On the Selection of the Number of Model Particles in DSMC Computations

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Abstract. The discretization errors of majorant frequency scheme (MFS) based Direct simulation Monte Carlo (DSMC) are analyzed numerically and compared to known results for no-time-counter (NTC) scheme DSMC on the example of the Fourier problem. Independence of error from an average number of particles in a cell is confirmed for MFS. Convergence on time step and cell size in MFS is verified to be second order as in NTC. New criterion for the number of model particles is proposed, invariant on local density and, in simplest case, coming to product of the mean number of particles in a cell and the number of cells along the local mean free path. First order convergence on the criterion value is demonstrated for both 1D and 2D grids.

Keywords: Fourier problem, number of model particles, repetitive collisions, majorant frequency scheme.
PACS: 44.15, 47.11, 47.45

INTRODUCTION

The Direct simulation Monte Carlo (DSMC) method is a standard for simulation of nonequilibrium rarefied gas flows described by Boltzmann equation. This method is based on tracking individual molecules (model particles), considering them moving independently with occasional discrete events of pair collisions applied according to a statistical model. Macroparameters of the flow are then calculated by time averaging parameters of particles after the steady state is reached. Two kinds or errors present in simulation result: statistical errors of averaging, and discretization errors of simulation process, only the latter are considered in this paper.

First, the displacement and collision phases are uncoupled to speed up a computation, that gives the time step parameter Δt. Second, a considerable finite number of particles is used to simulate a large number of physical molecules. The Boltzmann equation has a symmetry that allows reducing the density n of molecules by increasing the total collisional cross-section σ_T: $n \to \frac{n}{F_N}, \sigma_T \to \sigma_T F_N$, with local mean free path $\lambda = \frac{1}{\sqrt{2} n \sigma_T}$ being unchanged (however, $\sigma_T \ll \lambda^2$ is assumed in Boltzmann equation). With finite number of particles, collisions cannot be pointed like in Boltzmann equation. Thus, third, a space is divided into collisional cells of size h, and paired colliding molecules are selected from the same cell only yielding the spatial collision separation. Most known collisional schemes are: the majorant frequency scheme (MFS) [1] and the no-time-counter (NTC) scheme [2].

MFS assumes that each possible pair (i, j) of particles in a cell has a collision probability uniformly distributed over time, with the mean frequency $\nu_{ij} = \frac{F_N \cdot \{\sigma_T \mathrm{c}_r\}_{ij}}{V_C}$. Here F_N is a number of physical molecules represented by each model particle, c_r is a relative velocity, σ_T is a total collision cross-section as a function of c_r, V_C is a cell volume. The approach is to guess a maximal number of collisions in a cell during time step, first by sampling from Poisson distribution with the mean value $K_{max} = \frac{N_C(N_C-1)}{2} \cdot \frac{F_N \cdot \{\sigma_T \mathrm{c}_r\}_{max}}{V_C} \cdot \Delta t$, then select random pairs (i, j) within a cell and accept each collision with probability $\frac{\{\sigma_T \mathrm{c}_r\}_{ij}}{\{\sigma_T \mathrm{c}_r\}_{max}}$. The N_C is an instantaneous number of particles in a cell. The value $\{\sigma_T \mathrm{c}_r\}_{max}$ should be chosen so that only a negligible fraction of collisions exceed it. Generally, this work concerns MFS.

In classical NTC scheme, the number of collisions in a cell is determined by the number of particles in a cell but not by the number of particle pairs, so $K_{max} = \frac{N_C \overline{N_C}}{2} \cdot \frac{F_N \cdot \{\sigma_T \mathrm{c}_r\}_{max}}{V_C} \cdot \Delta t$. The mean number of particles in a cell $\overline{N_C}$

must be known a-priori[1]. Here and below, designations of mean values are marked with overline. As opposed to MFS, in NTC scheme the number K_{max} of collision tests is just rounded down, with fractional part of K_{max} postponed to next time step. If a single particle is in a cell, all collision tests are postponed. The NTC cell may be further divided into smaller subcells (so-called subcell logic), with a collision partner restricted to be in the same or closest non-empty subcell.

