigg[A_2(\nabla\mathbf{u}^A+\mathbf{\Omega})+(A_2+2B_2)\overline{\nabla\mathbf{u}^S}$$
$$+[A_2+(D+2)B_2]\frac{1}{D}\nabla\cdot\mathbf{u}\mathbf{1}\bigg]. \tag{73}$$

The antisymmetric part of the total stress tensor in the local equilibrium approximation to first order in gradients is given by (as an axial vector)

$$\mathbf{\Pi}^{A0}=\gamma m n^2\frac{A_2}{2}\left(\frac{1}{2}\nabla\times\mathbf{u}-\mathbf{\Omega}\right). \tag{74}$$

In a similar way one computes the quantities in Eq. (58) that appear in the balance equation for the spin (46). In particular, the last term in Eq. (58) is also given by $-2\mathbf{\Pi}^A$ in the local equilibrium approximation to first order gradients.

Substitution of the local equilibrium expressions for the stress tensor into the balance equations produce, the Euler equations,

$$\partial_t n=-\nabla n\mathbf{u},$$

$$\partial_t\mathbf{u}=-(\mathbf{u}\cdot\nabla)\mathbf{u}-\frac{k_BT}{m}\frac{1}{n}\nabla n+\frac{1}{n}\nabla\times\gamma\frac{A_2}{2}n^2\mathbf{\Omega}, \tag{75}$$

$$\partial_t\mathbf{\Omega}=-(\mathbf{u}\cdot\nabla)\mathbf{\Omega}+\gamma\frac{m}{I}A_2 n\left[\frac{1}{2}\nabla\times\mathbf{u}-\mathbf{\Omega}\right].$$

We have neglected a term of first order in gradients, which produces a term of order $\nabla^2$ in the momentum balance equation. We note that the time derivative of the angular velocity contains a term that is of *zeroth* order in gradients (the $\mathbf{\Omega}$ term in the last equation).

With the help of the Euler equations and the chain rule, we can now compute the time and space derivatives of the local equilibrium distribution, to first order in gradient. The result is

$$\partial_t f_0+\mathbf{v}\cdot\nabla f_0=f_0\bigg(-\nabla\cdot\mathbf{u}+\frac{m}{k_BT}(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u}):\nabla\mathbf{u}+\frac{I}{k_BT}(\boldsymbol{\omega}-\mathbf{\Omega})(\mathbf{v}-\mathbf{u}):\nabla\mathbf{\Omega}+\gamma n A_2\frac{m}{k_BT}\frac{1}{2n}(\mathbf{v}-\mathbf{u})\cdot\nabla\times n^2\mathbf{\Omega}$$
$$+\gamma A_2 n\frac{m}{k_BT}(\boldsymbol{\omega}-\mathbf{\Omega})\cdot\left[\frac{1}{2}\nabla\times\mathbf{u}-\mathbf{\Omega}\right]\bigg), \tag{76}$$

where the double dot ":" denotes double contraction.

The next step is the calculation of $I[f_0]$. To first order in gradients it is given by

$$I[f_0]=\gamma n A_2\frac{m}{k_BT}f_0\left(\frac{1}{2n}(\mathbf{v}-\mathbf{u})\cdot\nabla\times n^2\mathbf{\Omega}+(\boldsymbol{\omega}-\mathbf{\Omega})\cdot\left[\frac{1}{2}\nabla\times\mathbf{u}-\mathbf{\Omega}\right]\right). \tag{77}$$

Therefore, after some happy cancellations the right hand side of Eq. (69) has the simple form

$$\partial_t f_0+\mathbf{v}\cdot\nabla f_0-I[f_0]=f_0\left[-\nabla\cdot\mathbf{u}+\frac{m}{k_BT}(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u}):\nabla\mathbf{u}+\frac{I}{k_BT}(\boldsymbol{\omega}-\mathbf{\Omega})(\mathbf{v}-\mathbf{u}):\nabla\mathbf{\Omega}\right], \tag{78}$$

which contains only terms of first order in gradients.

Next, we consider the term $\partial_t f_1$ in Eq. (69). We note that it is of first order in gradients due to the term of zeroth order in the Euler equation for the angular velocity, that is,

$$\partial_t f_1=\frac{\partial f_1}{\partial\mathbf{\Omega}}\cdot\partial_t\mathbf{\Omega}+O(\nabla^2),$$

$$=-\frac{m}{I}\gamma A_2 n\mathbf{\Omega}\cdot\frac{\partial f_1}{\partial\mathbf{\Omega}}+O(\nabla^2), \tag{79}$$

$$=\frac{m}{I}\gamma A_2 n\mathbf{\Omega}\cdot\frac{\partial f_1}{\partial\boldsymbol{\omega}}+O(\nabla^2),$$

where we have assumed that the dependence of $f_1$ on $\mathbf{\Omega}$ appears in the combination $\boldsymbol{\omega}-\mathbf{\Omega}$. This assumption will be confirmed *a posteriori*.

