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Numerical modelling of finite-size particle collisions in a viscous fluid

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A general model is presented for short-range hydrodynamic interactions and head-on particle-particle/wall collisions. The model has been embedded in two distinct numerical methods for fully resolved simulation of finite-size particles in a viscous fluid. It accounts for the material properties of the particles and lubrication effects prior to collision that cannot be fully resolved on a fixed grid. We demonstrate that the model is able to reproduce experimental data for the coefficient of restitution of particle-wall collisions over a wide range of Stokes number based on the particle impact velocity. The set of model parameters we selected and more generally the modelling approach we propose can be efficiently used for fully resolved simulations of moderately dense solid-liquid suspensions. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4817382]

I. INTRODUCTION

Particulate flows are ubiquitous in industrial and natural processes, from coal combustors, reactive fluidized beds to sediment transport in coastal areas or rivers. According to the review paper of Elghobashi,[1] collisions play a role for particle volume fraction larger than 0.1%. Direct hydrodynamic interactions and particle-particle or particle-wall collisions are important features which control the overall dynamics of the flow for moderately concentrated suspension.[2] Efficient numerical models are highly desirable to predict the physics of those complex flows[3] and to optimize the design of industrial devices involving dispersed two-phase flows. Recent numerical techniques[4–6] provide useful tools to simulate suspension flows seeded with finite size particles. Although computing resources are continuously increasing, such simulations do not accurately capture short range hydrodynamic interactions and collisions. Indeed, for fixed grid methods (immersed boundary method,[7] fictitious domain,[8] penalty method, . . .), the flow resolution to simulate film drainage becomes insufficient when the number of grid points within the particle-particle gap is below four. Local refinement of the grid (see Refs. 9 and 10 and Figure 1) would be required but is far too expensive for three-dimensional simulations of thousands of particles. Alternatively, simplified models may be used to represent unresolved hydrodynamic interactions and solid collisions or simply to prevent numerical overlapping of particles. We propose a general approach to account simultaneously for lubrication forces and particle contact based on a multilayer soft sphere model.

The simulation of granular flows through discrete particle models is often used when hydrodynamic interactions are negligible. In such models, the drag force on the particles is parameterized, possibly with a correction for a finite volume fraction but the fluid flow is not solved. Particle contacts and collision events are modelled with spring-dashpot interaction forces[11,12] whose parameters have to be determined based on material properties. In another context, repulsive forces have been used to prevent particle overlapping[13] and to mimic hydrodynamic lubrication forces.[14]

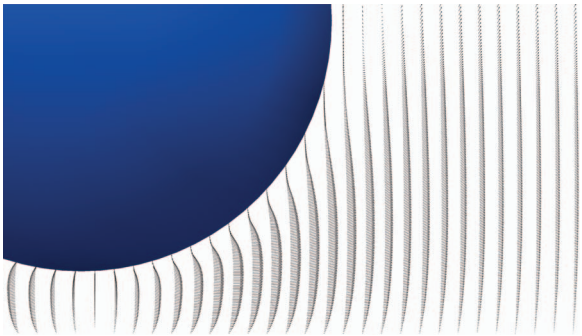

FIG. 1. Fully resolved drainage of an intervening film layer between a particle and a wall with 150 grid points over the particle radius and 40 grid points over the gap width.

In none of these studies, the local interaction between two approaching particles (or between a particle and a wall) has been compared to existing experiments on rebounds. When two solids are approaching and eventually collide, three interaction mechanisms are successively occurring for macroscopic particles. When the separation distance is large (more than one or two radii for spherical particles), fluid interactions generate a deceleration of the solid body. Those long range hydrodynamic interactions are readily captured by different methods (Immersed Boundary Method, Fictitious Domain-Distributed Lagrange Multiplier, . . .) for finite size particles simulations. When the separation distance is lower than one fourth of the particle radius, the Reynolds number (based on the relative velocity, the gap width, and the fluid kinematic viscosity) is often low and lubrication repulsive forces dramatically damp the impact velocity. Theoretically, for perfectly smooth surfaces actual contact never occur while the lubrication force becomes infinitely large in the limit of zero gap width. At very small gap width, the continuum approach underlying the Navier-Stokes equations breaks down as molecular effects are not included and solid contact occurs. Several phenomena may lead to lubrication breakdown (non-continuum effect,[15] surface roughness,[16] or residual Brownian motion). Then, a local deformation of solid surfaces due to rapid pressure increase in the liquid film (Refs. 17 and 18) or solid contact occurs. The solid-solid collision can be characterized by a dry restitution coefficient e_d (ratio of rebound velocity to particle impact velocity in the absence of fluid such as in vacuum) which depends on particle material. Including the effect of hydrodynamic interactions, several authors[19–21] proposed to model the overall collision process with an effective restitution coefficient e. This coefficient depends on particle and fluid properties through an impact Stokes number defined as $St = \frac{2}{9}\frac{RU\rho_p}{\mu_f}$, where U is the particle velocity prior to contact, μ_f the fluid viscosity, R the particle radius, and ρ_p its density. The correlation given by Legendre *et al.*,[22] based on multiple experimental data sets, reproduces this evolution $\frac{e}{e_d} = \exp\left(-\frac{35}{St}\right)$ over a wide range of physical properties for particle-wall rebound or particle-particle collision.[19]