The dependence of discretization errors on the number of model particles, the cell size and the time step for a long time was an open question. The consensus is that results should be accurate if the cell size is less than the local mean free path, most particles pass no more than one cell per time step, and each cell (or subcell in NTC scheme) contains on average at least few model particles. The theoretical estimation [3, 4] of convergence on the cell size and time step gives the second order for both. For reference, the heat conductivity deviation predicted by the theory is:

$$\frac{\kappa}{\kappa_{|\Delta\tilde{x}\to 0}} = 1 + \frac{32}{225\pi}\cdot\Delta\tilde{x}^2 \qquad (1); \qquad \frac{\kappa}{\kappa_{|\Delta\tilde{t}\to 0}} = 1 + \frac{64}{675\pi}\cdot\Delta\tilde{t}^2 \qquad (2);$$

where $\Delta\tilde{x} = \frac{h}{\lambda}$, $\Delta\tilde{t} = \frac{c_0\Delta t}{\lambda}$, local heat speed $c_0 = \sqrt{\frac{2kT}{m}}$, with local temperature T and molecule mass m.

For the required number of model particles, no theory is developed. It is believed the simulation error is inversely proportional to $\overline{N_C}$ [5]. Repetitive collisions (assumed impossible in Boltzmann equation) are thought as one of the problem of finite number of particles: with fewer particles in a cell, repetitive collisions are considered to be more probable.

However, in [6] the 1D shock wave is simulated using MFS and $\overline{N_C}$ is stated to be irrelevant. Instead, the criterion $\overline{N_\lambda} \gg 1$ is proposed, where $\overline{N_\lambda}$ is the average number of particles in a simulation area volume with linear size of the local mean free path. The probability of repetitive collisions is weakly dependent on $\overline{N_C}$ while $\overline{N_\lambda} = const$, according to [6].

In [5], a Fourier problem with a weak temperature gradient is simulated and the effective heat conductivity coefficient is measured. After performing a large set of simulations with NTC scheme, authors provide a polynomial fit for the heat conductivity deviation:

$$\begin{aligned}\frac{\bar{\kappa}_{DSMC}}{\kappa_{|h\to 0,\Delta t\to 0,\overline{N_C}\to\infty}} &= 1.0001 + 0.0287\Delta\tilde{t}^2 + 0.0405\Delta\tilde{x}^2 - 0.0009\Delta\tilde{x}^4 - 0.016\Delta\tilde{t}^2\Delta\tilde{x}^2 + 0.0081\Delta\tilde{t}^4\Delta\tilde{x}^2 \\ &+ \frac{-0.083 + 1.16\Delta\tilde{x} - 0.220\Delta\tilde{x}^2 + 1.56\Delta\tilde{t}^2 - 2.55\Delta\tilde{t}^2\Delta\tilde{x} + 1.14\Delta\tilde{t}^2\Delta\tilde{x}^2}{\overline{N_C}} \\ &+ \frac{-0.92\Delta\tilde{t}^3 + 1.91\Delta\tilde{t}^3\Delta\tilde{x} - 0.94\Delta\tilde{t}^3\Delta\tilde{x}^2}{\overline{N_C}} + \frac{0.095\Delta\tilde{t}^2}{\overline{N_C}^2}\end{aligned} \qquad (3).$$

Like (1) and (2), the (3) shows second order for cell size and time step as well, but with slight less coefficients. Also, (3) shows a first order dependence on $\frac{1}{\overline{N_C}}$ and $\frac{\Delta\tilde{x}}{\overline{N_C}}$. The [5] states that the latter term is important only if too few particles are used.

The present work proposes the new universal criterion for the number of model particles, valid for 1D, 2D and probably 3D grids. The efficiency of new criterion for MFS simulations is testified numerically. Additionally, spatial and time discretization errors are briefly studied and compared to known results for NTC scheme.

THE NEW CRITERION

If a pair of particles has just collided in MFS, the second (repetitive) collision of this pair will be possible until these particles separate enough not to be in a same cell. Let the $\Delta t_P \sim \frac{h}{\overline{c_r}}$ be the time needed for a pair to separate. We then have: $\nu_{ij}\Delta t_P = \frac{\sigma_T\cdot h}{V_C/F_N}\cdot\frac{c_r\Delta t_P}{h} \sim \frac{\overline{\sigma_T}\cdot h}{V_C/F_N} \ll 1$. The $\frac{V_C/h}{F_N\overline{\sigma_T}\cdot} \gg 1$ is actually the new criterion proposed in this work. If a single sort of molecules is used and no weight factors are applied, one can use the simplified form of the criterion: $\overline{N_C}\cdot \mathrm{Kn}_C \gg 1$; here $\mathrm{Kn}_C = \frac{\lambda}{h} = \frac{1}{\Delta\tilde{x}} = \frac{1}{\sqrt{2}n\overline{\sigma_T}h}$; $\overline{N_C} = \frac{nV_C}{F_N}$.