The linearization of the functional $I[f]$ might be easier to perform by expanding $I[f_0+f_1]$ to first order in gradients. The final result for the left hand side of Eq. (69) is

$$I[f_0+f_1]-I[f_0]-\partial_t f_1=\gamma n\left[[A_0+B_0]\mathcal{L}^T+\frac{m}{I}\frac{A_2}{2}\mathcal{L}^R\right]f_1$$
$$+O(\nabla^2), \tag{80}$$

where the operators are given by

$$\mathcal{L}^T=\frac{\partial}{\partial\mathbf{v}}\cdot\left[\mathbf{v}-\mathbf{u}+\frac{k_BT}{m}\frac{\partial}{\partial\mathbf{v}}\right],$$

$$\mathcal{L}^R=\frac{\partial}{\partial\boldsymbol{\omega}}\cdot\left[\boldsymbol{\omega}-\boldsymbol{\Omega}+\frac{k_BT}{I}\frac{\partial}{\partial\boldsymbol{\omega}}\right] \tag{81}$$

and the constants $A_0, B_0$ are given by

$$A_0\equiv\int d\mathbf{R}A(R),$$

$$B_0\equiv\frac{1}{D}\int d\mathbf{R}B(R). \tag{82}$$

Equation (69) can be written in compact form as

$$\mathcal{L}f_1=f_0\left[-\nabla\cdot\mathbf{u}+\frac{m}{k_BT}\mathbf{VV}:\nabla\mathbf{u}+\frac{I}{k_BT}\mathbf{OV}:\nabla\boldsymbol{\Omega}\right], \tag{83}$$

where the operator has the form

$$\mathcal{L}=\gamma n\left[[A_0+B_0]\mathcal{L}^T+\frac{m}{I}\frac{A_2}{2}\mathcal{L}^R\right] \tag{84}$$

and the peculiar velocities are $\mathbf{V}=\mathbf{v}-\mathbf{u},\mathbf{O}=\boldsymbol{\omega}-\boldsymbol{\Omega}$.

Equation (83) is an inhomogeneous second order partial differential equation. In order to obtain a special solution of the inhomogeneous equations (83), we introduce the following tensors:

$$\mathbf{J}_{\mu\nu}=\frac{m}{k_BT}\left\{\mathbf{V}_\mu\mathbf{V}_\nu-\frac{1}{D}V^2\delta_{\mu\nu}\right\},$$

$$\mathcal{J}=\frac{mV^2}{Dk_BT}-1, \tag{85}$$

$$\mathcal{T}_{\mu\nu}=\frac{I}{k_BT}\mathbf{O}_\mu\mathbf{V}_\nu.$$

With these quantities we write Eq. (83) in the form

$$\mathcal{L}f_1=f_0[\mathbf{J}:\overline{\nabla\mathbf{u}}^S+\mathcal{J}\nabla\cdot\mathbf{u}\mathbf{1}+\mathcal{T}:\nabla\boldsymbol{\Omega}]. \tag{86}$$

The quantities (85) satisfy

$$\mathcal{L}^Tf_0\mathbf{J}_{\mu\nu}=-2f_0\mathbf{J}_{\mu\nu},$$

$$\mathcal{L}^Rf_0\mathbf{J}_{\mu\nu}=\mathbf{0},$$

$$\mathcal{L}^Tf_0\mathcal{J}=-2f_0\mathcal{J},$$

$$\mathcal{L}^Rf_0\mathcal{J}=0, \tag{87}$$

$$\mathcal{L}^Tf_0\mathcal{T}_{\mu\nu}=f_0\mathcal{T}_{\mu\nu},$$

$$\mathcal{L}^Rf_0\mathcal{T}_{\mu\nu}=f_0\mathcal{T}_{\mu\nu},$$

and therefore, a special solution of Eq. (83) is given by

$$f_1=-f_0\left[\frac{1}{2\gamma n(A_0+B_0)}[\mathbf{J}:\overline{\nabla\mathbf{u}}^S+\mathcal{J}\nabla\cdot\mathbf{u}\mathbf{1}]-\frac{1}{\gamma n(A_0+B_0+(m/I)A_2/2)}\mathcal{T}:\nabla\boldsymbol{\Omega}\right] \tag{88}$$

as can be checked by substitution.

Now it remains to obtain a general solution of the homogeneous equation $\mathcal{L}f_1=0$. The solution of this homogeneous equation is an arbitrary linear combination of $f_0a$, where $a$ are the collisional invariants $a=\{1,\mathbf{v}-\mathbf{u},\boldsymbol{\omega}-\boldsymbol{\Omega}\}$. Nevertheless, the combination of Eqs. (53) and (68) imposes that the coefficients of the linear combination are zero.

### F. Transport coefficients

The phenomenological theory of viscous flow of an isotropic fluid [28] relates the trace tr$[\mathbf{\Pi}]$, the traceless symmetric $\overline{\mathbf{\Pi}}^S$, and antisymmetric $\mathbf{\Pi}^A$ parts of the stress tensor $\mathbf{\Pi}$ with the linear velocity gradients and angular velocity in the following way:

$$\frac{1}{D}\mathrm{tr}[\mathbf{\Pi}]=-\zeta\nabla\cdot\mathbf{u}+p,$$

$$\overline{\mathbf{\Pi}}^S=-2\eta\overline{\nabla\mathbf{u}}^S, \tag{89}$$

$$\mathbf{\Pi}^A=-2\eta_R\left[\frac{1}{2}\nabla\times\mathbf{u}-\boldsymbol{\Omega}\right],$$

where the antisymmetric part is written as an axial vector. Here $p$ is the isotropic hydrostatic pressure. The coefficients are the bulk viscosity $\zeta$, the shear viscosity $\eta$, and the rotational viscosity $\eta_R$.

