A high resolution collision algorithm for anisotropic particle populations

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July 2014

Collision algorithm, stochastic parcel method, anisotropic dispersions, adaptive control volumes, order of accuracy

Abstract

In turbulent particle laden flows such as liquid sprays, droplet collisions make a significant contribution to momentum transfer and energy dissipation. By Lagrangian particle tracking with the stochastic parcel method, only a computational subset of the particle population is simulated, known as computational parcels; the prediction of particle collisions is based on a statistical assessment of collision probabilities. Collision algorithms for stochastic particle tracking are generally built upon two assumptions: first, an isotropic dispersion of particles within the control volume; second, perfect representation of relative velocities by the parcel population [1].

Prior to the preparation of this work, various collision algorithms have been investigated with respect to exactness, robustness, and convergence. Within these preliminary studies, two significant errors were identified, namely voidage errors and gradient errors, which are unresolved in any collision algorithm found today:

Voidage errors are a well known issue in stochastic collision algorithms, and have promoted the development of adaptive collision algorithms in the past [2, 3]. Voidage errors occur if the control volumes of a collision mesh grow into the void regions outside the parcel population, which leads to a systemic under-prediction of collision probabilities. In cases where the parcel population is highly anisotropic as particles do not populate all spatial directions, increasing resolution isotropically does not lead to convergence. In such cases, the control volumes must be adapted in an anisotropic manner, as has been presented initially in a previous publication [4].

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Gradient errors have not been identified since the introduction of the O’Rourke algorithm [1]. Physically, the mean velocity gradient in the disperse phase does not contribute to particle collisions. In stochastic parcel simulations, the mean velocity gradient adds to relative velocities proportionally with control volume size, which has been identified as gradient error [5].

To address these issues, a hybrid deterministic-stochastic formulation for the collision probability has been derived, which treats parcel collisions in a deterministic manner, i.e. based on their trajectories and distances, while the collisions of the represented particles are predicted in a stochastic manner. Parcels are represented by isotropic spheres-of-influence [6], introducing an explicit Gaussian kernel function for spatial filtering. In extension to similar existing algorithms, a non-parametric estimator for the diameter of the sphere-of-influence has been found, which makes the collision algorithm independent of user-defined numerical parameters.

To resolve voidage errors in anisotropic populations, the spheres-of-influence are further refined to ellipsoidal volumes-of-influence, which are fit to the local parcel population by a weighted principal component analysis of parcel positions. By that method, the collision probability is found to be convergent for isotropic three-dimensional dispersions, and for anisotropic one- and two-dimensional dispersions [4].

For the reduction of gradient errors, the velocity decomposition method is introduced, which reconstructs the mean velocity gradient and eliminates its spurious contribution to the collision probability. The velocity decomposition method gains second-order convergence even in the presence of strong velocity gradients, where common formulations provide first-order convergence only [5].

The methods derived are not introducing additional numerical parameters, i.e. spatial and temporal resolution are defined by the number of parcels and the numerical time-step only. The formulations have undergone a rigorous analytical and numerical validation, and show advanced accuracy and convergence behavior when compared to other formulations for stochastic collision algorithms. The methodology, convergence tests, and exemplary applications are subject to this presentation.

References

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The work in this presentation is based on four publications over the recent two years:


In this presentation, the focus is put on the concepts, not on the mathematics, numerics or implementation.
The purpose of a collision algorithm is to predict the incidence of collision. In direct simulations, where all particles are resolved and particle positions are known, collisions can be found deterministically by intersecting trajectories.
In stochastic parcel simulations, only a weighted subset of the entire parcel population is simulated. Thus, information on particle positions is lost. Collisions must be described statistically by stochastic collision algorithms. This is the topic of this work.
Stochastic collision algorithms are based on the prediction of a collision probability $P$.

Here, the variables are

- $q_i$ the statistical weight of the parcel considered
- $N/V$ the parcel number density in a given control volume
- $\pi (d_i + d_j)^2/4$ the collision cross-section
- $u_{ij} \Delta t$ the displacement per time-step

The exactness of the collision calculations depends strongly on a resolution-independent prediction of those quantities.
As will be shown, the number density and the relative velocity between two parcels are subject to strong numerical dependencies, which cause "voidage errors" and "gradient errors", as will be introduced in the following presentation.

\[
P_{ij} = q_i \frac{N}{V} \pi \frac{(d_i + d_j)^2}{4} u_{ij} \Delta t
\]
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**Anisotropic populations** have a number density which is a function of direction. Thus, resolution requirements strongly depend on the orientation of the population. Isotropic control volumes tend to grow into void regions, which we refer to as „voidage errors“ in the following.
The most extreme case of an anisotropic population occurs if parcels populate a lower-dimensional subspace only. Here, two examples are given, a two-dimensional (homogeneous) population (left), and a one-dimensional (anisotropic) population (right), which both reside in a two-dimensional control volume.
The most extreme case of an anisotropic population occurs if parcels populate a lower-dimensional subspace only. Here, two examples are given, a two-dimensional (homogeneous) population (left), and a one-dimensional (anisotropic) population (right), which both reside in a two-dimensional control volume.

