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Short Note

Conservative method for the reduction of the number of particles in the Monte Carlo simulation method for kinetic equations

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Abstract

A method for the reduction of the number of particles in the weighted Monte Carlo method for kinetic equations is described. The method randomly redistributes statistical weights over the particle ensemble in such a way that the weight of some particles becomes 0, i.e., the particles are cancelled, while all physically relevant macroscopic moments (e.g., mass, energy, momentum) of the ensemble do not change. The method has been applied to the spatially uniform relaxation of a gas of hard spheres.

Keywords: Monte carlo; Population balances; Weighted particles method; Random weight transfer

1. Introduction

The Monte Carlo simulation method (DSMC) is a statistical method for the computation of particulate flows, either rarefied gas flows or aerosol flows [1,4,7]. The method can be formulated as follows. The flow volume is divided into cells. The particle ensemble is represented by computational particles such that a group of W identical molecules or particles in the physical system is substituted by one computational particle. The parameter W_i is the statistical weight of the ith computational particle. In the particular case when $W_i = W$ for all i, the method is called the direct simulation Monte Carlo (DSMC) method, while the more general case is the stochastic weighted particle method (SWPM) [2,9,8,6]. Provided that the

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particles' sizes, positions and other necessary parameters are known at a time t, the particles' distribution at time $t + \Delta t$ can be calculated by an operator-splitting technique which comprises free flow and a spatially homogeneous relaxation step. In the free flow phase the particles move, without any collisions occurring, during the time interval Δt. Their positions, velocities, sizes, temperatures, etc., are determined from the equations of motion, and heat and mass transfer. In the second splitting step binary collisions between particles in each cell are sampled randomly. At this step, a particle can collide only with those particles that are in the same cell irrespective of the relative positions of the particles within the cell.

The accuracy of the method depends both on the size of the cells and on the number of particles in a computational cell. Since the number of physical particles in a cell is proportional to the volume of the cell, reduction of the cell size does not necessarily increase the precision of the calculations. For an accurate resolution of the collision physics one needs a minimum number of computational particles in each spatial cell. If the number of computational particles in a cell is small, both averaged physical properties of the ensemble, such as mass and momentum, and the collision rate of the particles are subjected to large spurious fluctuations. A comprehensive discussion of the dependence of the number of particles on the particles density and the geometry of the flows is given in [3].

The direct way to control the optimal number of computational particle in each cell is the use of statistical weights [1,9]. If a particle weight decreases as it passes from one cell to another, the particle is cloned, i.e., several copies of the mother particle with smaller weights are created. This procedure leads to an increase in the number of particles in the system. Note, that in the case of the Boltzmann equation a collision of two particles with different statistical weights forms at least three particles. Thus, a procedure for reduction of the number of particles in SWPM is necessary in order to keep the system computationally tractable.

The simplest method for reducing of number of particles is proposed in [1]. The trajectory of a particle is either terminated with probability p, or the statistical weight of the particle is multiplied by $1/(1-p)$. While this method is algorithmically simple, it satisfies the law of mass, momentum and energy conservation only in a statistical sense. Thus, random creation/dissapearence of the particles leads to large spurious oscillations of the macroscopic parameters of the ensemble and impairs the accuracy of the calculations [3].

Boyd [2] proposed a conservative method for the simulation of trace species in nonequilibrium gas flows. If a particle with smaller statistical weight which represent a trace species collides with a particle with larger weight, three particles, one trace and two nontrace are created. Then, the nontrace molecules are merged in such a way as to conserve the linear moment explicitly. The energy that is lost at this step is added to the next nontrace interparticle collision. If the statistical weights of a trace species is much smaller than the statistical weights of the nontrace species, the proposed scheme introduces only very small fluctuations of energy.

A method that preserves the number (or mass) of the particles in the Monte Carlo simulation of Smoluchowski's equation is presented in [10,5]. If a randomly chosen particle is removed, its statistical weight is redistributed among the other particles of the ensemble. If this method is conservative with respect to the total mass, it is not conservative with respect to the number of particles and vice versa. When applied to a multidimensional problem, this method does not preserve the momentum of the particles (for gas flow simulations) or the mass of the components (for multicomponent population balance).