We now compute the stress tensor (56) using the molecular chaos assumption (64) for the pair distribution function and the approximate solution $f_0+f_1$ for the single particle distribution function. This will produce $\mathbf{\Pi}=\mathbf{\Pi}_0+\mathbf{\Pi}_1$ where the local equilibrium contribution $\mathbf{\Pi}_0$ has been already computed in Eq. (70). Regarding the term $\mathbf{\Pi}_1$ computed with $f_1$ one observes that the only contribution that is of first order in gradients is $\mathbf{\Pi}_1^K$, which is computed along similar lines to Ref. [22]. The final result is

$$\mathbf{\Pi}^K=nk_BT\mathbf{1}-\frac{k_BT}{\gamma[A_0+B_0]}\overline{\nabla\mathbf{u}}^S-\frac{k_BT}{D\gamma[A_0+B_0]}\nabla\cdot\mathbf{u}\mathbf{1}. \tag{90}$$

The remaining contributions $\mathbf{\Pi}_1^D$ are of order $\nabla^2$ and will be neglected. The final expression of the stress tensor in linear order of gradients is given by collecting Eqs. (73), (74), and (90):

$$\frac{1}{D}\mathrm{tr}[\boldsymbol{\Pi}]=-\left\{\gamma m n^2\left[\frac{A_2}{2D}+\frac{(D+2)}{2D}B_2\right]+\frac{k_BT}{\gamma D[A_0+B_0]}\right\}\nabla\cdot\mathbf{u}$$
$$+nk_BT,$$

$$\overline{\boldsymbol{\Pi}}^S=-\left\{\gamma m n^2\left[\frac{A_2}{2}+B_2\right]+\frac{k_BT}{\gamma[A_0+B_0]}\right\}\overline{\nabla\mathbf{u}^S}, \tag{91}$$

$$\boldsymbol{\Pi}^A=-\gamma m n^2\frac{A_2}{2}\left[\frac{1}{2}\nabla\times\mathbf{u}-\boldsymbol{\Omega}\right].$$

Comparison of Eqs. (89) and (91) allows one to identify the viscosities as

$$\zeta=\left\{\gamma m n^2\left[\frac{A_2}{2D}+\frac{(D+2)}{2D}B_2\right]+\frac{k_BT}{\gamma D[A_0+B_0]}\right\},$$

$$\eta=\frac{1}{2}\left\{\gamma m n^2\left[\frac{A_2}{2}+B_2\right]+\frac{k_BT}{\gamma[A_0+B_0]}\right\}, \tag{92}$$

$$\eta_R=\gamma m n^2\frac{A_2}{2}.$$

In order to compare these expressions with those obtained by Marsh *et al.* [22], we should note that for the original DPD algorithm we have

$$A(r)=0,$$
$$B(r)=\omega(R). \tag{93}$$

Simple substitution of Eq. (93) into Eq. (92) shows that the transport coefficient (92) coincides with those provided in Ref. [22].

### G. Transport equations

Substitution of the stress tensor $\boldsymbol{\Pi}=\mathrm{tr}[\boldsymbol{\Pi}]\mathbf{1}/D+\overline{\boldsymbol{\Pi}}^S+\boldsymbol{\Pi}^A$, Eq. (89), into the momentum balance equation (42) produces the Navier-Stokes equations for a fluid with spin [28] ($D=3$),

$$\rho\frac{d}{dt}\mathbf{u}=-\nabla p+\nabla\cdot(2\eta\nabla\mathbf{u}^S)+\nabla(\zeta-2\eta/3)\nabla\cdot\mathbf{u}+\nabla$$
$$\times[2\eta_R(\boldsymbol{\Omega}-\tfrac{1}{2}\nabla\times\mathbf{u})], \tag{94}$$

where we have used the substantial derivative $d/dt=\partial_t+\mathbf{u}\cdot\nabla$. The last term in Eq. (94) is the gradient of the antisymmetric part of the stress tensor and describes the effect of the spin on the momentum transport.

On the other hand by neglecting the term $\boldsymbol{\Phi}$ in the angular momentum balance equation (50) [28] we obtain

$$\partial_t\mathbf{J}=-\nabla[\mathbf{J}\mathbf{v}+\mathbf{r}\times\boldsymbol{\Pi}], \tag{95}$$

which in combination with Eq. (47) produces the following balance equation for the spin density:

$$\partial_t\mathbf{S}=-\nabla[\mathbf{S}\mathbf{u}]-2\boldsymbol{\Pi}^A, \tag{96}$$

which implies the following dynamic equation for the angular velocity:

$$nI\frac{d}{dt}\boldsymbol{\Omega}=-2\boldsymbol{\Pi}^A. \tag{97}$$

Substitution of $\boldsymbol{\Pi}^A$ in Eq. (89) into this equation gives

$$\frac{d}{dt}\boldsymbol{\Omega}=-\frac{4\eta_R}{nI}\left[\boldsymbol{\Omega}-\frac{1}{2}\nabla\times\mathbf{u}\right]=-\frac{1}{\tau}\left[\boldsymbol{\Omega}-\frac{1}{2}\nabla\times\mathbf{u}\right]. \tag{98}$$

The final closed set of equations for the hydrodynamic fields is given by Eqs. (94) and (98), together with the continuity equation

$$\frac{d}{dt}\rho=-\rho\nabla\cdot\mathbf{u} \tag{99}$$

and the equation of state

$$p=k_BTn=\frac{k_BT}{m}\rho\equiv c^2\rho, \tag{100}$$

where we have introduced the speed of sound $c$.

Equation (98) shows that the spin relaxes towards the vorticity with a relaxation time scale given by $\tau=nI/4\eta_R$ [28]. In the model of this paper, substitution of $\eta_R$ in (92) gives the following time scale

$$\tau=\frac{I}{2\gamma n m A_2}. \tag{101}$$

### H. Summary of kinetic theory

In summary, it has been shown in this section that the macroscopic behavior of the fluid particle model is hydrodynamical and the mass, momentum and angular momentum transport equations have been derived [Eqs. (99), (94), and (98)]. In doing this, explicit expressions for the transport coefficients in terms of the original model parameters have been obtained [Eqs. (92) and (101)]. The equations cited here are the main results of the kinetic theory of the fluid particle model.