If the control volume dimensions $L$ are changed, the number density $N/A$ of the isotropic population scales with $L^2/L^2$, and thus is constant except for statistical scatter; the number density $N/A$ of the anisotropic population scales with $L/L^2$, i.e. the number density is a function of resolution and does not converge for either large or small control volumes. This is the voidage error discussed before.
The present algorithm replaces the fixed control volume typically found in collision algorithms by a moving (Lagrangian) control volume bound to each parcel (hard-sphere-model/sphere-of-influence-model, common in molecular gas dynamics, not specific to this algorithm).
Typically, collision probabilities obey a box filter, i.e. the collision probability is a constant value if parcels are within the same control volume, and zero otherwise. This formulation is not differentiable, which leads to numerical artifacts, and the definition of the control volume size is arbitrary, either given by a parcel population target per control volume (adaptive algorithms), or by fixed dimensions (non-adaptive algorithms).

The present algorithm involves a Gaussian filter, and a novel formulation of the filter width, which is adaptive and non-parametric. See Pischke, 2012.
Finally, to cope with anisotropic dispersions, the spheres-of-influence are reduced to ellipsoidal volumes-of-influence by a weighted least-squares-approximation of their neighborhood. Spatial resolution is given by the Gaussian filter.
One of the validation cases presented in Pischke, 2012. A cylindrical particle population is collapsed to a 1D population, i.e. from isotropic to anisotropic. One particle is moving through the population, and the number of collisions is counted.
The number of collisions over the degree of anisotropy 
($R/R_0 = 0 = \text{anisotropic}, \ R/R_0 = 1 = \text{isotropic}$)
- If there were one single control volume of constant diameter $R_0$, the number of collisions would be constant as $N/V = \text{const}$.
- The direct simulation of all particles shows an increase of the number of collisions as the local number density grows as the population turns anisotropic.
- The isotropic sphere-of-influence approach cannot follow the increase of the number density, as isotropic refinement is insufficient. The number of collisions at $R/R_0 = 0$ is non-convergent, i.e. increasing the resolution does not lead to a converged result for the reasons given on slide (10).
- The anisotropic volume-of-influence approach follows the direct scheme accurately, leading to an exact prediction for $R/R_0 = 0$. 
As discussed before, the relative velocity between two parcels is another variable to influence the collision probability. In the presence of velocity gradients, it is subject to strong numerical dependencies.
Assume a one-dimensional control volume. All parcels within the control volume are considered collision partners. The parcel number density is homogeneous, so there is no influence from that side.

If there is a velocity gradient within the particle population, the maximum relative velocity and thus mean relative velocities are a function of control volume sizes, as larger control volumes extend over a wider range of the velocity gradient.
In Pischke 2012, the velocity decomposition method is introduced, splitting velocities into a velocity gradient with zero fluctuations, and velocity fluctuations with zero gradient.

Physically, the velocity gradient does not contribute to collisions, as droplets at the same location (i.e. at the moment of collision) have the same velocity. Thus, the velocity gradient is dropped, and the velocity fluctuations are used to calculate collision probabilities.

In Pischke, 2012, the scheme is shown to be second-order accurate, contrary to all other schemes, which are second-order only in the absence of velocity gradients, and drop to first-order in the presence of velocity gradients.
For demonstration, a simulation of a hollow-cone spray is shown. In hollow-cone sprays, droplets align almost two-dimensionally on a conical sheet before they are dispersed. Thus, the spray is highly anisotropic near the nozzle.

Other authors tend to check convergence of collision algorithms by macroscopic quantities of the simulated spray, e.g. by investigating the sensitivities of liquid penetration, velocities, or drop sizes. However, these quantities may depend on other models, or may exhibit little sensitivity to collisions.

Thus, in Pischke 2012 the sensitivity of collisional quantities is checked, e.g. the number of collisions, or momentum transfer and energy dissipation by droplet-droplet interaction.
The figure shows the spheres-of-influence of a 1/8th segment of the hollow-cone spray. The spheres-of-influence extend in regions where there are no droplets. If the resolution is coarsened, the spheres-of-influence are enlarged and outgrow the parcel population even further, leading to the voidage errors discussed on slide (10).
With the anisotropic volume-of-influence approach, the spheres collapse to discs, representing the two-dimensional sheet very accurately. Note that the anisotropic adaptation takes place locally by using the Gaussian filter of slide (12). Far off the nozzle, the volumes-of-influence are near spherical, as the spray is dispersed isotropically.
Here, the accumulated momentum transfer is shown over time. The momentum transfer is strongly dependent on the number of parcels, thus on resolution. The reason is (i) the voidage errors of the isotropic sphere-of-influence approach, and (ii) the gradient errors, which lead to resolution dependent relative velocities, collision regimes and momentum transfer.
With the anisotropic volume-of-influence approach and velocity decomposition, the solution converges almost immediately, as first-order gradient errors are eliminated.
Advantages of the new collision algorithm (to be found in Pischke 2012):
- It’s non-parametric; except for time-step and number of parcels, there are no resolution determining parameters or arbitrary model constants.
- It is consistent in itself by using the same spatial filter throughout all formulations, and consistent with other formulations of collision probabilities, e.g. direct schemes.
- It is differentiable, which avoids collision artifacts such as clover leaf patterns.
- It is convergent, as was shown in a previous example.
- It is adaptive, maxing out resolution for any given number of parcels
- It is anisotropic, leading to converged results even for populations in lower-dimensional subspaces.
- It is second-order where other algorithms are first-order only.
- It is validated analytically and numerically against direct simulations.

Accuracy has a price tag: numerical performance. The scheme relies on exponential functions, error functions and eigenwert problems, leading to high numerical effort. Parallelization is difficult.
Here, only the concept of the collision algorithm was shown. For derivation and validation, consider our publications: