Imitation Monte Carlo methods for problems of the Boltzmann equation with small Knudsen numbers, parallelizing algorithms with splitting

To cite this article: A I Khisamutdinov and N N Velker 2014 J. Phys.: Conf. Ser. 510 012021

You may also like
- Rapid detection of the authenticity of silver jewelry by laser induced shockwave plasma spectroscopy using Nd:YAG laser 1064 nm
  R W Septianti, W S Budi, H Sugito et al.
- Evolutionary game dynamics of combining the Moran and imitation processes
  Xian-Jia Wang, , Cui-Ling Gu et al.
- Predictability of imitative learning trajectories
  Paulo R A Campos and José F Fontanari

Recent citations
- Algorithms and Numerical Implementation of Imitation Monte Carlo Methods with Splitting for Problems of the Boltzmann Equation
  Alfred Khisamutdinov and Nikolay Velker
Imitation Monte Carlo methods for problems of the Boltzmann equation with small Knudsen numbers, parallelizing algorithms with splitting

A I Khisamutdinov¹,², N N Velker²
¹ Novosibirsk State University, 2 Pirogova Str., Novosibirsk, Russia
² A.A. Trofimuk Institute of Petroleum Geology and Geophysics SB RAS, 3 Akademika Koptyuga Prosp., Novosibirsk, Russia
E-mail: KhisamutdinovAI@ipgg.sbras.ru

Abstract. The talk examines a system of pairwise interaction particles, which models a rarefied gas in accordance with the nonlinear Boltzmann equation, the master equations of Markov evolution of this system and corresponding numerical Monte Carlo methods. Selection of some optimal method for simulation of rarefied gas dynamics depends on the spatial size of the gas flow domain. For problems with the Knudsen number $Kn$ of order unity “imitation”, or “continuous time”, Monte Carlo methods (²) are quite adequate and competitive. However if $Kn \leq 0.1$ (the large sizes), excessive punctuality, namely, the need to see all the pairs of particles in the latter, leads to a significant increase in computational cost (complexity). We are interested in to construct the optimal methods for Boltzmann equation problems with large enough spatial sizes of the flow. Speaking of the optimal, we mean that we are talking about algorithms for parallel computation to be implemented on high-performance multi-processor computers. The characteristic property of large systems is the weak dependence of sub-parts of each other at a sufficiently small time intervals. This property is taken into account in the approximate methods using various splittings of operator of corresponding master equations. In the paper, we develop the approximate method based on the splitting of the operator of master equations system “over groups of particles” (⁷). The essence of the method is that the system of particles is divided into spatial subparts which are modeled independently for small intervals of time, using the precise “imitation” method. The type of splitting used is different from other well-known type “over collisions and displacements”, which is an attribute of the known Direct simulation Monte Carlo methods. The second attribute of the last ones is the grid of the “interaction cells”, which is completely absent in the imitation methods. The main of talk is parallelization of the imitation algorithms with splitting using the MPI library. New constructed algorithms are applied to solve the problems: on propagation of the temperature discontinuity and on plane Poiseuille flow in the field of external forces. In particular, on the basis of numerical solutions, comparative estimates of the computational cost are given for all algorithms under consideration.

1. Introduction
The paper examines a system of pairwise interaction particles to model a rarefied gas in accordance with the nonlinear smoothed Boltzmann equation, the master equations of Markov evolution of this system and corresponding numerical Monte Carlo methods. Selection of an optimal simulation method of rarefied gas dynamics depends on the spatial size of the gas flow
domain. “Imitation“ or “continuous time“ Monte Carlo methods ([1, 2, 3, 4]) are quite adequate and competitive for problems with the Knudsen number $Kn \simeq 1$. However if $Kn < 0.1$ (the large sizes), excessive punctuality, namely, a need to see all the pairs of particles in the latter, leads to a significant increase of the computational cost (complexity). In this study we have been interested in developing optimal solution methods for the Boltzmann equations with spatial sizes of the flow that are large enough. Saying optimal, one has meant the algorithms for parallel computation should be implemented on high-performance multi-processor computers. The characteristic property of large systems is the weak dependence of its sub-parts on each other at a sufficiently small time intervals. This property is considered in the approximate methods using various splittings for the operator of the corresponding master equations. In the paper we have presented the approximate method based on the splitting of a master-equation-system operator “over groups of particles“ ([5, 6, 7]). The essence of the method is that the system of particles is divided into spatial subparts which are modeled “quasi“-independently for small intervals of time, using the precise imitation method. The type of splitting used is different from another well-known type “over collisions and displacements“ being an attribute of the known direct simulation Monte Carlo methods ([8, 9]). The second attribute of the last ones is a grid of “interaction cells“ that is completely absent in the imitation methods. The main issue this paper addresses to is parallelization of the imitation algorithms with splitting performed using MPI library. The new constructed algorithms have been applied to solve problems: on propagation of the temperature discontinuity and on the plane Poiseuille flow in external-force field both for cases with small $Kn$. In the paper we have also given some estimates of the computational cost for all the algorithms considered which are in agreement with numerical results.