## VII. RESOLUTION ISSUES OF THE FLUID PARTICLE MODEL

Within the picture of the Voronoi coarse-graining sketched in Sec. II, it is possible to consider different levels of coarse graining in which the number of atomic particles within a Voronoi cell is different. We expect that, provided that the number of atomic particles within the cell is large enough, the description of the hydrodynamic behavior will be more and more accurate as the number of Voronoi cells increases. In other words, we expect to reach a ''continuum limit'' as the number density of *fluid* particles goes to infinity. The discussion resembles that of the resolution in the numerical solution of partial differential equations. Actually, the resemblance can be made more accurate by comparing the structure of the equations of motion of the fluid particle model with those of smoothed particle hydrodynamics. Smoothed particle hydrodynamics is a Lagrangian discretization of the continuum equations of hydrodynamics that allows one to interpret the nodes of the grid in terms of ‘‘smoothed particles.’’

For the case in which there is no coupling between the Navier-Stokes equation and the energy equation (the pressure does not depend on the temperature, for example), Takeda *et al.* [3] propose a discretization of the Navier-Stokes equations that produce equations of motion for the smoothed particles that correspond exactly in structure with the postulated equations of motion of the fluid particle model in this paper. The correspondence is

$$V(r)=2\frac{p_0}{mn_0^2}W(r),$$

$$\gamma A(r)=\frac{1}{mn_0^2}\left[\eta W''(r)+\left[2\eta+\left(\zeta+\frac{\eta}{3}\right)\right]\frac{W'(r)}{r}\right], \tag{102}$$

$$\gamma B(r)=\frac{1}{mn_0^2}\left(\zeta+\frac{\eta}{3}\right)\left[W''(r)-\frac{W'(r)}{r}\right],$$

where, $p_0,n_0$ are the equilibrium pressure and number density, respectively, and $W(r)$ is the 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).

In this respect, the fluid particle model postulated in this paper is simply the smoothed particle hydrodynamics with two additional bonuses: (1) thermal noise is introduced consistently (that is, the fluid particle model can be interpreted as a Lagrangian discretization of the nonlinear fluctuating hydrodynamic equations), and (2) the angular momentum is conserved exactly in the fluid particle model, in contrast with the smoothed particle hydrodynamics model. The first bonus allows one to apply smoothed particle hydrodynamics to microhydrodynamic problems as those appearing in complex fluids where Brownian fluctuations are due to the fluctuating hydrodynamic environment. It can be also useful in studying the effect of thermal fluctuations near convective instabilities and, in general, in the study of nonequilibrium thermal fluctuations in hydrodynamic systems. The actual relevance of the second bonus will be discussed later.

The comparison of SPH with the fluid particle model points to an inconsistency that appears when using some particular selections for the weight function like the Lucy weight function [5] or a Gaussian weight function [3]. In these cases, it is easily seen that the function $A(r)$ can become negative for certain values of $r$. This is unacceptable in view of Eq. (34). From a physical point of view this means that if two particles are at a distance such that $A(r)$ is negative, then the viscous forces will try to *increase* its relative velocities.

In the derivation of the SPH model [2,3] it becomes apparent that the weight function $W(r)$ must be normalized to unity in order to have correct discrete (Monte Carlo) approximations for integrals. If $W(r)$ is normalized to unity, then one expects that by increasing the number density of smoothed particles one is increasing the numerical resolution of the simulation. The normalization implies that as the range of the weight function decreases with higher resolution, its height increases and, in the limit of infinite resolution it becomes a Dirac delta function $W(r)\to\delta(r)$. Because the weight function is steeper when the resolution is higher, the time step used in the SPH model has to be reduced as the resolution increases. This is also encountered in any finite difference algorithm for solution of partial differential equations in order to maintain stability.

Let us investigate the effect of the resolution effects on the macroscopic parameters defining the fluid on hydrodynamic scales and which have been computed by means of the kinetic theory in the previous section. The parameters that characterize the evolution of the velocity field are, as can be appreciated from Eq. (94), the speed of sound defined in Eq. (100) and the *kinematic* viscosities defined by $\nu=\eta/\rho$, $\nu_b=\zeta/\rho$, and $\nu_r=\eta_R/\rho$. From Eq. (92) they have the form

$$\nu_b=\left[\gamma n\left\{\frac{A_2}{2D}+\frac{(D+2)}{2D}B_2\right]+c^2\frac{1}{\gamma Dn[A_0+B_0]}\right\},$$

$$\nu=\frac{1}{2}\left\{\gamma n\left[\frac{A_2}{2}+B_2\right]+c^2\frac{1}{\gamma n[A_0+B_0]}\right\}, \tag{103}$$

$$\nu_R=\gamma n\frac{A_2}{2}.$$

We are assuming, for the sake of the argument, that $n=n_0$, that is, the density field is constant. The conclusions, however, are valid in the compressible case also.

Let us focus first on the dimensionless functions $A(r),B(r)$ that determine the range of the dissipative and random forces. We expect that the clusters interact only with their neighbors, which are a typical distance λ apart. Therefore, these functions will be of the form

$$A(r)=a(r/\lambda),$$
$$B(r)=b(r/\lambda), \tag{104}$$

where $a,b$ are functions that do not depend explicitly on λ. This ensures that as the resolution is increased, the range of the force decreases, and this has the computationally appealing feature that the interaction between fluid particles remains always local. By using these scaling functions and after a change to the dimensionless variable $\mathbf{x}\equiv\mathbf{r}/\lambda$, we have