The above criterion is invariant on a local density. Therefore, increasing the size of collisional cells is not necessary if a local density drops, and a wide class of problems can be solved using regular grid. However, one should still take into account that the mean collision cross-section $\overline{\sigma_T}$ may depend on local temperature.

[1] The one described in [2] is meant everywhere in this paper, though other NTC schemes exist and are used recently, with different selection of K_{max} not needing the average density.

For 1D case, the $\overline{N_C} \cdot \mathrm{Kn}_C$ criterion is identical to $\overline{N_\lambda}$ and is invariant on a cell size as well, therefore, increasing cell size cannot balance the lack of model particles. For 2D and 3D cases, the decrease of the cell size still has to be accompanied by the increasing number of model particles. In general, the cell size might be adapted to local cell volume (for example, in axisymmetric problems), local temperature and local F_N (in the case of spatial weight factors).

COMPUTATIONAL VALIDATION

Simulation of the Fourier problem was chosen to numerically test the criterion in practice. In first case, the following conditions were set: Kn_0=0.1, $T_2 / T_1 = 4$, diffuse reflection, HS (hard sphere) model. MFS scheme was used. Knudsen number is determined by the mean density n_0 and the distance between planes. T_1 and T_2 are wall temperatures. These conditions are identical to [7], allowing direct comparison of results.

The choice of Knudsen number was determined by the possibility to perform both 1D and 2D simulations with as little as 0.01 particles per cell keeping reasonable heat flux error and less than 1000 x 1000 grids.

First, the reference simulation was performed with certainly sufficient selection of total number of particles, cell size and time step. Comparing with [7] shows negligible difference in wall heat flux (0.29589 ± 0.22% vs 0.295) and wall pressure (1.12311 ± 0.080% vs 1.124), both related to free-molecular value. Then, different combinations of total particles and grids were tested. Cell size was chosen to be a minor source of error. Table 1 groups these simulations sorted by wall heat flux Q deviation, calculated as: $\left|\frac{Q}{Q_{ref}} - 1\right|$. The confidence interval is 99.73%. In 2D simulations, a square area was used with two additional mirror planes.

TABLE 1. Wall heat flux deviation from the reference value for different 1D and 2D simulations. Bold italic marks VS model based simulations, other simulations use HS model.

Wall heat flux error, ×100%	**Criterion $\overline{N_C} \cdot \mathrm{Kn}_C$**	**$\overline{N_\lambda}$**	**$\overline{N_C}$**	**Kn_C**	**Total particles**	**Total cells**
reference	10000	10000	100	100	100000	1000 x 1
0.17 ± 0.18	***13333 / 10000[2]***	***13333 / 10000[2]***	***100***	***133 / 100[2]***	***100000***	***1000 x 1***
0.58 ± 0.29	100	100	4	25	1000	250 x 1
5.09 ± 0.58	***13.3 / 10[2]***	***13.3 / 10[2]***	***5***	***2.66 / 2[2]***	***100***	***20 x 1***
5.36 ± 0.47	10	10	5	2	100	20 x 1
5.57 ± 1.05	10	10	0.1	100	100	1000 x 1
11.62 ± 0.80	***5.33 / 4[2]***	***5.33 / 4[2]***	***2***	***2.66 / 2[2]***	***40***	***20 x 1***
12.13 ± 0.87	4	4	2	2	40	20 x 1
40.56 ± 1.40	1	1	0.5	2	10	20 x 1
0.41 ± 0.25	100	1000	10	10	100000	100 x 100
2.94 ± 0.48	***13.3 / 10[2]***	***133 / 100[2]***	***1***	***13.3 / 10[2]***	***10000***	***100 x 100***
3.16 ± 0.62	10	1000	0.1	100	100000	1000 x 1000
3.17 ± 0.35	10	100	1	10	10000	100 x 100
27.71 ± 3.35	1	100	0.01	100	10000	1000 x 1000
28.32 ± 0.71	1	10	0.1	10	1000	100 x 100
238	*free molecular flow*					

Simulations with VS (variable spheres) scattering model [8] were performed as well. In VS model, the deflection angle cosine is not random but fixed. Changing this cosine allows balancing diffusion and viscosity. Fixed cosine yields the smallest possible σ_T. Deflection angle 109.47° and total cross-section $\frac{3}{4}\sigma_T$ were chosen to represent HS.