In order to avoid these difficulties an alternative method based on the clustering of particles has been proposed in [9,8]. According to this approach, the particles are divided into groups (clusters) such that the distance between the particles in the phase space (diameter of the cluster) is small. Then the cluster can be replaced by a few particles which have the same physically important first statistical moments (mass, momentum, energy, etc.) as the original cluster. Thus, the method creates some new ''synthetic'' particles that approximate the ensemble in a mean-square sense, i.e., the solution of the Boltzmann equation is smoothed as the algorithm proceeds further. The efficiency of the method depends on the efficiency of the clustering algorithm, and the method introduces some systematic errors that decrease with the diameter of the clusters.

In the present study we propose a method that does not require a time-consuming clustering procedure and does not smooth the solution of the equation. The method redistributes statistical weights of the particles in such a way that all physically relevant moments of the ensemble remain unchanged. We test this method on the spatially homogeneous relaxation of a gas of hard spheres, but this method has a more general area of applicability and can be used for any other population balance problem.

2. Description of the SWPM

Consider the spatially homogeneous Boltzmann equation for a gas of hard Spheres

$$\frac{\partial f(t,\vec{u})}{\partial t} = \int B(\vec{u},\vec{v},\vec{e})\{f(t,\vec{u}')f(t,\vec{v}') - f(t,\vec{u})f(t,\vec{u})\}\,\mathrm{d}\vec{v}\mathrm{d}\vec{e}, \tag{1}$$

where

$$\vec{u}' = \frac{\vec{u}+\vec{v}}{2} + \frac{|\,\vec{u}-\vec{v}\,|}{2}\vec{e}, \quad \vec{v}' = \frac{\vec{u}+\vec{v}}{2} - \frac{|\,\vec{u}-\vec{v}\,|}{2}\vec{e}, \tag{2}$$

where $\vec{e}$ is a uniformly distributed unit vector, and $\vec{u}$, $\vec{v}$ and $\vec{u}'$, $\vec{v}'$ are the velocities of the particles before and after the collision, repectively. The formula for the collision kernal $B(\vec{u},\vec{v},\vec{e})$ is given by

$$B(\vec{u},\vec{v},\vec{e}) = \frac{1}{4\sqrt{2}\pi Kn}\,|\,\vec{v}-\vec{u}\,|, \tag{3}$$

where Kn is the Knudsen number.

The main idea of the weighted particles method [9] is the representation of the solution of Eq. (1) as

$$f(\vec{u}) \approx \sum_{i=1}^{N} W_i \delta(\vec{u}-\vec{u}_i). \tag{4}$$

As the ith and jth particles collide, four new particles appear. Two of them with weights and velocities $W_i - w$, $W_j - w$ and $\vec{u}_i, \vec{u}_j$, respectively. While the others have weight w and velocities $\vec{u}'_i$ and $\vec{u}'_j$ that are calculated according to Eq. (2). The parameter w ($w \leqslant W_i$, $w \leqslant W_j$) is the weight transfer function [9]. In the partial case $W_i = W_j = w$ the method is equivalent to DSMC and the number of particles does not increase.

Integration of Eq. (3) over the unit sphere yields the formula for the collision rate between two particles:

$$\hat{B}(\vec{u},\vec{v}) = \frac{1}{\sqrt{2}Kn}|v-\vec{u}|.$$

The total collision rate is given by

$$\rho = \sum_{1\leqslant i<j\leqslant N} \hat{B}(\vec{u}_i,\vec{v}_j)\frac{W_i W_j}{w}.$$

The Monte Carlo algorithm [9] reads:

1. Generate an exponentially distributed time increment with parameter ρ.
2. Choose the pair for collision with probability

$$\frac{\hat{B}(\vec{u}_i,\vec{v}_j)W_i W_j}{\rho w}.$$

3. Generate a uniformly distributed unit vector $\vec{e}$ and create the new particles with parameters

$$(W_i - w, \vec{u}_i), \quad (W_j - w, \vec{u}_j), \quad (w, \vec{u'}_i), \quad (w, \vec{u'}_j).$$