$$A_0=\frac{a_0}{n_0},$$

$$B_0=\frac{b_0}{n_0},$$

$$A_2=\frac{a_2}{n_0}\lambda^2, \tag{105}$$

$$B_2=\frac{b_2}{n_0}\lambda^2,$$

where the dimensionless coefficients are given by

$$\begin{gathered} a_0 = \int a(x)\, d^D\mathbf{x}, \\ b_0 = \frac{1}{D}\int b(x)\, d^D\mathbf{x}, \\ a_2 = \frac{1}{D}\int x^2 a(x)\, d^D\mathbf{x}, \\ b_2 = \frac{1}{D(D+2)}\int x^2 b(x)\, d^D\mathbf{x} \end{gathered} \tag{106}$$

and do not depend on the resolution. By using Eq. (105) in Eq. (103) we obtain

$$\begin{gathered} \nu_b = \left\{ \gamma\lambda^2\left[\frac{a_2}{2D} + \frac{(D+2)}{2D} b_2\right] + c^2 \frac{1}{D\gamma(a_0+b_0)} \right\}, \\ \nu = \frac{1}{2}\left\{ \gamma\lambda^2\left[\frac{a_2}{2} + b_2\right] + c^2 \frac{1}{\gamma(a_0+b_0)} \right\}, \\ \nu_R = \gamma \frac{\lambda^2}{2} a_2 . \end{gathered} \tag{107}$$

We observe that all the dependence on the resolution ($\lambda$ or $n_0$) has been made explicit. In the limit of high resolution ($\lambda \to 0$ or $n_0 \to \infty$) the only contribution to the bulk $\nu_b$ and shear $\nu$ viscosities comes from the kinetic contribution that depends linearly on the temperature. This means that at zero temperature the system would not display any viscosity in the limit of high resolution. We find this behavior undesirable and we are led to the conclusion that the friction coefficient $\gamma$ must depend on $\lambda$. In particular, if we define $\tilde{\gamma} \equiv \gamma\lambda^2$ (which has dimensions of a kinematic viscosity) and assume that $\tilde{\gamma}$ remains constant as the resolution varies, we will have

$$\begin{gathered} \nu_b = \left\{ \tilde{\gamma}\left[\frac{a_2}{2D} + \frac{(D+2)}{2D} b_2\right] + c^2 \frac{\lambda^2}{D\tilde{\gamma}} \right\}, \\ \nu = \frac{1}{2}\left\{ \tilde{\gamma}\left[\frac{a_2}{2} + b_2\right] + c^2 \frac{\lambda^2}{\tilde{\gamma}} \right\}, \\ \nu_R = \frac{\tilde{\gamma}}{2} a_2 , \end{gathered} \tag{108}$$

where the normalization $a_0 = b_0 = 1$ has been used as in the original DPD algorithm [15]. The relaxation time (101) will take the form

$$\tau = \frac{I}{2m}\frac{\lambda^2}{\tilde{\gamma} a_2}. \tag{109}$$

In this way, in the limit of high resolution ($\lambda \to 0$) the viscosities are given essentially by $\tilde{\gamma}$ and the relaxation time goes to zero (note that the moment of inertia $I$ must be of the form $\propto m \times \lambda^2$ so $\tau$ must tend to zero very fast). In the high resolution limit the spin becomes equal to the vorticity in a short time scale. The spin becomes a slaved variable and can be dropped from the description. Note also that in this situation the last term in the Navier-Stokes equation with spin (94) vanishes and one recovers the actual Navier-Stokes equation. This explains why, in SPH, the violation of angular momentum does not pose a serious problem *for sufficiently high resolutions* [3]. If low resolutions are to be used in problems where the correct transfer of angular momentum is relevant (as in rotational diffusion of concentrated colloidal suspensions, for example), then the use of spin might suppose a real advantage.

We have arrived at the conclusion that in order to have a well-defined continuum limit the friction coefficient $\gamma$ must increase as the resolution increases. This can be understood physically in the following way. The number of particles in between two reference fluid particles at a given distance of each other increases as the resolution increases. If we require that the viscous interaction between these two reference particles must remain the same as the resolution increases, the mediating particles must interact stronger in order to transmit the same response between the two reference particles. From a mathematical point of view, the $\lambda^2$ factor can be interpreted as the ‘‘lattice spacing’’ that is lacking in the original equations and that would be present in a numerical discretization of a *second* order derivative term. Preliminary simulation results for the DPD model ($A(r) = 0$) with energy conservation [30] shows that the correct continuum limit is obtained when the model parameter equivalent to $\gamma$ increases with $\lambda^2$ [37].

We would like to comment finally on an apparent inconsistency between SPH and the fluid particle model, which is summarized as follows: if one discretizes the hydrodynamic equations on a set of points and then constructs the kinetic theory of these points, one would expect that the computed transport coefficients would coincide with the input transport coefficients of the hydrodynamic equations. If one naively uses the results (102) in the calculation of the transport coefficients in (92), one arrives at an inconsistent result. The viscosities computed through the kinetic theory (92) do not coincide with the input values. This could be traced back to the fact that the kinetic theory for the fluid particle model has been developed in the limit where no conservative forces are present, whereas the pressure term in the hydrodynamic equations (even for an ideal gas) produces a conservative term given by the first equation in Eq. (102) in SPH. The kinetic theory with conservative forces is a bit more involved but the modifications can be summarized simply. The molecular chaos assumption (64) now involves the pair distribution function (which in the absence of conservative forces is equal to 1). This means that the parameters $\overline{A_2}, \overline{B_2}$ appearing in the transport coefficients will be modified by the presence of the pair distribution function within the integral defining these parameters. Also a new contribution to the transport coefficients arises due to the conservative forces. It is an open question whether these modified transport coefficients due to conservative forces do coincide with the input transport coefficients. The opposite case could also be possible simply due to the fact that the discretization procedure in SPH may induce ‘‘artificial viscosities’’ in the language of numerical resolution of the hydrodynamic partial differential equations.