2. Common construction and notations

Evolution of rarefied gas is simulated in a bounded connected domain $(V)$, $(V) \subset R^3$, with the piecewise smooth boundary $(\partial V)$. Translatory movement and pairwise elastic collisions are simulated for the gas particles. It is assumed that the boundary has been split into two nonintersecting subdomains $(\partial V_1)$ and $(\partial V_2)$. Particles may fly in and fly out of the surface $(\partial V_1)$ and reflect back to $(V)$ from $(\partial V_2)$ with account for the given boundary conditions. Particles flying out of $(V)$ do not return.

Here are some common designations:

$(\bar{V}) = (V) \cup (\partial V)$, $(G) = (V) \times R^3$, $(\bar{G}) = (V) \times R^3$; where $\|V\|$ is the volume of domain $(V)$; $N = N_1$ is the random number of particles in $(V)$ at the moment of time $t$, $t \geq 0$, $0 \leq N_1 < \infty$, $N$ is realization of $N$;

$(r^i, v^i), i = 1, \ldots, N$, are the particles' radius vectors and velocities;

$x^i = (r^i, v^i)$, $R = (r^1, \ldots, r^N)$, $V = (v^1, \ldots, v^N)$, $X \equiv X^{(N)} = (R, V) = (x^1, \ldots, x^N)$;

$\mathcal{P}_0 = \{N_t, X_t\}_{t=0}^{\infty}$ is the Markov jump process of gas-particle evolution with states in $S$;

$S = \bigcup_{N=0}^{\infty} S_N; S_N = N \times (\bar{G})^N$; $S_0$ - is the state when the domain $(\bar{V})$ does not contain particles; $\mu_i^{(N)}(X) = \mu_i^{(N)}(x^1, \ldots, x^N)$ are the phase densities of gas at the moment of time $t$ defined on $S$;

$p_i^{(N)}(t) \equiv p_i^{N}(t) = \int_{(\bar{G})^N} \mu_i^{(N)}(x^1, \ldots, x^N)dx^1 \ldots dx^N; p_0^{(0)}(t) \equiv p_0^0(t)$ is the probability that the domain $(\bar{V})$ does not contain particles at the moment of time $t$; $f(t, x)$ is the density of an average number of particles in a random process at the moment of time $t$; $\mathcal{N}_0 = \mathcal{M}(N_0) = \int f(0, x)dx = \bar{n}_0 \cdot \|V\|$; we note that the density $f(t, x)$ is an approximation to the solution of the smoothed Boltzmann equation; $E_r(x)$ is the given function measurable in $(G)$, $t^*$ is some given moment of time, $0 < t^* < \infty$; so that all considered functionals can be represented as $I_{t^*} = \int f(t^*, x) \cdot E_r(x)dx$.

Note, that if the integration domain is not specified, the integration is performed over $(\bar{G})$. 


3. Imitation methods

3.1. Algorithms of Imitation methods

Imitation, or “continuous time“, Monte Carlo method to model rarefied gas evolution has been proposed in ([1, 2]). In this method, gas evolution is considered as predetermined process $P_0$ with the following jumps: changing of velocities of a pair of particles due scattering; changing of the velocity and coordinates during flying out of a particle on the boundary ($\partial V_2$); changing of the number of particles in domain ($V$) as a result of flying out or flying in of a particle through the boundary ($\partial V_1$). The algorithm implementing this process was proposed, for example, in ([4]), and it will not be presented below. It should be noted only, that this algorithm has two distinctive features. First, it uses the well-known method of “fictitious collisions” for pair interactions modeling (see [10, 11]). Second, pair scattering frequency at arbitrary time depends on the relative velocity of the particles and the differences of their coordinates. In this paper one will refer to this algorithm as $A_0$.

