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Estimating the Collision Rate of Inertial Particles in a Turbulent Flow: Limitations of the "Ghost Collision" Approximation

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Abstract. Most studies of collisions in turbulent flows are based on the "ghost collision" approximation, whereby one follows a number of particles, and simply counts the number of times the distance between two particles becomes less than the sum of their radii; particles are kept in the flow after they collided. We discuss here the limitations of this approximation, and demonstrate, using a simple model flow, that it leads to overestimates of the real collision rate by as much as $\sim 30\%$ at small Stokes numbers.

1. Introduction

Coagulation processes in turbulent suspensions play a crucial role in many phenomena, both in industrial and natural contexts. To quantitatively understand the time scales involved in these processes, one needs to estimate the collision rates between particles. Most estimates of collision rates in turbulent flows are based on the so-called "ghost collision" approximation, whereby one simulates the dynamics of a set of particles in a turbulent flow, and simply counts the number of times the particles come within a given distance, equal to the sum of their radii. As explained by Gustavsson *et al.* (2008), this potentially leads to biases in the estimates of the collision rates, induced by the finite time correlation of the velocity of the flow.

We study here the problem of determining collision rates in turbulent flows. To this end we use a simplified flow model, known as "kinematic simulations". We determine in such a flow the collision rates, both using the "ghost particle" approximation, and in a more realistic configuration whereby one systematically removes colliding particle pairs once they have collided. The dependence of the results as a function of the parameters of the problem is determined.

1.1. The Saffman-Turner Theory and "Ghost Collisions"

Saffman & Turner (1956) argued that for small particles which follow the streamlines of the flow (i.e. $St \rightarrow 0$) the collision rate is given by

$$\mathcal{N} = -n_0 \int \mathrm{d}\Omega \, v_r(2a,\Omega,t) \Theta(-v_r(2a,\Omega,t)). \tag{1}$$

This integral makes use of the Heaviside step function $\Theta(x)$ to sum up all regions on a sphere of two times the particle radius a where the the radial velocity v_r is directed inwards. The

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underlying idea is to follow particles as they move in the flow. Then the above integral multiplied by the particle density n_0 in the surrounding fluid will give the rate at which other particles come in contact with the particle at the system's origin. Averaging the above expression (1) and taking into account that for very small particles the radial relative velocity v_r can be approximated by the strain, which is assumed to be persistent and hyperbolic, Saffman & Turner (1956) finally arrive at their famous result

$$\mathcal{N} = \frac{n_0^2}{2} (2a)^3 \left(\frac{8\pi\epsilon}{15\nu}\right)^{1/2} = \frac{n_0^2}{2} \underbrace{1.294 \frac{(2a)^3}{\tau_\eta}}_{\Gamma_{\rm ST}},\tag{2}$$

where we introduced the Saffman–Turner collision kernel Γ_{ST} . The remaining undefined quantities are the rate of turbulent energy dissipation ϵ , the kinematic viscosity ν and the Kolmogorov time τ_{η} .

In the special limit case of persistent hyperbolic strain that Saffman & Turner (1956) investigate, there is no reason to take into consideration what happens after two particles have collided. In such a system the particles would just separate and never come close again. This leads to the method, consisting in counting collisions, while keeping colliding particles in the flow, known in the literature as "ghost collisions". This method enables a simple collision treatment in numerical simulations (e.g. in Wang *et al.*, 2000; Zhou *et al.*, 2001; Bec *et al.*, 2005; Franklin *et al.*, 2005; Bec *et al.*, 2010). In a turbulent flow, however, the strain will not stay constant along the trajectory of a particle (Brunk *et al.*, 1998) and it may be elliptic in some regions (Chong *et al.*, 1990). Thus two particles can get close to each other, separate and come close again. If in such a case the distance falls two times below the particle diameter 2a, two collisions would be counted within the framework of "ghost collisions". These re-collisions augment the collision rate in an unphysical way.

In the present paper we propose to study the effect of "ghost collisions" in detail and we will be especially interested in the error they impose on the estimates of the collision kernel Γ . To this end we define an alternative method to deal with colliding particles, which shall be described in more detail in Section 3. But before coming to this we will give an overview of the numerical methods used.