Table 1 shows clear correlation of error and $\overline{N_C} \cdot \mathrm{Kn}_C$. Criterion $\overline{N_\lambda}$ shows some interdependence with error as well, but non-universal. Oppositely, the $\overline{N_C}$ does not show any clear interdependence with error at all. Once can see, the VS model gives almost the same error as corresponding HS model, while the formal Knudsen number is 4/3 times higher. This shows the error depends on the scattering model as well.

Figure 1 is plotted by HS data from Table 1. It shows, that the error linearly depends on $\overline{N_C} \cdot \mathrm{Kn}_C$. The error is 40% less for 2D grid. The reason is, with the more dimensions available, particles are mixed better by random movement; because of larger cell boundary per cell volume, a collided pair leave a cell easier and separates faster.

One more series of simulations was performed with Kn_0=0.025 keeping the same wall temperatures. This time, the reference value of heat flux is 0.0986 +/- 0.18% (again, related to free molecular value). Lower Knudsen number

[2] First number is the true value for VS model, second number is the value for corresponding HS model.

is selected to flatten gradients and study the effect of cell size; it is close to [5], though using their small temperature factor would slow down statistical convergence 25 times. Figure 2 shows the dependence of error on $\overline{N_C} \cdot \mathrm{Kn}_C$ with different cell size. The dependence is linear at low $\overline{N_C} \cdot \mathrm{Kn}_C$ as well, and stabilizes on high $\overline{N_C} \cdot \mathrm{Kn}_C$, when the error is determined mostly by cell size. Comparing fitting curves, one can notice that dependence of error determined by cell size is close to the second order.

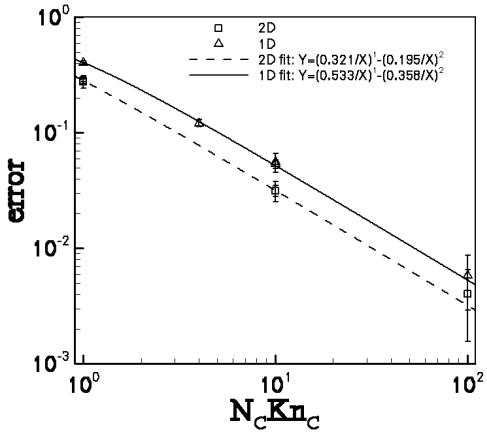

FIGURE 1. Heat flux error on different $\overline{N_C} \cdot \mathrm{Kn}_C$, in 1D and 2D cases. Kn_0=0.1.

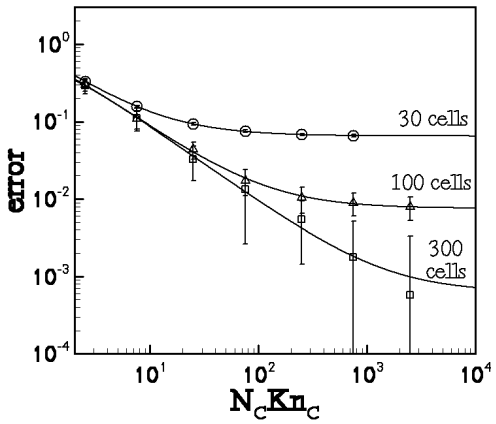

FIGURE 2. Dependence of heat flux error on $\overline{N_C} \cdot \mathrm{Kn}_C$. 1D grid, different cell size. Kn_0=0.025.

EFFECT OF TIME STEP AND CELL SIZE

Using equation (2), assuming the distortion of heat conductivity is small, considering theoretical [9] temperature gap near walls, one can solve Fourier problem analytically and predict the dependence of wall heat flux on the time step. Figure 3 shows both actual dependence for three collision grids and the prediction. The unit of time step is: $\lambda_0 / \sqrt{\frac{2k\sqrt{T_1 T_2}}{m}}$., where $\lambda_0 = \frac{1}{\sqrt{2} n_0 \sigma_T}$. The $\overline{N_c} \cdot \mathrm{Kn}_c$ values were chosen large enough to neglect its contribution to error. When time step is small, the error is determined mostly by cell size. With the increase of time step, it approaches the predicted quadratic curve, although it does not fit it perfectly.