Approximate simulation method, based on splitting the operator, corresponding to the exact master equations, “over groups of particles“ has been proposed in [5, 6]. This method is based on the idea stated in the introduction: if we divide the particle system into multiple spatial subparts, then particles from the different sub-parts will rarely interact with each other at short time intervals. This feature virtually allows to model evolution of gas in the sub-parts almost independently from each other. Simulation inside an arbitrary splitting intervalis carried out in two stages. At the first stage, gas evolution is modeled independently in each of the $K_{sub}$ groups, and modeling within a group is carried out the way is done for the process $P_0$. At the second stage, one performs correction for interaction of the particles that belong to different groups. The algorithm, implementing this method, has been presented in [7]. Its description is given below, and what will follow is the way of how to parallelize it.

(i) The time axis is split into intervals $[t_d-1, t_d)$ , $d = 1, 2, ..., M$. All the particles in the system are split into the $K_{sub}$ groups. Simulation of the evolution of rarefied gas inside each $d$-th interval is performed in two stages.

   (a) At the first stage, the evolution of gas is simulated independently in each group. Simulation is performed based on algorithm, implementing the process $P_0$.

   (b) The Simulation is considered as complete when the condition $t' \geq t_d$ for the current moment of time $t'$ is satisfied.

(ii) After the first stage is complete, the particles are redistributed by the new $K_{sub}$ groups. At the same time, the distribution of particles over old groups at the first stage is stored in the memory. Then, one starts the second stage of the simulation.

   (a) Value $t_{d-1}$ is selected as the initial (zero) jump at the $d$-th step, while all the coordinates and velocities of the particles are fixed at this moment of time in the same way as they were at the moment of time $t_d$ at the end of the first stage.

   (b) Gas evolution is modeled in each of the new groups independently as in the algorithm that implements the process $P_0$, but with account for two features:

   1. state of the system does not change between jumps (that means, that the particles remain stationary)

   2. only one type of jump (pair scattering) is considered, and the scattering may be physical only for the particles that have belonged to different groups at the first stage.

   (c) The second-stage simulation is considered complete when the condition $t' \geq t_d$ is satisfied for the current moment of time $t'$. At the same time, the distribution of particles by groups performed at the beginning of the second stage is used for the implementation of the first stage at the next $(d + 1)$-th step.

(iii) The trajectory is interrupted when the M-th step is complete.
3.2. Parallelization of the algorithm \( A_1 \)

The structure of the algorithm \( A_1 \) causes its natural parallelization. Its basic idea is that the simulation of particles evolution in each group at the first and second stage of an arbitrary step of splitting by time should be carried out on different processors of a multiprocessor device. One has used MPI library for the code implementation of this parallelism. The algorithm \( A_1^{\text{Par}} \) for parallel computation based on the algorithm \( A_1 \) is described below.

(i) The number of groups \( K_{\text{sub}} \) is chosen to be equal to the number of parallel processes. Paragraph 1 of the algorithm \( A_1 \) is implemented in parallel for all the processes. In each \( i \)-th process, \( i = 1, \ldots, K_{\text{sub}} \), the initial spatial energy and angular distribution has been given only for the particles that belong only to the \( i \)-th group.

(ii) Paragraphs 1.1 and 1.2 of the algorithm \( A_1 \) is implemented simultaneously in all processes. It should be noted, that since only the \( i \)-th group has been defined in the \( i \)-th process, it is equivalent to the simultaneous modeling of gas evolution in all the \( K_{\text{sub}} \) groups.

(iii) The particles, defined in each process, are sorted into two subgroups at the end of the first phase. The first subgroup includes the particles, which by the end of the first stage still belong to the group, corresponding to the process. The second subgroup includes the particles that have fallen into any of the other groups or taken off the system. For example, if a particle's belongs to the \( i \)-th group means it is located in some \( i \)-th spatial subdomain of the system. The division into subgroups in \( i \)-th group has been performed as follows: the particle belongs to the first subgroup, if it have not left the \( i \)-th subdomain at the end of the first stage; the particle belongs to the second subgroup, when it has flown out of the \( i \)-th subdomain.