The fluid particle model is a consistent model by itself, without having to resort to the smoothed particle model for its validity. Actually, the fluid particle model, together with the kinetic theory developed in this paper, has its advantages with respect to SPH: precise predictions can be made from the initial model parameters about the transport properties of the fluid. In this way, to obtain a prescribed fluid of known transport properties, one simply adjusts the model parameters according to the formulas of kinetic theory (slight errors stemming from the failure of the molecular chaos assumption might play a minor role [22]). In SPH, on the contrary, the only way to specify the fluid is through the input transport coefficients in the original hydrodynamic equations. The discretization procedure then produces a ‘‘fluid’’ whose transport properties do not in general correspond with those of the fluid intended to be modeled, and there is no systematic control on the appearance of artificial viscosities.

It is apparent that this whole discussion about resolution issues can be applied to the DPD model, which is a particular case of the fluid particle model, and for which a kinetic theory has been formulated previously in Ref. [22]. One of the main motivations for introducing shear forces between dissipative particles into the original algorithm of DPD was the identification of the following elementary motion between dissipative particles that produces no force in that algorithm. Let us focus on two neighboring dissipative particles, the first one at rest at the origin and the second one orbiting in a circumference around the first one. This relative motion produces no force in DPD because the relative approaching velocity is exactly zero. Nevertheless, on simple physical grounds one expects that the motion of the second particle must drag in some way the first particle. This is taken into account through the shear forces in the fluid particle model presented in this paper. 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.

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## APPENDIX

The derivation of the FPE is best achieved by considering the differential of an arbitrary function $f$ to second order [32]:

$$\begin{aligned} df=&\sum_i \; d\mathbf{r}_i\cdot\frac{\partial f}{\partial \mathbf{r}_i}+d\mathbf{v}_i\cdot\frac{\partial f}{\partial \mathbf{v}_i}+d\boldsymbol{\omega}_i\cdot\frac{\partial f}{\partial \boldsymbol{\omega}_i}+\frac{1}{2}\sum_{ij}\; d\mathbf{v}_i\; d\mathbf{v}_j\,\frac{\partial^2 f}{\partial \mathbf{v}_i\;\partial \mathbf{v}_j}+d\mathbf{v}_i\; d\boldsymbol{\omega}_j\colon\frac{\partial^2 f}{\partial \mathbf{v}_i\;\partial \boldsymbol{\omega}_j}+d\boldsymbol{\omega}_i\; d\mathbf{v}_j\colon\frac{\partial^2 f}{\partial \boldsymbol{\omega}_i\cdot\partial \mathbf{v}_j}\\ &+d\boldsymbol{\omega}_i\; d\boldsymbol{\omega}_j\colon\frac{\partial^2 f}{\partial \boldsymbol{\omega}_i\cdot\partial \boldsymbol{\omega}_j}. \end{aligned} \tag{A1}$$

One then substitutes the SDE’s (19) and uses the Ito stochastic rules (17), keeping terms up to order $dt$ (the cross terms involving positions have been neglected in Eq. (A1) on account of the fact that $d\mathbf{r}$ is already of order $dt$). Then after averaging with respect to the distribution function $\rho(r,v,\omega;t)$, one performs a partial integration and uses the fact that $f$ is arbitrary, to obtain the Fokker-Planck equation in the form

$$\partial_t\rho(r,v,\omega;t)=[L^C+L^T+L^R]\rho(r,v,\omega;t), \tag{A2}$$

where we have defined the operators

$$\begin{aligned} L^C&\equiv-\left[\sum_i \;\mathbf{v}_i\frac{\partial}{\partial \mathbf{r}_i}+\sum_{i,j\neq i}\frac{1}{m}\mathbf{F}^C_{ij}\frac{\partial}{\partial \mathbf{v}_i}\right],\\ L^T&\equiv\sum_{i,j\neq i}\frac{\partial}{\partial \mathbf{v}_i}\cdot\left[-\frac{1}{m}(\mathbf{F}^T_{ij}+\mathbf{F}^R_{ij})+\frac{1}{2}\frac{\partial}{\partial \mathbf{v}_j}\cdot\sum_{i'j'}\frac{1}{dt}d\tilde{\mathbf{v}}_{ii'}d\tilde{\mathbf{v}}_{jj'}-\frac{1}{2}\frac{\partial}{\partial \boldsymbol{\omega}_j}\cdot\frac{m}{I}\sum_{i'j'}\frac{1}{dt}d\tilde{\mathbf{v}}_{ii'}\left(\frac{\mathbf{r}_{jj'}}{2}\times d\tilde{\mathbf{v}}_{jj'}\right)\right], \end{aligned} \tag{A3}$$

$$L^R\equiv\frac{m}{I}\sum_{i,j\neq i}\frac{\partial}{\partial \boldsymbol{\omega}_i}\cdot\left[\frac{1}{m}\frac{\mathbf{r}_{ij}}{2}\times(\mathbf{F}^T_{ij}+\mathbf{F}^R_{ij})-\frac{1}{2}\frac{\partial}{\partial \mathbf{v}_j}\cdot\sum_{i'j'}\frac{1}{dt}\left(\frac{\mathbf{r}_{ii'}}{2}\times d\tilde{\mathbf{v}}_{ii'}\right)d\tilde{\mathbf{v}}_{jj'}+\frac{1}{2}\frac{\partial}{\partial \boldsymbol{\omega}_j}\cdot\frac{m}{I}\sum_{i'j'}\frac{1}{dt}\left(\frac{\mathbf{r}_{ii'}}{2}\times d\tilde{\mathbf{v}}_{ii'}\right)\left(\frac{\mathbf{r}_{jj'}}{2}\times d\tilde{\mathbf{v}}_{jj'}\right)\right].$$