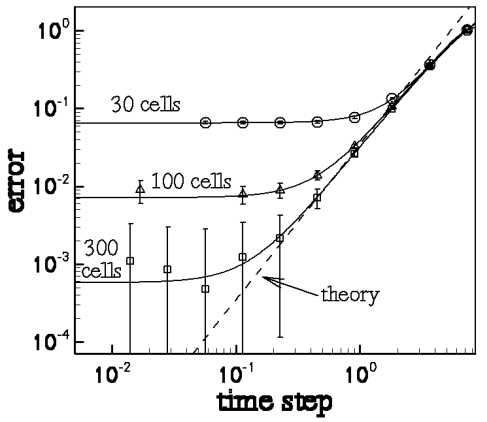

FIGURE 3. Effect of the time step size on different grids (actual points and fitting) for Kn_0=0.025 in comparison with the theoretical estimation.

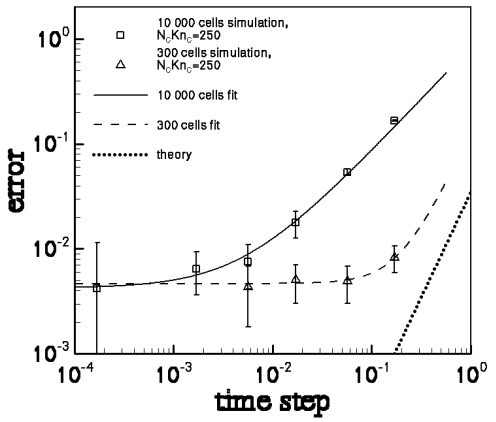

FIGURE 4. Comparison of time step determined error for 10 000 cell and 300 cell grids. Minimal error is determined by the limited $\overline{N_C} \cdot \mathrm{Kn}_C$ value.

Figure 4 shows the dependence of error on time step for two grids: 10 000 cells and 300 cells. With 10 000 total particles used, it gives $\overline{N_C} \sim 1$ and $\overline{N_C} \sim 33$ correspondingly. In both cases the spatial discretization error is negligible and the minimal error is determined by fixed $\overline{N_C} \cdot \mathrm{Kn}_C = 250$, therefore it is higher for 300 cells case than on previous figure. For 300 cells, the error is constant up to $\Delta t \sim 0.1$. In the case of 10 000 cells, the error increase linearly within a time step, starting at $\Delta t \gtrsim 0.0015$; for reference, $\Delta t_P \sim 0.0025$. This demonstrates the necessity of balancing the time step and cell size. While $\Delta t \ll \Delta t_P$, time step error dependence is quadratic. But in the case

$\Delta t \gg \Delta t_P$, the linear term might exceed the quadratic one. This effect is due to many collisions between rare movement phases. The effective pair lifetime becomes Δt instead of Δt_P, and repetitive collisions are more probable.

In Figure 4, one can note that error converges to the same value for both cases when time step is small. This confirms the absence of $\overline{N_C}$ effect. In contrary, the $1/\overline{N_C}$ term of equation (3) predicts ~8% deviation in heat conductivity with $\overline{N_C}\sim 1$. For comparison, the $\frac{\Delta\tilde{x}}{\overline{N_C}} = \frac{1}{\overline{N_C}\cdot \mathrm{Kn}_C}$ term predicts ~0.5% error that is close to experienced error of heat flux. Although the (3) is inapplicable at $\overline{N_C}\sim 1$, more likely, MFS outperforms NTC scheme on small $\overline{N_C}$. Nevertheless, $\frac{1}{\overline{N_C}\cdot \mathrm{Kn}_C}$ term exceeds $1/\overline{N_C}$ term if $\mathrm{Kn}_C < 14$. In practical range of $1 < \mathrm{Kn}_C < 10$, the $\overline{N_C}\cdot \mathrm{Kn}_C$ criterion is still more important for NTC scheme as well, with number of particles in a cell not needed to be especially planned. The 10 000 cells example above has $\mathrm{Kn}_C \sim 250 \gg 10$.