3. Reduction of the number of particles

As the number of particles in the system becomes too large, some of them have to be removed and their statistical weights to be redistributed over the remaining particles. Our purpose is to construct an algorithm that keeps the distribution function (4) statistically intact and also conserves physically important statistical moments. These moments for gas flow are mass, momemtum and energy. Thus, no transformation of the statistical weights can change the following moments:

$$m_1 = \sum_i W_i, \quad m_2 = \sum_i W_i u_{xi}, \quad m_3 = \sum_i W_i u_{yi}, \quad m_4 = \sum_i W_i u_{zi}, \quad m_5 = \sum_i W_i |\vec{u}|_i^2. \tag{5}$$

Let us divide the particles into 6 groups I_k, $i \in I_k$. The jth moment of the kth group is m_{jk}, these moments form a 5×6 matrix M. Consider a vector $\vec{g} = (g_1, \ldots g_6)$ and multiply all the statistical weights of the kth group by $1 + \alpha g_k$, where α is a scalar parameter. In order to keep the moments (5) unchanged one needs

$$m_{jk} g_k = 0, \tag{6}$$

i.e, the vector $\vec{g}$ has to be orthogonal to the subspace formed by the rows of the matrix M. Thus, the algorithm for the reduction of the number of particles reads:

1. Generate a uniformly distributed unit vector $\vec{g}$.
2. In order to satisfy Eq. (6) recalculate $\vec{g}$ as

$$\vec{g} := \vec{g} - M^T (M M^T)^{-1} M \vec{g}.$$

3. Find

$$\alpha_1 = \min_{g_k < 0} \left\{ -\frac{1}{g_k} \right\}.$$

4. Find

$$\alpha_2 = \min_{g_k > 0} \left\{ \frac{1}{g_k} \right\}.$$

5. With probability $\alpha_2/(\alpha_1 + \alpha_2)$ multiply all the statistical weights of the kth group by $1 + \alpha_1 g_k$.
6. Otherwise multiply all the statistical weights of the kth group by $1 - \alpha_2 g_k$.

In order to demonstrate that the procedure described above keeps the solution of Eq. (1) statistically intact, consider an arbitrary functional $H(f(\vec{u}_i))$:

$$H(f(\vec{u})) = \int f(\vec{u}) h(\vec{u}) \, \mathrm{d}(\vec{u}) \approx \sum_i W_i h(\vec{u}_i) = \sum_{k=1}^{6} \sum_{i \in I_k} W_i h(\vec{u}_i). \tag{7}$$

After the reduction of the number of particles, Eq. (7) becomes

$$H_1(f(\vec{u})) \approx \sum_{k=1}^{6} \sum_{i \in I_k} (1 + \alpha_1 g_k) W_i h(\vec{u}_i),$$

with probability $\alpha_2/(\alpha_1 + \alpha_2)$, or

$$H_2(f(\vec{u})) \approx \sum_{k=1}^{6} \sum_{i \in I_k} (1 - \alpha_2 g_k) W_i h(\vec{u}_i),$$

with probability $\alpha_2/(\alpha_1 + \alpha_2)$. Direct calculation shows that

$$\langle H(f(\vec{u})) \rangle = \frac{\alpha_2}{\alpha_1 + \alpha_2} H_1(f(\vec{u})) + \frac{\alpha_2}{\alpha_1 + \alpha_2} H_2(f(\vec{u})) = H(f(\vec{u})),$$

and the estimation (7) remains statistically intact for arbitrary $h(\vec{u})$, while the statistical weights of one of the groups of particles is 0.