In this article a general model including lubrication and collision forces is proposed and validated over the whole range of impact Stokes number (from complete viscous damping to dry collision). The interaction model will be detailed together with proposed parameters provided by extensive testing. The paper is concluded by simulations of particle colliding onto a plane wall for a wide range of impact Stokes number. We fix the particle diameter to be discretized with 16 grid points which is of common use for the simulation of finite size particles in a viscous fluid. A fictitious domain approach based on a Cartesian fixed grid has been chosen as a computational framework for the implementation of the complete collision model. An implicit tensorial penalty method allows to account for solid behavior in the volume occupied by particles, while the fluid incompressibility is achieved with an augmented Lagrangian method. To prevent particle deformations, the solid volume fraction in each cell is updated assuming an exact spherical shape. A detailed presentation of the finite size particle simulations and precise validations are presented elsewhere.[23] It is worthwhile to mention that the present model can be easily implemented in any code (based on IBM, Immersed Interface Method, etc.) accounting for finite size particles.

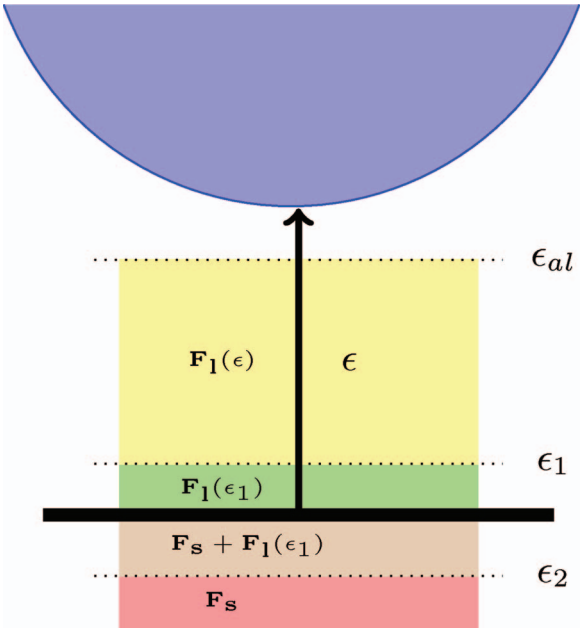

FIG. 2. Multilayer model for hydrodynamic interaction and head-on collision of a spherical particle onto a plane wall.

II. DESCRIPTION OF THE MODEL

The multilayer interaction model is sketched in Figure 2 for particle-particle or particle-wall collision where ϵ is the ratio between the distance δ separating solid surfaces and the particle radius. It is positive before contact and negative when the particle overlaps the wall. Lubrication interaction prior to collision is supplemented by a soft-sphere model for solid contact which becomes active when the particle overlaps with the wall. Originally, this approach has been proposed by Breugem,[24] who embedded the multilayer model in a direct-forcing immersed boundary method for finite-size particles.[25] We demonstrate the capability of the model to reproduce experimental data for the head-on collision of a spherical particle onto a plane wall with both numerical approaches of finite size particle simulation. Based on extensive testing and validation, we have derived optimal values for the model parameters, which can be used for fully resolved simulations of moderately concentrated particle suspensions.