(iv) Numbers and phase coordinates of the particle that belong to the second subgroup in each process, is forwarded to the processes of the respective groups to which they belong. Afterwards, they are included in the lists of new groups of particles, and the information about them in the old group is erased. Thus there has been an automatic redistribution of particles on the new \( K_{\text{sub}} \) groups, referred to the paragraph 2 of the algorithm \( A_1 \). Doing so, one should keep in mind, how the particles have been distributed in the old groups at the first stage.

(v) Paragraphs 2.1-2.3 of the algorithm \( A_1 \) is implemented in parallel in each of the processes.

(vi) Paragraph 3 of the algorithm \( A_1 \) is implemented in parallel in each of the processes.

4. Results of numerical modelling and analysis of computation costs

4.1. Problem of temperature discontinuity propagation

Algorithm \( A_1^{\text{Par}} \) has been applied to model a problem of temperature discontinuity propagation. Studying this issue has been conducted and reported in a number of papers, however, using of the algorithm \( A_1^{\text{Par}} \) has allowed us to consider the problem for the sufficiently small values of \( Kn \). In the problem monoatomic gas is placed in a halfspace \( z > 0 \) bounded by the plane \( z = 0 \). Diffuse reflection with temperature \( T_0 \) is realized on the plane. The gas is in equilibrium with the temperature \( T_0 \) and (numerical) density \( n_0 \) until to time \( t = 0 \); at \( t = 0 \), the temperature of the plane \( z = 0 \), changes abruptly from \( T_0 \) to \( 2 \cdot T_0 \) causing temperature discontinuity. Its propagation is studied further.

In the numerical simulation the evolution of the gas is regarded in a rectangular parallelepiped \( (V) : 0 \leq z \leq L, \quad -d_x \leq x \leq d_x, \quad -d_y \leq y \leq d_y \). The periodic conditions are set on the parallel to the axis \( OZ \) faces. Diffuse reflection is modeled on the face \( z = 0 \), with a temperature of \( 2 \cdot T_0 \). Departure and entry of particles in accordance with the equilibrium conditions of \( z = \infty \) are modeled on the face \( z = L \). Scattering of particles pairs is modeled following the law of hard spheres, and the scattering cross section is constant and equal to \( \sigma \). Dimensionless variables

25th IUPAP Conference on Computational Physics (CCP2013) IOP Publishing
Journal of Physics: Conference Series 510 (2014) 012021
doi:10.1088/1742-6596/510/1/012021
are used in the problem: $[L_0] = \frac{1}{\sqrt{2\pi n_0\sigma}}$ is the length unit (mean free path of equilibrium gas); $[v_0] = \sqrt{\frac{2kT_0}{m}}$ is the velocity unit; $[E_0] = kT_0$ is the energy unit. Here $n_0$ is the initial density of particles, $T_0$ is the initial temperature of the equilibrium gas, $m$ is the mass of a gas particle, $k$ - the Boltzmann constant. The parameters defining the lateral dimensions of the parallelepiped $(V)$ in terms of dimensionless quantities are: $d_x = d_y = 0.5$. Any two particles with the numbers $k$ and $l$ are considered interacting if the condition $|z_k - z_l| < 0.1$ is satisfied.

Modeling of temperature discontinuity propagation problem for $L = 20$ ($Kn = 0.05$) has been carried out to compare the algorithms $A_1$, $A_{\text{Par}1}$ and $A_0$. The initial density of particles is equal to 100. Figure 1. shows the calculated density profiles at times $t = 5$ and $t = 15$. The simulation has implemented six thousand trajectories. Standard statistical error of the calculated density is not more then 0.5%. From the figure you can see that the results of simulation are in agreement with each other within the statistical error specified. The same good agreement presents for graphs displaying such physical quantities as the longitudinal velocity, longitudinal and transverse components of temperature and heat flux.

**Figure 1.** Density profiles. The temperature discontinuity propagation problem, $L = 20$.

**Figure 2.** Velocity $v_z$ component profiles. The temperature discontinuity propagation problem, $L = 100$.

**Figure 3.** Temperature components profiles. The temperature discontinuity propagation problem, $L = 100$.

**Figure 4.** Heat flux $Q_z$ component profiles. The temperature discontinuity propagation problem, $L = 100$. 

$[v_0] = \sqrt{\frac{2kT_0}{m}}$ is the velocity unit; $[E_0] = kT_0$ is the energy unit. Here $n_0$ is the initial density of particles, $T_0$ is the initial temperature of the equilibrium gas, $m$ is the mass of a gas particle, $k$ - the Boltzmann constant. The parameters defining the lateral dimensions of the parallelepiped $(V)$ in terms of dimensionless quantities are: $d_x = d_y = 0.5$. Any two particles with the numbers $k$ and $l$ are considered interacting if the condition $|z_k - z_l| < 0.1$ is satisfied.