4. Numerical experiment

We calculated spatially uniform, relaxation of a gas of hard spheres with Knudsen number $Kn = \sqrt{2}$. Two groups of particles with equal momenta and velocities $\vec{u}_1 = (1, 0, 0)$ and $\vec{u}_2 = (-9, 0, 0)$, respectively, collide and the process evolves toward thermodynamic equilibrium. The initial distribution reads:

$$f_0(u_x, u_y, u_z) = \frac{9}{10} \delta(u_x - 1) \delta(u_y) \delta(u_z) + \frac{1}{10} \delta(u_x + 9) \delta(u_y) \delta(u_z).$$

Three varients of the Monte Carlo particle method have been used in the simulations. Since the standard DSMC method [1] has been well studied in the past, we refer to the results obtained by this method as ''exact''. The SWPM has been run with two strategies for the reduction of the number of particles, namely, the constant-number Monte Carlo method that was described in [10] and the conservative method proposed in the present work. Initially the two colliding fractions has the same number of particles, while the fast particles have statistical weights which are nine times smaller. The weight transfer function w during a collision

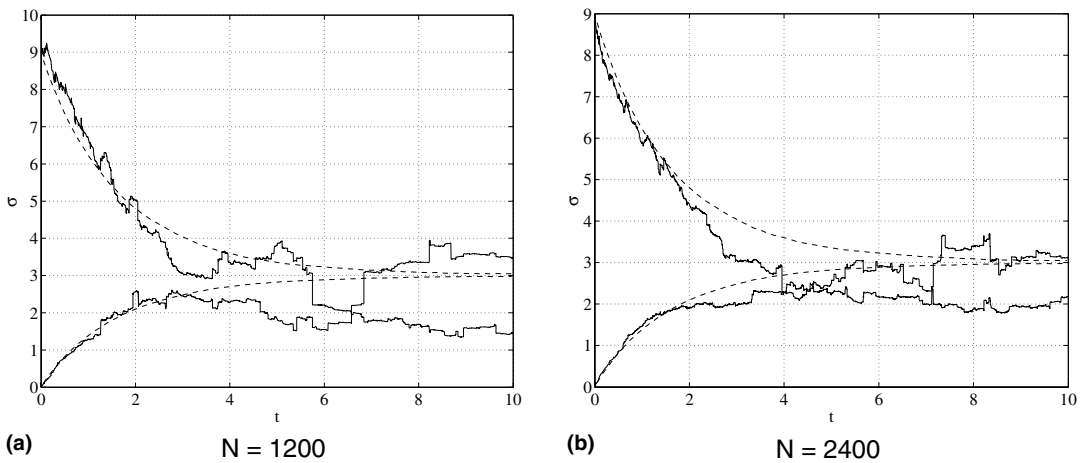

Fig. 1. Time evolution of σ_n (upper lines) and σ_t (low lines), DSMC method (dashed lines), constant-number MC (solid lines) for different number N of particles.

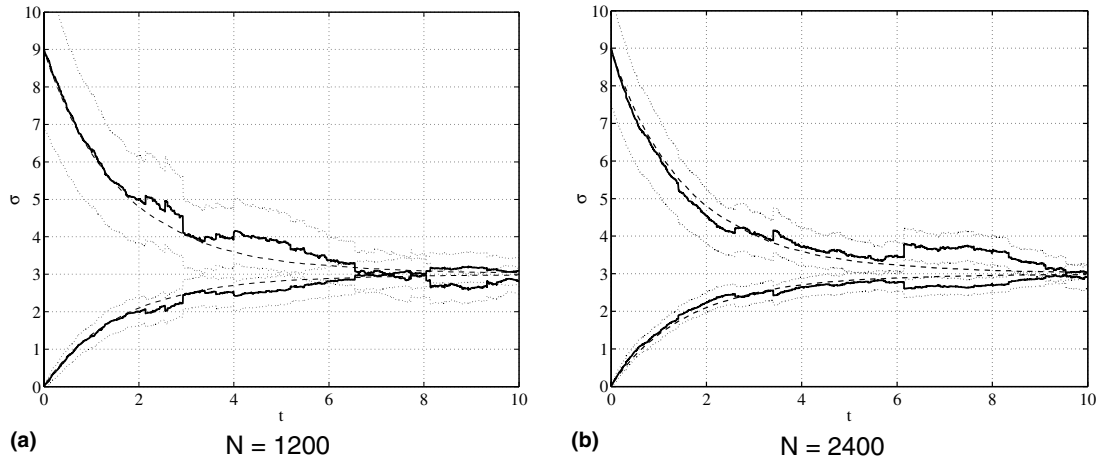

Fig. 2. Time evolution of σ_n (upper lines) and σ_t (low lines), DSMC method (dashed lines), conservative method (solid lines) for different number N of particles. The confidence intervals are shown by dotted lines.

of two particles with weights W_i and W_j is $w = \min(W_i, W_j)$ and three new particles grows, a special procedure is necessary to tractable. In the present case as the number of particles reaches the maximum allowed value, the reduction procedure is applied which terminates one sixth of the particles.