2. Numerical Methods

Maxey & Riley (1983) have derived a system of equations that describes the motion of small spheres in a turbulent flow. For heavy particles, i.e. particles with a mass density ρ_p much larger than the density of the surrounding fluid ρ_f , whose diameter is much smaller than the Kolmogorov length scale η , these equations take the simplified form

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{v}, \qquad \qquad \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \frac{\boldsymbol{u}(\boldsymbol{x},t) - \boldsymbol{v}}{\tau_p} + \boldsymbol{g}. \tag{3}$$

Here \boldsymbol{x} and \boldsymbol{v} denote the particle's position and velocity respectively, $\boldsymbol{u}(\boldsymbol{x},t)$ is the fluid velocity at point \boldsymbol{x} and \boldsymbol{g} represents the gravitational acceleration. The particle response time $\tau_p = 2a^2\rho_p/9\nu\rho_f$ describes the particle's inertia induced by the Stokes drag. Comparing it to the Kolmogorov time τ_{η} , i.e. the fastest time scale of the surrounding fluid flow, gives the relevant dimensionless parameter, the Stokes number $\mathrm{St} = \tau_p/\tau_{\eta}$.

We are interested in collisions induced by the turbulent motion of the fluid and for the present purpose, we set g to zero. Equations (3) are integrated using an ordinary second order Runge–Kutta scheme. This integration demands the knowledge of the fluid velocity at each particle's position and the usual way to provide it, would be to perform a direct numerical

simulation of the Eulerian velocity field u(x, t). This however is numerically very expensive and it is especially difficult to obtain higher Reynolds numbers. Therefore we opt for a simple model flow introduced by Fung *et al.* (1992) as "kinematic simulations".

2.1. Kinematic Simulations

Our kinematic simulations follow closely those described by Ducasse & Pumir (2009). The Eulerian velocity field is given by a superposition of N_k randomly chosen Fourier modes

$$\boldsymbol{u}(\boldsymbol{x},t) = \sum_{n=1}^{N_k} \boldsymbol{a}_n \cos(\boldsymbol{k}_n \cdot \boldsymbol{x} + \omega_n t) + \boldsymbol{b}_n \sin(\boldsymbol{k}_n \cdot \boldsymbol{x} + \omega_n t), \qquad (4)$$

which fulfills certain additional conditions. First the wave vectors $\mathbf{k}_n = k_n \hat{\mathbf{k}}_n$ are chosen pointing in random directions $\hat{\mathbf{k}}_n$ with their amplitudes k_n distributed according to

$$k_n = k_1 \left(\frac{L}{\eta}\right)^{(n-1)/(N_k-1)}, \qquad k_1 = \frac{2\pi}{L}, \qquad k_{N_k} = \frac{2\pi}{\eta}, \qquad (5)$$

where L signifies the large (integral) length scale and η the small (Kolmogorov) one. The coefficient vectors \boldsymbol{a}_n and \boldsymbol{b}_n are also chosen randomly but perpendicular to the wave vectors thus ensuring incompressibility

$$\boldsymbol{a}_n \cdot \boldsymbol{k}_n = \boldsymbol{b}_n \cdot \boldsymbol{k}_n = 0. \tag{6}$$

Furthermore a Kolmogorov spectrum is imposed on the flow by defining the amplitudes of the coefficient vectors as $a_n^2 = b_n^2 = E(k_n)\Delta k_n$ with $E(k_n) = E_0 k_n^{-5/3}$ ($E_0 = 1$ in our simulations). The discrete differences between the wave vectors Δk_n are defined as

$$\Delta k_n = \begin{cases} (k_2 - k_1)/2, & n = 1\\ (k_{n+1} - k_{n-1})/2, & n \in [2, N_k - 1]\\ (k_{N_k} - k_{N_k - 1})/2, & n = N_k. \end{cases}$$
(7)

We kept $L/\eta = 64$ in all our simulations and chose $N_k = 109$. It has been shown by Malik & Vassilicos (1999) that for $N_k \gtrsim 100$ one obtains good agreement between kinematic simulations and DNS.

Finally, a further parameter, λ , shows up in the definition of the frequencies ω_n , which are chosen to be proportional to the eddy turnover time on each length scale,

$$\omega_n = \lambda \sqrt{k_n^3 E(k_n)}.$$
(8)

It has been shown by Malik & Vassilicos (1999); Nicolleau & ElMaihy (2004) and others, that a value of $\lambda = 0.5$ is consistent with known Lagrangian properties of the flow. This has been used in the simulations discussed here.