The operator $L^C$ is the usual Liouville operator of a Hamiltonian system interacting with conservative forces $\mathbf{F}^C$. We need to arrange a bit the operators $L^T$ and $L^R$ by using the Ito rules (18)

$$\begin{aligned}\frac{1}{dt}d\tilde{\mathbf{v}}^{\mu}_{ii'}d\tilde{\mathbf{v}}^{\nu}_{jj'}&=\sigma^2\Bigg[\frac{1}{2}[\tilde{A}(r_{ii'})\tilde{A}(r_{jj'})+\tilde{C}(r_{ii'})\tilde{C}(r_{jj'})]\delta^{\mu\nu}\mathbf{e}_{ii'}\cdot\mathbf{e}_{jj'}+\frac{1}{2}[\tilde{A}(r_{ii'})\tilde{A}(r_{jj'})-\tilde{C}(r_{ii'})\tilde{C}(r_{jj'})]\mathbf{e}^{\nu}_{ii'}\mathbf{e}^{\mu}_{jj'}\\&\quad+\frac{1}{D}[\tilde{B}(r_{ii'})\tilde{B}(r_{jj'})-\tilde{A}(r_{ii'})\tilde{A}(r_{jj'})]\mathbf{e}^{\mu}_{ii'}\mathbf{e}^{\nu}_{jj'}\Bigg][\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{ji'}]\\&\equiv\sigma^2\mathbf{T}^{\mu\nu}_{ii'jj'}[\delta_{ij}\delta_{i'j'}+\delta_{ij'}\delta_{ji'}].\end{aligned}\tag{A4}$$

The second order tensor $\mathbf{T}^{\mu\nu}_{ii'jj'}$ satisfies

$$\mathbf{T}^{\mu\nu}_{ijij}=\mathbf{T}^{\nu\mu}_{ijij}=-\mathbf{T}^{\mu\nu}_{ijji}.\tag{A5}$$

If we define

$$\mathbf{T}_{ij}\equiv\mathbf{T}_{ijij}=\frac{1}{2}[\tilde{A}^2(r_{ij})+\tilde{C}^2(r_{ij})]\mathbf{1}+\left[\left(\frac{1}{2}-\frac{1}{D}\right)\tilde{A}^2(r_{ij})+\frac{1}{D}\tilde{B}^2(r_{ij})-\frac{1}{2}\tilde{C}^2(r_{ij})\right]\mathbf{e}_{ij}\mathbf{e}_{ij}\tag{A6}$$

then the following identities are obtained:

$$\begin{aligned}\frac{1}{2}\sum_{ij}\frac{\partial}{\partial\mathbf{v}_i}\frac{\partial}{\partial\mathbf{v}_j}:\sum_{i'j'}\frac{1}{dt}d\tilde{\mathbf{v}}_{ii'}d\tilde{\mathbf{v}}_{jj'}&=\frac{\sigma^2}{2}\sum_{ij}\frac{\partial}{\partial\mathbf{v}_i}\cdot\mathbf{T}_{ij}\cdot\left[\frac{\partial}{\partial\mathbf{v}_i}-\frac{\partial}{\partial\mathbf{v}_j}\right]\\-\frac{1}{2}\sum_{ij}\frac{\partial}{\partial\mathbf{v}_i}\frac{\partial}{\partial\boldsymbol{\omega}_j}:\sum_{i'j'}\frac{1}{dt}d\tilde{\mathbf{v}}_{ii'}\left(\frac{\mathbf{r}_{jj'}}{2}\times d\tilde{\mathbf{v}}_{jj'}\right)&=\frac{\sigma^2}{2}\sum_{ij}\frac{\partial}{\partial\mathbf{v}_i}\cdot\mathbf{T}_{ij}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times\left[\frac{\partial}{\partial\boldsymbol{\omega}_i}+\frac{\partial}{\partial\boldsymbol{\omega}_j}\right]\right)\\-\frac{1}{2}\sum_{ij}\frac{\partial}{\partial\boldsymbol{\omega}_i}\frac{\partial}{\partial\mathbf{v}_j}:\sum_{i'j'}\frac{1}{dt}\left(\frac{\mathbf{r}_{ii'}}{2}\times d\tilde{\mathbf{v}}_{ii'}\right)d\tilde{\mathbf{v}}_{jj'}&=-\frac{\sigma^2}{2}\sum_{ij}\frac{\partial}{\partial\boldsymbol{\omega}_i}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\left[\frac{\partial}{\partial\mathbf{v}_i}-\frac{\partial}{\partial\mathbf{v}_j}\right]\right)\\\frac{1}{2}\sum_{ij}\frac{\partial}{\partial\boldsymbol{\omega}_i}\frac{\partial}{\partial\boldsymbol{\omega}_j}:\sum_{i'j'}\frac{1}{dt}\left(\frac{\mathbf{r}_{ii'}}{2}\times d\tilde{\mathbf{v}}_{ii'}\right)\left(\frac{\mathbf{r}_{jj'}}{2}\times d\tilde{\mathbf{v}}_{jj'}\right)&=-\frac{\sigma^2}{2}\sum_{ij}\frac{\partial}{\partial\boldsymbol{\omega}_i}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times\mathbf{T}_{ij}\cdot\left[\frac{\mathbf{r}_{ij}}{2}\times\left[\frac{\partial}{\partial\boldsymbol{\omega}_i}+\frac{\partial}{\partial\boldsymbol{\omega}_j}\right]\right]\right).\end{aligned}\tag{A7}$$