Modeling of temperature discontinuity propagation problem for $L = 20$ ($Kn = 0.05$) has been carried out to compare the algorithms $A_1$, $A_{\text{Par}1}$ and $A_0$. The initial density of particles is equal to 100. Figure 1. shows the calculated density profiles at times $t = 5$ and $t = 15$. The simulation has implemented six thousand trajectories. Standard statistical error of the calculated density is not more then 0.5%. From the figure you can see that the results of simulation are in agreement with each other within the statistical error specified. The same good agreement presents for graphs displaying such physical quantities as the longitudinal velocity, longitudinal and transverse components of temperature and heat flux.

**Figure 1.** Density profiles. The temperature discontinuity propagation problem, $L = 20$.

**Figure 2.** Velocity $v_z$ component profiles. The temperature discontinuity propagation problem, $L = 100$.

**Figure 3.** Temperature components profiles. The temperature discontinuity propagation problem, $L = 100$.

**Figure 4.** Heat flux $Q_z$ component profiles. The temperature discontinuity propagation problem, $L = 100$. 

$[v_0] = \sqrt{\frac{2kT_0}{m}}$ is the velocity unit; $[E_0] = kT_0$ is the energy unit. Here $n_0$ is the initial density of particles, $T_0$ is the initial temperature of the equilibrium gas, $m$ is the mass of a gas particle, $k$ - the Boltzmann constant. The parameters defining the lateral dimensions of the parallelepiped $(V)$ in terms of dimensionless quantities are: $d_x = d_y = 0.5$. Any two particles with the numbers $k$ and $l$ are considered interacting if the condition $|z_k - z_l| < 0.1$ is satisfied.

Modeling of temperature discontinuity propagation problem for $L = 20$ ($Kn = 0.05$) has been carried out to compare the algorithms $A_1$, $A_{\text{Par}1}$ and $A_0$. The initial density of particles is equal to 100. Figure 1. shows the calculated density profiles at times $t = 5$ and $t = 15$. The simulation has implemented six thousand trajectories. Standard statistical error of the calculated density is not more then 0.5%. From the figure you can see that the results of simulation are in agreement with each other within the statistical error specified. The same good agreement presents for graphs displaying such physical quantities as the longitudinal velocity, longitudinal and transverse components of temperature and heat flux.

**Figure 1.** Density profiles. The temperature discontinuity propagation problem, $L = 20$.

**Figure 2.** Velocity $v_z$ component profiles. The temperature discontinuity propagation problem, $L = 100$.

**Figure 3.** Temperature components profiles. The temperature discontinuity propagation problem, $L = 100$.

**Figure 4.** Heat flux $Q_z$ component profiles. The temperature discontinuity propagation problem, $L = 100$. 

$[v_0] = \sqrt{\frac{2kT_0}{m}}$ is the velocity unit; $[E_0] = kT_0$ is the energy unit. Here $n_0$ is the initial density of particles, $T_0$ is the initial temperature of the equilibrium gas, $m$ is the mass of a gas particle, $k$ - the Boltzmann constant. The parameters defining the lateral dimensions of the parallelepiped $(V)$ in terms of dimensionless quantities are: $d_x = d_y = 0.5$. Any two particles with the numbers $k$ and $l$ are considered interacting if the condition $|z_k - z_l| < 0.1$ is satisfied.

Modeling of temperature discontinuity propagation problem for $L = 20$ ($Kn = 0.05$) has been carried out to compare the algorithms $A_1$, $A_{\text{Par}1}$ and $A_0$. The initial density of particles is equal to 100. Figure 1. shows the calculated density profiles at times $t = 5$ and $t = 15$. The simulation has implemented six thousand trajectories. Standard statistical error of the calculated density is not more then 0.5%. From the figure you can see that the results of simulation are in agreement with each other within the statistical error specified. The same good agreement presents for graphs displaying such physical quantities as the longitudinal velocity, longitudinal and transverse components of temperature and heat flux.
The further series of calculations presented have been obtained for the same problem at $Kn = 0.01$. For the modeling the algorithm $A_{1}^{Par}$ has been obtained. Fig. 2, 3 and 4 show the average velocity (particle flow), the temperature components and the heat flux at various time instants. In total, the simulation has implemented six thousand trajectories. Standard statistical error has been not more then 2.2% for the velocity, 3.7% - for the temperature, 9% - for the heat flow.