2.2. Particle dynamics

A total of N particles are confined to a periodic box of side length αL and the volume fraction occupied by those particles, $\Phi = 4N\pi a^3/3(\alpha L)^3$, is kept constant in all our simulations. It has to be small to make sure that the approximations leading to Equations (3) are valid and that collisions involving three and more particles may be neglected. We took $\Phi = 1.2 \times 10^{-4}$ in all our simulations. The parameter $\alpha \in \mathbb{N}$ adapts the box size allowing to have more particles in one simulation while keeping the volume fraction Φ constant.

3. Collision Detection

To detect particle collisions we perform a neighborhood search—similar to the method described by Sundaram & Collins (1996)—at each time step. For every particle pair within a small distance of one another the trajectories between the current and the precedent time step are interpolated by a cubic polynomial and it is checked if the distance between the particles' centers falls below 2a anywhere along these trajectories. If this is the case a collision is counted and the two particles get marked for an eventual post-collision processing. We used two different schemes for post-collision treatment: Either

- (i) the particles were kept in the flow and allowed to (re-)collide right at the next time step—this is the "ghost collision" approach and statistics derived using this method will be denoted by the index "gh" in the following—or
- (ii) one of the two particles is replaced by another one coming from a "particle bath". This "particle bath" consists of a sufficiently large number of particles, which are not accounted for during collision detection. But they are advected in the flow just like usual particles and therefore already "thermalized" at the time when they replace a colliding particle. For numerical reasons the replaced particle is added to the reservoir and will be allowed to replace itself another colliding particle at a much later time (usually several large eddy turnover times). Statistics obtained within this frame will be denoted by the index "re".

We performed simulations for different Stokes numbers in the range $0.125 \leq \text{St} \leq 5$. For each Stokes number ten runs, each with a different set of randomly chosen Fourier modes, were started. It is especially crucial in the case of kinematic simulations to investigate independent realizations, as for those the properties of the flow are strongly dependent on a small set of (frozen) random wavenumber modes (comp. Sec. 2.1). The total integration time was chosen such that a total of $\mathcal{O}(10^6)$ collisions per Stokes number could be provided.

The relevant factor when comparing these two approaches will be the collision kernel Γ . Averaged over time it can be expressed as

$$\langle \Gamma \rangle_T = \frac{1}{T} \int_0^T \frac{2\mathcal{N}(t)}{n_0^2} \,\mathrm{d}t = \frac{2VN_c([0,T])}{TN_p^2},$$
(9)

where we introduced $N_c([0, T])$, the number of collisions in the time interval [0, T]. Further averaging is performed over different realizations of each simulation. An estimate of the error can be obtained from the fluctuations. We shall now drop the angular brackets again and denote by Γ the collision rate averaged over time and realizations.

4. Numerical Results: The "Ghost Particle" Overestimates the Collision Rates

The numerically evaluated collision kernel for different Stokes numbers St and both post-collision treatments (see Sec. 3) is shown in Figure 1. For small Stokes numbers the "ghost particle" collision kernel tends to the value $\Gamma_{\rm ST}$ (see Eq. (2)) as predicted by Saffman & Turner (1956). The proper collision kernel, obtained by replacing colliding particles, however, falls below this value. In fact the "ghost collision" approach overestimates the collision kernel for all Stokes numbers. This result is especially prominent in Figure 2, where we show the relative error of the "ghost" collision kernel, $(\Gamma_{\rm gh} - \Gamma_{\rm re})/\Gamma_{\rm re}$. This error falls with growing Stokes number but reaches up to ~ 30% for small values of the Stokes number.

The diminishing of the error made by using the "ghost collision" approach can be understood, when one takes into consideration the growing importance of the "sling effect" (Falkovich *et al.*, 2002; Falkovich & Pumir, 2007; Ducasse & Pumir, 2009) or "caustics" (Wilkinson *et al.*, 2006). These describe collision events, where the two colliding particles have velocities very different



St

Figure 1. The numerically estimated collision kernel using "ghost collisions" (squares) and the replacement particle approach (circles) for different Stokes numbers. The ghost collision method overestimates the collision kernel for all Stokes numbers but both estimates approach for larger Stokes numbers. Furthermore the dashed line segment shows the collision kernel theoretically predicted by Saffman & Turner (1956) and clearly $\Gamma_{\rm gh}$ tends to this value for St $\rightarrow 0$.