A. Lubrication effect

When two solid surfaces embedded in a viscous fluid come close to contact, lubrication theory[26,27] provides analytical expressions of the hydrodynamic force (Eq. (1)) due to viscous fluid drainage. For a head-on or normal collision, the force is parallel to the line of centers of two colliding particles or orthogonal to the wall in case of a particle-wall collision. u_n is the particle velocity along the normal direction (for particle-particle collision, u_n is the particle velocity in the relative framework). An extension to lubrication corrections for non-normal collision or with rotating particles could be achieved following Breugem.[24] The amplification factor λ for the Stokes drag acting on a single sphere is given in Eqs. (2) and (3) for particle-particle and particle-wall interaction, respectively. The short range lubrication force is activated for a prescribed distance, ϵ_{al} (Fig. 2). When $\epsilon > \epsilon_{al}$, no correction to the hydrodynamic interaction is needed ($F_l = 0$ for $\epsilon = \epsilon_{al}$) while the primary numerical simulation can resolve the dynamics sufficiently until lubrication dominates

$$F_l(\epsilon, u_n) = -6\pi\mu_f R u_n \left[\lambda(\epsilon) - \lambda(\epsilon_{al})\right], \tag{1}$$

$$\lambda_{pp} = \frac{1}{2\epsilon} - \frac{9}{20}\mathrm{Ln}(\epsilon) - \frac{3}{56}\epsilon\mathrm{Ln}(\epsilon) + 1.346 + \mathcal{O}(\epsilon), \tag{2}$$

$$\lambda_{pw} = \frac{1}{\epsilon} - \frac{1}{5}\mathrm{Ln}(\epsilon) - \frac{1}{21}\epsilon\mathrm{Ln}(\epsilon) + 0.9713 + \mathcal{O}(\epsilon). \tag{3}$$

The lubrication force for smooth particles diverges as the separation distance tends to zero. Breakdown of continuum assumptions and/or roughness effects yields saturation of the hydrodynamic force. The lubrication force is kept constant (constant Stokes amplification factor when ϵ is lower than ϵ_1 and larger than ϵ_2) until it is largely dominated by solid-solid interaction corresponding to slight numerical overlapping of surfaces.

Surface roughness can be accounted for in the present model by adapting the Stokes amplification factor for ϵ lower than ϵ_1. Note that we model surface roughness in this study, rather than resolving it for reason of computational feasibility as the typical height of the surface roughness elements is assumed to be very small compared to the sphere radius for polished spheres.[20] The location of the solid surface can be thought as the nominal position of the rough wall.

B. Solid-solid interaction

For collision of steel spheres, the collision time is typically 10^{-9} s. This is much smaller than a typical time step for suspension flow simulation; resolving a collision in time is thus computationally not feasible. Instead, slight overlap (negative overlap distance δ) of solid surfaces is allowed for a limited number of time steps and the spring-dashpot model (Eq. (4)) provides a simple way to reproduce elastic ($e_d = 1$, where e_d is the dry collision coefficient) or inelastic collisions ($e_d < 1$), following the soft sphere approach. m_e characterizes the mass of solids involved in the collision, $m_e = \left(m_1^{-1} + m_2^{-1}\right)^{-1}$ for particle-particle collision and $m_e = m$ for particle-wall collision

$$F_s = -k_n\delta - \beta_n u_n, \tag{4}$$

$$k_n = -\frac{m_e\left(\pi^2 + [\mathrm{Ln}e_d]^2\right)}{[N_c\Delta t]^2}, \beta_n = -\frac{2m_e[\mathrm{Ln}e_d]}{[N_c\Delta t]}. \tag{5}$$

k_n is the stiffness of the spring and β_n the damping coefficient of the dashpot. The numerical collision duration corresponds to N_c fluid time steps: $N_c\Delta t$. The spring-dashpot representation of particle-particle collision comes from the Hertz-Mindlin theory of elastic contact. Equation (4) is a linearized model and has the advantage to give an analytic expression[28] for β_n for a dry inelastic collision $e_d = \exp(-\beta_n t_n/2m_e)$ where $t_n = N_c\Delta t$ is the contact time. Therefore, the physical properties of the solid (Young modulus, Poisson coefficient) are lumped in the dashpot coefficient. The value of k_n fixes the duration of the collision. It comes from a compromise between the computational cost (if the contact time is too short CPU overhead will be huge due to very small Δt) and the physics of the suspension flow. Granular flows[29] are well represented when the collision time is small compared to flow characteristic time scales (either collective or single particle dynamics). The collision time has to be at least one order of magnitude lower than the shortest time scale of the suspension flow dynamics. Therefore, N_c has to be selected as small as possible. Note that the collision cannot be resolved on too few time steps, as otherwise the method becomes numerically inaccurate (dry collision will not be reproduced when N_c is too small). The determination of k_n and β_n proceeds as follows. Based on an estimate of the relevant time scales of the particulate flow, the collision time t_n is fixed which gives the value of k_n for a particular value of the dry restitution coefficient e_d (which accounts for the physical properties of the solid). Then, the dashpot parameter β_n is fixed accordingly.