We calculated the second moments, the longitudinal moment $\sigma_n = \int (f(\vec{u})u_x^2 \, \mathrm{d}\vec{u}$ and the transversal moment $\sigma_t = 1/2 \int f(\vec{u})(u_y^2 + u_z^2) \, \mathrm{d}\vec{u}$. We also controlled energy, momentum and mass conservation in DSMC and in the conservative method (which are not conserved in constant-number MC). As the collision process proceeds further, the moments relax from their initial values $\sigma_n = 9$ and $\sigma_t = 0$, respectively, toward the equilibrium values $\sigma_n = \sigma_t = 3$. The results are presented in Figs. 1 and 2. In order to obtain reliable results we run the DSMC method 100 times with $N = 1000$ particles in each run. The results of a single run of the constant-number and conservative methods for different values of N are plotted in Figs. 1 and 2, respectively. Since the constant-number MC method does not conserve momentum and energy of the particles,

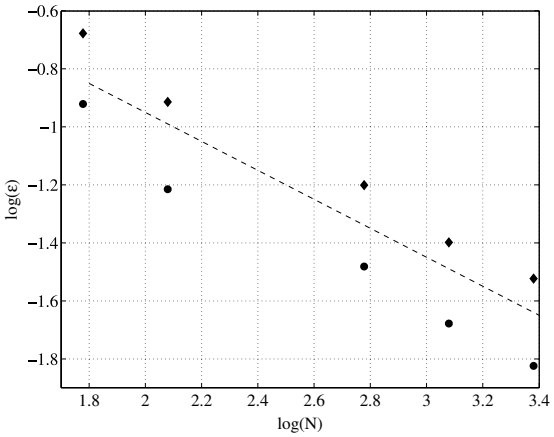

Fig. 3. Error of the conservative method versus number N of the particles in each run of the algorithm σ_n (diamonds) and σ_n (circles). The $-1/2$ slope is shown by the dotted line.

the solution significantly deviates from those by the DSMC method. As one can see, the solution obtained by the conservative method is close to the "exact" one and is free from the large spurious fluctuations, unlike the solution calculated by the constant-number method. In order to investigate how the maximum number of particles N in a single run of the conservative methods affects the results, we run the method L times. Since the total number of particles $N \times L = 1{:}2 \times 10^5$ was kept constant, the error in the calculations has a systematic character. We use maximum deviation

$$\in (N) = \max \|\sigma(N) - \sigma^{\text{exact}}\|,$$

as a measure of the error. Then the results for different values of N are plotted in Fig. 3. As one can see, $\in(N) \sim N^{-1/2}$.

5. Conclusion

We have proposed a conservative method for the reduction of the number of particles in the particle Monte Carlo method. Although the method was tested on monoatomic gas relaxation, it can be applied to arbitrary population balance problem such as fragmentation and coagulation. The method is based on the redistribution of statistical weights in such a manner that it does not affect the physically relevant statistical moments. The key idea of the proposed method is the division of the particles into groups and the multiplication of the statistical weights of the kth group by a factor $1 - g_k$. If our purpose is to conserve the α moments and the particles are divided into β groups ($\beta > \alpha$), the moments conservation condition means that the vector $\vec{g}$ is orthogonal to the rows of the $\alpha \times \beta$ matrix of moments M. The condition $M\vec{g} = 0$ together with the requirement that $g_k \leqslant 1$ (the moments are non-negative) implies that the vector $\vec{g}$ belongs to a $(\beta - \alpha)$-dimensional convex polygon. Thus, $(\beta - \alpha)$ particles groups can be cancelled by choosing randomly a corner point of the polygon. Additional research is necessary in order to find the optimal distribution of particles into the groups and the optimal proportion between number of the groups and number of the moments to be conserved by the transformation.

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