**Figure 5.** The position of $v_z$ maximum at different time instants.

**Figure 6.** Energy flux through the surface $z = 0$. The temperature discontinuity propagation problem, $L = 100$.

These results show that the perturbation caused by the wall's temperature jump propagates with approximately constant speed. It can be best seen from the average velocity component $v_z$ behavior, demonstrated in Fig. 2. Fig. 5 shows the position of the $v_z$ maximum at different time instants. The figure shows that it is changing linearly with time, and its velocity is approximately $v_0 = 0.87$. The fig. 5 shows that in the region of the front temperature komponets’ inversion is present, indicating the non-uniform redistribution of the internal energy between the longitudinal and transverse degrees of freedom. The heat flux profiles, shown in Fig. 4 have prominent features near the heated wall and in the vicinity of the disturbance front. The flux $Q_z$ is decreasing with time, asymptotically tending toward zero, near the plane $z = 0$. The flow has a characteristic hump, in the vicinity of the front disturbance, moving with approximately constant velocity. The humps height is decreasing with time, while it is spreading. Fig. 6 demonstrates the time dependence of energy flux through the surface $z = 0$, computed in ([12]) using the BGK for times from the interval $[1, 10]$ and using the algorithm of $A_{1}^{Par}$ for times from the interval $[1, 100]$. It is clear From Fig. 6 that, as well as the heat flow, the flow of energy through the surface $z = 0$ is asymptotically approaching zero. The difference between the results obtained with BGK and $A_{1}^{Par}$ can be explained by the fact that BGK is an approximate method in contrast to the Monte Carlo ones.

4.2. **Comparison and estimating of the algorithms computation costs**

Fig. 7 shows the ratio of the computation costs for the $A_0$ and $A_1$ algorithms and for the $A_0$ and $A_{1}^{Par}$ algorithms depending on the number of splitting groups. The data are presented for the temperature discontinuity propagation problem with a typical size $L = 100$. The figure demonstrates that the algorithms $A_1$ and $A_{1}^{Par}$ have been more beneficial in terms of computation costs if compared with the algorithm $A_0$. In the case of $A_1$ the simulation is performed using a single processor. In the case when the $A_{1}^{Par}$ is applied the number of processors involved in the simulation is equal to $K_{sub}$. Saying computation costs one means product of
the algorithm implementation time and the dispersion of the corresponding method. In accord
with the theoretical ideas the numerical experiments have showed that all three methods under
consideration have close dispersions, so the ratio of computational costs is equivalent to the ratio
of implementation times.

\[
T_{A_1} = C \cdot \frac{n_0^2}{K_{sub}} \cdot (1 + O\left(\frac{1}{n_0}\right))
\] (1)

This estimate can be detailed, highlighting explicitly the member responsible for the
redistribution of particles on the new \(K_{sub}\) groups between the first and second stage of the
simulation.

**Figure 7.** The ratio of the computation costs for the \(A_0\) and \(A_1\) algorithms and for the \(A_0\) and
\(A_1^{Par}\) algorithms as a functions of the splitting groups number \(K_{sub}\). The temperature discontinuity
propagation problem, \(L = 100\)
Since the simulation of the evolution of the particles within the groups in the algorithm \( A_{1}^{\text{Par}} \) is implemented in parallel, rather than sequentially, as in the algorithm of \( A_1 \), then implementation of the first and second stages is reduced to \( K_{\text{sub}} \) times in this case. The estimate also contains a term that describes the exchange of information between the \( K_{\text{sub}} \) parallel processes between the first and second stage of the simulation. Each of \( K_{\text{sub}} \) parallel processes sends information about particles field out from the corresponding group to other \( K_{\text{sub}} - 1 \) processes. The number of such particles is proportional to \( n_0 \). Therefore the estimate for the \( T_{A_1}^{\text{Par}_1} \) should be written as:

\[
T_{A_1}^{\text{Par}_1} = C \cdot \frac{n_0^2}{K_{\text{sub}}} \cdot (1 + O(\frac{1}{n_0})) + C_1 \cdot K_{\text{sub}} \cdot n_0
\]  