III. NUMERICAL VALIDATION

The lubrication activation and deactivation region, ϵ_{al} and ϵ_2, the region where the lubrication remains constant, ϵ_1 and the number of time steps per solid collision, N_c has to be determined. Next,

we discuss how these parameters are selected. To test the response of the model to each parameter variation, we first neglected the effect of long range hydrodynamic interaction yielding simplified interaction in 1D (Eq. (6)). It is then discretized in Eqs. (7) and (8) which is similar to Lagrangian tracking coupled to the Navier-Stokes solver

$$m\ddot{x} = F_l(x, \dot{x}) + F_s(x, \dot{x}), \tag{6}$$

$$V^{n+1} = V^n + \frac{\Delta t}{m}\left(F_l(\tilde{X}^{n+\frac{1}{2}}, \tilde{V}^{n+\frac{1}{2}}) + F_s(\tilde{X}^{n+\frac{1}{2}}, \tilde{V}^{n+\frac{1}{2}})\right), \tag{7}$$

$$\tilde{V}^{n+\frac{1}{2}} = \frac{3}{2}V^n - \frac{1}{2}V^{n-1}, \tilde{X}^{n+\frac{1}{2}} = X^n + \frac{1}{2}\Delta t V^n. \tag{8}$$

The time step Δt has to be adapted to the lubrication gap and the typical relative velocity V_0. For the simulation of colliding particles, we limited the time step to $\Delta t < 0.2\frac{\epsilon_{al}R}{V_0}$. In complex situations, such as turbulent flows, the time step will be evaluated by comparing this constraint to numerical stability criterion. The use of quasi-static lubrication theory requires two assumptions: low Reynolds number within the gap and momentum diffusive time scale much smaller than the time step. Both assumptions lead to the condition $St < \mathcal{O}(\rho^* \epsilon^{-1})$ where ρ^* stands for the ratio of particle to fluid density. The condition is fulfilled over a wide range of impact Stokes numbers for particles or droplets in air. It is more restrictive for liquid-solid suspensions. When the lubrication force is activated, we are surely on the upper bound of lubrication theory validity ($\epsilon_{al} = 0.1$ would restrict the simulations to $St < 3.5$) but very rapidly when $\epsilon < 0.01$ the limit on impact St number spans all the range of behaviors from $St \ll 1$ (no rebound) to $St \sim 400$ corresponding to $e/e_d = 0.9$.

IV. NUMERICAL TEST

Extensive testing has been carried out and the following conclusions are drawn:

- If $N_c < 8$, the dry collision corresponding to high Stokes number is not well reproduced. So, $N_c = 8$ has been chosen to keep the solid collision time as short as possible. Higher values can be used with an increased computational cost and no significant enhancement of the reliability of the results.
- The lubrication activation distance ϵ_{al} modifies the collision total time although it does not change significantly the restitution coefficient over the range $0.25 > \epsilon_{al} > 0.03$. $\epsilon_{al} = \frac{\Delta x}{R}$ is suitable for the simulation of finite size particles with $\frac{R}{\Delta x}$ ranging from 4 to 15 depending on the flow structure at the particle scale. In our case, $\frac{R}{\Delta x} = 8$ yields $\epsilon_{al} = 0.125$.
- ϵ_1 accounts for the breakdown of the analytic lubrication solution due to the effect of surface roughness (and to a lesser extent elastic deformation). Extensive numerical tests gave a range of appropriate values for the model to give correct results over the full range of impact Stokes numbers. For $\epsilon_1 < 10^{-4}$, the model gives unphysical behavior of the particle-wall interaction. Above this value, the net effect of this parameter is an increase of the restitution coefficient. $\epsilon_1 = 10^{-3}$ has been selected.
- The value of ϵ_2 accounts for the complete breakdown of lubrication after many surface roughness elements have been connected with each other. Varying ϵ_2 does not modify the restitution coefficient. When the overlapping time is long enough, the solid-solid force dominates (see Figure 3). The particle experiences successively fluid and solid interactions. The velocity and forces are continuous and evolve smoothly. $\epsilon_2 = -10^{-2}$ is adequate.

To test the model, we carried out simulations for the following physical parameters: a steel particle with a diameter 3×10^{-3}m and density 7780 kg m^{-3} is approaching the wall with different initial velocities in a viscous fluid (density $\rho_f = 1000$ kg m^{-3} and viscosity $\mu_f = 3.82 \times 10^{-3}$Pa s). The domain is large enough to prevent confinement effects.