Figure 2. The error in estimating the collision rate using the "ghost collision" approximation. The difference between the collision rate estimated with the "ghost collision" approximation $\Gamma_{\rm gh}$ and by replacing colliding particles $\Gamma_{\rm re}$ divided by $\Gamma_{\rm re}$, as a function of the Stokes number St. The error decreases when St increases, due to the increased importance of the "sling effect".

from the surrounding fluid. Thus such two particles will veer away from each other quickly and are unlikely to re-collide afterward. Therefore, when collisions resulting from this kind of phenomenon prevail, the unphysical re-collisions accounted for by the "ghost collision" approach are of minor importance.

To verify our hypothesis, that collisions resulting from the "Sling effect" are lesser affected by the "ghost collision" approach, we calculated the average collision kernel conditioned on the relative velocity of the two particles at the moment of their collision $\langle \Gamma | v_{\ell} \rangle$. The relative collision velocity v_{ℓ} can be determined from the particles' positions, \mathbf{r}_i , and velocities, \mathbf{v}_i , i = 1, 2, via $v_{\ell} = (\mathbf{v}_2 - \mathbf{v}_1) \cdot (\mathbf{r}_2 - \mathbf{r}_1) / |\mathbf{r}_2 - \mathbf{r}_1|$ and the conditionally averaged collision kernel fulfills

$$\int \langle \Gamma | v_{\ell} \rangle \, \mathrm{d}v_{\ell} = \Gamma. \tag{10}$$

This measure describes the contribution from each interval dv_{ℓ} to the overall collision kernel Γ . In Figure 3 we show the conditionally averaged collision kernel for the "ghost collision" approach, $\langle \Gamma_{\rm gh} | v_{\ell} \rangle$, and for our "particle bath" approach, $\langle \Gamma_{\rm re} | v_{\ell} \rangle$ in the case of St = 0.5. Furthermore the difference between those two, $\langle \Gamma_{\rm gh} - \Gamma_{\rm re} | v_{\ell} \rangle$, is shown. The bulk of this difference is concentrated at small relative velocities v_{ℓ} and it vanishes at intermediate values, where the contribution to the collision kernel, as given by the conditionally averaged collision kernels $\langle \Gamma_{\rm gh} | v_{\ell} \rangle$ and $\langle \Gamma_{\rm re} | v_{\ell} \rangle$, is still significant. Thus the overestimation of the "ghost collision" approach results mainly from collisions with small relative velocities; collisions with large relative velocities don't contribute to this error. This is in accordance with our hypothesis.



Figure 3. The conditionally averaged collision kernels for the two different schemes, $\langle \Gamma_{\rm re} | v_{\ell} \rangle$ (solid) and $\langle \Gamma_{\rm gh} | v_{\ell} \rangle$ (dashed), as well as their difference (dash-dotted) for St = 0.5. Vertical lines describe the median-type values \bar{v}_{ℓ} defined as $\int_{-\infty}^{\bar{v}_{\ell}} \langle \Gamma | v_{\ell} \rangle dv_{\ell} = \Gamma/2$. Clearly the error made using the "ghost collision" approach results mainly from collisions with small relative velocities. The inset shows the tails of the conditionally averaged collision kernels $\langle \Gamma_{\rm re} | v_{\ell} \rangle$ and $\langle \Gamma_{\rm gh} | v_{\ell} \rangle$. For large values of v_{ℓ} the difference between the two collision schemes vanishes.

5. Conclusion

We have demonstrated that the widely used "ghost collision" approach overestimates the collision kernel by up to ~ 30 %. This deviation diminishes with growing Stokes number and we argue that this is due to the growing importance of "Sling collisions". This argument is supported by our investigation of the average collision kernels conditioned on the relative velocity. Nevertheless it may be worthwhile to confirm these results, using techniques along the lines of Ducasse & Pumir (2009). These would allow to decide between ordinary and "Sling" collisions. Thus it would be possible to directly measure which of these two types of collision is more affected by using the "ghost collision" approach.

As pointed out in the introduction (Sec. 1.1) there are two reasons why "ghost collisions" lead to incorrect estimates of the collision rate: the existence of regions of elliptic strain and its non-persistence. Both are true as well for frozen turbulent flows. In fact, Zhou *et al.* (1998), who use a frozen field, do also find a difference in the collision kernels obtained using "ghost collisions" on the one hand and using another post-collision treatment, similar to our "particle bath," on the other hand. Especially with respect to the non-persistent strain, it may be interesting to investigate the influence of the time-dependence of the flow in more detail.

Finally the challenging task of extending the Saffman & Turner (1956) approach to properly take into account the unwanted "ghost collisions" remains to be addressed.

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