Figure 5 shows the dependence of error on cell size, summarizing 6 points acquired by polynomial fitting. Three of them are from time step dependence (Figure 3), and three from $\overline{N_C}\cdot \mathrm{Kn}_C$ dependence (Figure 2). The theoretical curve, based on equation (1) is shown as well. The cell size unit equals λ_0. Again, the fitting is good but not perfect, actual points are slightly under the theoretical curve.

One more interesting (3) term is: $\frac{\Delta\tilde{x}^2}{\overline{N_C}} = \frac{1}{\overline{N_C}\cdot \mathrm{Kn}_C{}^2}$, that is linear on a cell size if $\overline{N_C}\cdot \mathrm{Kn}_C$ is fixed. Corresponding $\frac{1}{\overline{N_C}\cdot \mathrm{Kn}_C}$ coefficients of fitting curves from Figure 2 actually fit straight line quite well, yielding $\ldots + \frac{0.908}{\overline{N_C}\cdot \mathrm{Kn}_C} - \frac{0.156}{\overline{N_C}\cdot \mathrm{Kn}_C{}^2} + \cdots$ terms in heat flux error, somewhat close to those in (3).

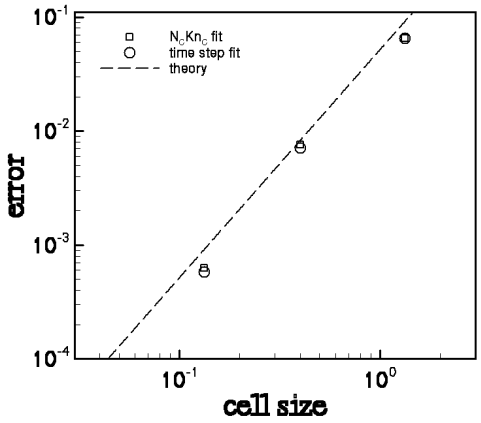

FIGURE 5. Actual heat flux error points for different cell sizes and theoretical curve.

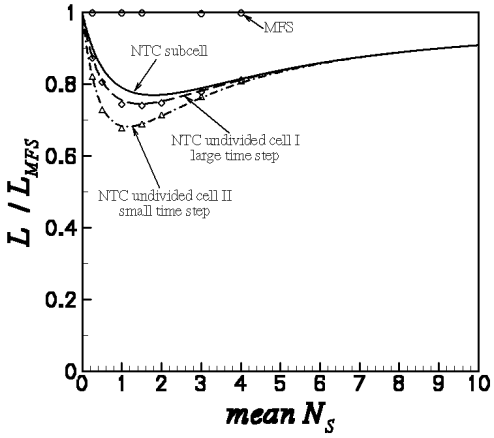

FIGURE 6. The comparison of the mean number of available collision partners in NTC scheme and MFS

POSSIBLE EFFECTS OF AVERAGE NUMBER OF PARTICLES IN A CELL

In the MFS, each time step the collision frequency is random, depending on the instantaneous number of particles in a cell N_C. Collisions tend to happen on greater N_C. NTC scheme conceptually assigns the known maximal per-particle collision frequency to each particle in a cell. One macroscopic parameter – the average density in a cell – must be known a-priori to calculate collision frequency in NTC scheme. As the per-particle collision frequency is independent on N_C, repetitive collisions are more probable on smaller N_C.