In Fig. 4, we present our results together with simulations of Breugem[24] for similar parameters. The agreement with experiments is very good over the full range of impact Stokes number. With the prescribed parameters, this simple model which accounts successively for long-range hydrodynamic

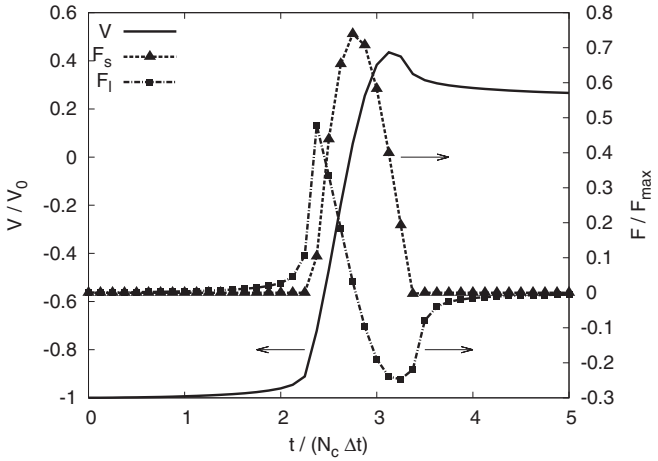

FIG. 3. Comparison of the different force contributions (F_S, F_l) during a collision onto a wall. V is the particle velocity. $St = 18$ and $\epsilon_{al} = 0.125$. The model parameters are: $N_c = 8$, $\epsilon_1 = 10^{-3}$, and $\epsilon_2 = -10^{-2}$.

interactions (by solving the Navier-Stokes equations with fully resolved particles), the short-range lubrication effect and finally the solid-solid collision is able to reproduce particle-particle or particle-wall collision. The dissipation of particle kinetic energy by the fluid is correctly reproduced. This is a major effect in solid-liquid suspensions. This approach is suitable for any numerical method handling finite size particles simulation in a viscous fluid.

Three or more particles interacting at the same time with each other is no problem. The contacts are treated one by one and the net collision force acting on a particle is the sum of the collision forces from each contact. The model have been used in configurations with volume fraction varying up to 40% without any problem.

V. PARTICLE COLLISIONS IN A TURBULENT FLOW

To test the collision model under realistic conditions encountered in particle laden flows, the response of finite size particles in isotropic homogeneous turbulence has been analyzed. Direct numerical simulations of the Navier-Stokes equations for a tri-periodic domain have been performed. The turbulence level is sustained by renormalization of the fluctuation intensity at each time step.[30] This provides a base flow which is statistically steady although preserving the temporal and spatial

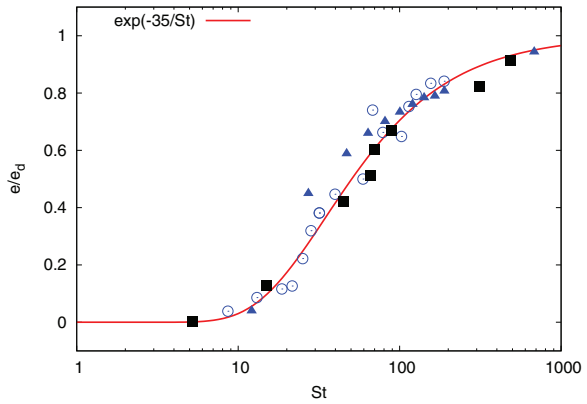

FIG. 4. Simulations results compared to the correlation[22] based on experiments. Triangles (blue online), cases presented by Breugem[24] reproduced with our numerical approach and implicit scheme. Circles, results obtained by Breugem[24] with a direct-forcing IBM. Squares, our results with a Lagrangian Volume Of Fluid tensorial penalty method.