By using these results into Eq. (A3) the operators take the following compact form:

$$L^T=\sum_{i,j\neq i}\frac{\partial}{\partial\mathbf{v}_i}\cdot[\mathbf{L}^T_{ij}+\mathbf{L}^R_{ij}],\quad L^R=-\frac{m}{I}\sum_{i,j\neq i}\frac{\partial}{\partial\boldsymbol{\omega}_i}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times[\mathbf{L}^T_{ij}+\mathbf{L}^R_{ij}]\right),\tag{A8}$$

where we have introduced the vector operators

$$\mathbf{L}^T_{ij}\equiv-\frac{1}{m}\mathbf{F}^T_{ij}+\frac{\sigma^2}{2}\mathbf{T}_{ij}\cdot\left[\frac{\partial}{\partial\mathbf{v}_i}-\frac{\partial}{\partial\mathbf{v}_j}\right],\quad\mathbf{L}^R_{ij}\equiv-\frac{1}{m}\mathbf{F}^R_{ij}+\frac{m}{I}\frac{\sigma^2}{2}\mathbf{T}_{ij}\cdot\left(\frac{\mathbf{r}_{ij}}{2}\times\left[\frac{\partial}{\partial\boldsymbol{\omega}_i}+\frac{\partial}{\partial\boldsymbol{\omega}_j}\right]\right).\tag{A9}$$

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[1] L. B. Lucy, Astrophys. J. **82**, 1013 (1977).

[2] J. J. Monaghan, Annu. Rev. Astron. Astrophys. **30**, 543 (1992).

[3] H. Takeda, S. M. Miyama, and M. Sekiya, Prog. Theor. Phys. **92**, 939 (1994).

[4] H. A. Posch, W. G. Hoover, and O. Kum, Phys. Rev. E **52**, 1711 (1995).

[5] O. Kum, W. G. Hoover, and H. A. Posch, Phys. Rev. E **52**, 4899 (1995).

[6] W. G. Hoover and H. A. Posch, Phys. Rev. E **54**, 5142 (1996).

[7] L. D. Landau and E. M. Lifshitz, *Fluid Mechanics* (Pergamon Press, New York, 1959).

[8] See the Proceedings of 1996 Conference on Discrete Models for Fluid Mechanics, edited by B. M. Boghosian, F. J. Alexander, and P. V. Coveney, in special issue of Int. J. Mod. Phys. C **8**, (1997).

[9] U. Frisch, B. Hasslacher, and Y. Pomeau, Phys. Rev. Lett. **19**, 155 (1992).

[10] S. Wolfram, J. Stat. Phys. **45**, 471 (1986).

[11] A. J. C. Ladd, J. Fluid Mech. **285**, 311 (1994).

[12] G. A. Bird, in *Rarefied Gas Dynamics: Theoretical and Computational Techniques*, Proceedings of the 16th International Symposium, *Progress in Astronautics and Aeronautics*, Vol. 118, edited by E. P. Muntz, D. P. Weaver, and D. H. Campbell (AIAA, Washington, D.C., 1989); G. A. Bird, *Molecular Gas Dynamics* (Oxford University Press, London, 1976).

[13] D. L. Ermak and J. A. McCammon, J. Chem. Phys. **69**, 1352 (1978).

[14] J. F. Brady and G. Bossis, Annu. Rev. Fluid Mech. **20**, 111 (1988).

[15] P. J. Hoogerbrugge and J. M. V. A. Koelman, Europhys. Lett. **19**, 155 (1992).

[16] J. M. V. A. Koelman and P. J. Hoogerbrugge, Europhys. Lett. **21**, 369 (1993).

[17] P. Español, M. Serrano, and I. Zúñiga, Int. J. Mod. Phys. C **8**, 899 (1997).

[18] P. Español and P. Warren, Europhys. Lett. **30**, 191 (1995).

[19] P. V. Coveney and P. Español, J. Phys. A **30**, 779 (1997).

[20] P. Español, Phys. Rev. E **53**, 1572 (1996).

[21] P. Español, Phys. Rev. E **52**, 1734 (1995).

[22] C. Marsh, G. Backx, and M. H. Ernst, Europhys. Lett. **38**, 411 (1997); C. Marsh, G. Backx, and M. H. Ernst, Phys. Rev. E **56**, 1976 (1997).

[23] C. A. Marsh and J. M. Yeomans, Europhys. Lett. **37**, 511 (1997).

[24] E. S. Boek, P. V. Coveney, H. N. W. Lekkerkerker, and P. van der Schoot, Phys. Rev. E **55**, 3124 (1997).

[25] E. S. Boek, P. V. Coveney, and H. N. W. Lekkerkerker, J. Phys.: Condens. Matter **8**, 9509 (1997).

[26] A. G. Schlijper, P. J. Hoogerbrugge, and C. W. Manke, J. Rheol. **39**, 567 (1995).

[27] P. V. Coveney and K. Novik, Phys. Rev. E **54**, 5134 (1996).

[28] S. R. de Groot and P. Mazur, *Non-equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962).

[29] P. Español, e-print cond-mat/9705183.

[30] P. Español, Europhys. Lett. **40**, 631 (1997).

[31] J. Bonet Avalós and A. D. Mackie, Europhys. Lett. **40**, 141 (1997).

[32] C. W. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, Berlin, 1983).

[33] H. Risken, *The Fokker-Planck Equation* (Springer-Verlag, Berlin, 1984).

[34] H. Mori, Prog. Theor. Phys. **33**, 423 (1965).

[35] H. Grabert, *Projection Operator Techniques in Nonequilibrium Statistical Mechanics*, Springer Tracts in Modern Physics Vol. 95 (Springer-Verlag, Berlin, 1982).

[36] L. E. Reichl, *A Modern Course in Statistical Physics* (University of Texas Press, Austin, 1980).

[37] M. Ripoll and P. Español (unpublished).