Now let consider a single cell for MFS and single subcell in NTC scheme and evaluate a mean number $\bar{L}$ of available collisional partners. With fewer available partners, repetitive collisions may be considered more probable. Let assume, the number of particles N_S in a cell (for MFS) or in each subcell (for NTC scheme) obeys Poisson distribution. For MFS scheme, the calculation is easy: $\bar{L}_{MFS} = \sum_{N_S} \frac{N_S(N_S-1)}{\overline{N_S}^2} \times (N_S - 1) \cdot \frac{\overline{N_S}^{N_S}}{N_S!} e^{-\overline{N_S}} = \overline{N_S} + 1$. For NTC, a set of cases should be considered: 1) $N_S = 0$, probability $p_0 = e^{-\overline{N_S}}$; 2) $N_S \geq 2$, number of collision partners $L_{N_S} = N_S - 1$, $p_{N_S} = \frac{\overline{N_S}^{N_S}}{N_S!} e^{-\overline{N_S}}$; 3) $N_S = 1$, no partners in adjacent subcells, $p_0{}' = \overline{N_S} e^{-\overline{N_S}} \cdot e^{-\overline{N_S}(S-1)}$, where S is a number of subcells in a composite cell; 4) $N_S = 1$, $p_1 = \overline{N_S} e^{-\overline{N_S}} \cdot \left(1 - e^{-\overline{N_S}(S-1)}\right)$, $L_1 = \frac{\overline{N_S}}{1-e^{-\overline{N_S}}}$. Summing it up: $\bar{L}_{NTC-I} = \sum_{N_S} \frac{\bar{M}+N_S}{\overline{N_S}} L_{N_S} p_{N_S} = \overline{N_S} + \frac{e^{-\overline{N_S}} + \overline{N_S} e^{\overline{N_S}(S-1)} - 1}{e^{\overline{N_S}S} - e^{\overline{N_S}(S-1)} - \overline{N_S}}$, here $\bar{M}$ is the average number of postponed collisions. The

derivation of these is omitted. If time step is small, N_S changes gradually and cannot be considered independent each time step. Thus, if subcell logic is not used ($S = 1$), postponed collisions tend to proceed when N_S switches from 1 to 2. For this case, assuming that all postponed collisions have a single partner, we get: $\bar{L}_{NTC-II} = \overline{N_S} + e^{-\overline{N_S}}$.

The dependence of $\bar{L}_{NTC}/\bar{L}_{MFS}$ ratio on $\overline{N_S}$ is plotted in Figure 6 for three cases: an NTC subcell of very large composite cell ($S \to \infty$) compared to the MFS cell of the same size as NTC subcell, and an undivided NTC cell ($S = 1$) versa equal volume MFS cell for both small and large time steps, together with actual points obtained in simulation. $\bar{L}_{NTC}/\bar{L}_{MFS} \to \frac{\overline{N_S}}{\overline{N_S}+1}$ on $\overline{N_S} \to \infty$ for all NTC cases. NTC scheme shows strictly lower $\bar{L}$ compared to MFS. It testifies that repetitive collisions are less likely to happen in MFS. Thus, in spite of no visible effect of $\overline{N_S}$ on a heat flux error in MFS simulations, some weak effect in NTC scheme may be still expected.

The second issue is the local density required in NTC scheme. Practically, the mean density is determined by averaging N_C. One needs to use a sort of iterative or convolution logic to keep good estimation of density before the steady state is reached. With small $\overline{N_C}$, average density converges slower. This elevates statistic and systematic errors in mean density, and, as a result, in collision frequency. That may explain the dependence on $\overline{N_C}$ found in [5]. MFS is free of this issue.

One more $\overline{N_C}$ issue is important for both NTC scheme and MFS: $(\sigma_T c_r)_{max}$. In practice $(\sigma_T c_r)_{max}$ is often not known a-priori, so some initial value is taken and then updated every time it is exceeded. Overestimating $(\sigma_T c_r)_{max}$ just slows down the simulation. But on underestimation, too few collision tests are performed each time step. Together with $\overline{N_C} \ll 2$ this slows down the convergence of $(\sigma_T c_r)_{max}$ enough to accumulate considerable systematic error through statistic accumulation period, just because collisional logic is skipped in the majority of time steps. The solution is to modify collision loop slightly: a collision pair is now selected as well as $(\sigma_T c_r)_{max}$ is updated before the necessity of individual collision test is decided. Thus, whenever collisions are possible ($N_C \geq 2$), at least one pair is selected to update $(\sigma_T c_r)_{max}$ even if the logic yields $\ll 1$ collision tests per time step.

CONCLUSION

The new universal criterion for a number of model particles for MFS is proposed and successfully verified on the example of 1D and 2D Fourier problem simulations. The weak effect of the number of particles in a cell is demonstrated by getting less than 30% heat flux error in simulations with as little as 0.01 particles in a cell. Second order convergence on the cell size and the time step is verified for MFS, similar to NTC scheme. MFS is proven to give more available collisional partners on average compared to NTC scheme.

ACKNOWLEDGMENTS

The present work was supported by the Russian Foundation for Basic Research (grant 09-01-92432), Federal program "Scientific and scientific-pedagogical personnel of innovating Russia for 2009-2013 years" (contract 02.740.11.0109).

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