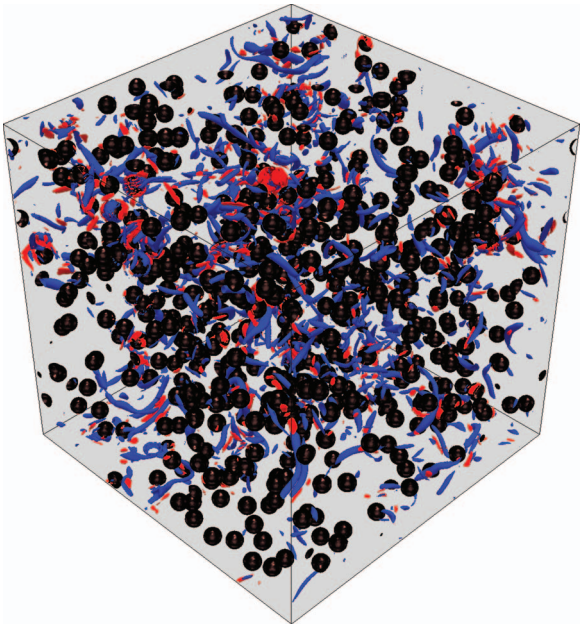

FIG. 5. Snapshot of 512 particles seeded in a tri-periodic cubic domain with vorticity contours in red and blue colors. The particulate volumetric fraction is 3%.

fluctuations of the turbulent structures. The Reynolds number based on the Taylor microscale is equal to 73 with a total resolution of 256^3 grid cells. In this flow, 512 spherical particles (the solid material is characterised by a dry coefficient $e_d = 0.97$) have been randomly seeded (Fig. 5) and their dynamics followed over more than ten integral time scales to get converged statistics. Following the numerical requirements to obtain a precise representation of the particle induced perturbation and the correct simulation of collisions, the particle diameter has been fixed to 22 Kolmogorov length scales. The overall particle volumetric concentration is 3% which generates minor modification of the flow statistics when gravity is neglected. The particle to fluid density ratio is one which corresponds to Stokes numbers 26 based on the Kolmogorov time scale and 1.5 based on the large-eddy turnover time scale (in this context the Stokes number compares the particle relaxation time to the fluid flow time scale). For this moderate particle concentration, only binary collisions are likely to occur. Statistics of the two-phase flow correspond to a particle agitation close to the fluid velocity fluctuation ($\frac{u'_p}{u'_f} = 0.92$).

Due to the finite size of the particles and the presence of local shear and vortices, particle collisions do occur. The characteristic time between two collisions in the domain is 100 Kolmogorov time scales. Examples of particle trajectories highlighting the occurrence of collisions are presented in Fig. 6.

Under the particle laden turbulence conditions we simulated, the major conclusion which can be drawn is that including the solid-fluid model of collision reduces the effective collision coefficient from $e_d = 0.97$ to below 0.1 on many collisions. This is an important insight which can have dramatic effect of the turbulent suspension dynamics.

Assuming that the mesh grid is the same for single phase and two-phase simulations, the CPU overhead of our model will be simply related to the reduction of the time step to account for particle collisions. The Courant–Friedrichs–Lewy criterion and the requirement of ten time steps within a collision generates moderate CPU overhead to include particle collisions in the fluid flow solver. Further development of the model[24] will lead to a complete modelling of general rebounds including oblique collisions, rotation, and friction (see Schäfer *et al.*,[28] Rosa *et al.*,[31] and Deen *et al.*[32] for a review in the context of fluidized beds).

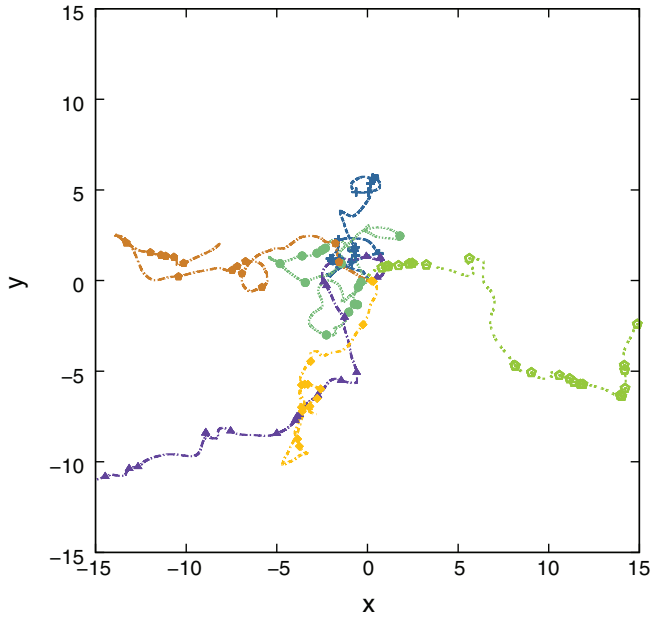

FIG. 6. Trajectories of six particles. The origin of each trajectory has been translated to coincide at the initial time. Symbols materialize collisions with another particle of the turbulent suspension.

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