(2)

(3)

It should be noted that constants \( C, C_1 \) and \( C_2 \) in (2) and (3) depend on the properties of multiprocessor system used for simulation. Data exchange in the algorithms \( A_1 \) and \( A_{1}^{\text{Par}} \) has been implemented in such a way, that \( C_1 > C_2 \) (it is possible, that \( C_1 \gg C_2 \) ). The formulas (2) and (3) are asymptotic expressions of the \( A_1 \) and \( A_{1}^{\text{Par}} \) realization times for large \( n_0 \) and for small and large values of \( K_{\text{sub}} \). If one neglects the remainder term \( O(\frac{1}{n_0}) \) in (2) and (3) and considers \( T_{A_1} \) and \( T_{A_{1}^{\text{Par}}} \) as functions of \( K_{\text{sub}} \), approximate estimates of the positions of the minima on \( K_{\text{sub}} \) can be obtained:

\[
K_{\text{sub}}^{A_1} = \sqrt{\frac{C \cdot n_0}{C_1}}, K_{\text{sub}}^{A_{1}^{\text{Par}}} = \sqrt{\frac{C \cdot n_0}{C_2}}
\]  

(4)

The minimum values of the expressions \( T_{A_1} \) and \( T_{A_{1}^{\text{Par}}} \) are, respectively:

\[
(T_{A_1})_{\text{min}} = 2 \cdot n_0 \cdot (C \cdot C_1 \cdot n_0)^{\frac{1}{2}}, (T_{A_{1}^{\text{Par}}} )_{\text{min}} = 2 \cdot n_0 \cdot (C \cdot C_2 \cdot n_0)^{\frac{1}{2}}
\]  

(5)

As follows from (4), \( K_{\text{sub}}^{A_1} > K_{\text{sub}}^{A_{1}^{\text{Par}}} \) under the condition \( n_0 > \frac{C_1^2}{CC_2} \). This condition is valid for sufficiently large \( n_0 \). Hence, the ratio of the implementation time minima should be written as:

\[
\frac{(T_{A_{1}^{\text{Par}}})_{\text{min}}}{(T_{A_1})_{\text{min}}} = \frac{C_2^{\frac{1}{2}}}{C_1^{\frac{1}{2}}}
\]  

(6)

The conclusions of the above analysis demonstrate good agreement with the curves in fig. 7. The similar computation costs behavior has been also got for the problem on plane Poiseuille flow in the field of external forces. In general, it has been obtained that the algorithm \( A_{1}^{\text{Par}} \) has good enough gain in the computational cost.

Algorithm \( A_{1}^{\text{Par}} \) does not contain any restrictions on the dimension of the problems. Volumes of the sub-parts in the method should not be small. Therefore, we suppose that the estimates and the conclusions retain their validity for the spatially multi-dimensional cases.

[1] Khisamutdinov A I 1985 Ob imitatsionnom metode Monte-Karlo dlya modelirovaniya dinamiki razrezhennykh gazov (On Imitation Method of Monte-Carlo for Simulation of Dynamics of Rarefied Gases) Preprint VTs SO AN SSSR 599.

[2] Khisamutdinov A I 1988 Imitatsionnoe statisticheskoe modelirovanie kineticheskogo uravneniya razrezhennykh gazov Dokl. Akad. Nauk SSSR 302 no.1 75-79.

[3] Khisamutdinov A I 2005 On some properties of Markov processes and Monte Carlo methods for inhomogeneous Boltzmann equation Russ. J. Numer. Anal. Math. Modelling 20 no.2 131-60.

[4] Khisamutdinov A I 2004 On development of Continuous Time Monte Carlo methods for problems of Boltzmann equation with external forces Transport. Theor. Stat. Phys. 33 No.1 69-89.
[5] Khisamutdinov A I 1989 Priblizhennyi metod statisticheskogo modelirovaniya, ispolzuemuyushchii slabuyu zavisimost' podchastei (Approximated Method of Static Simulation Using Weak Dependence of Subparts) Vopr. Korrekt. Zad. Anal. IM SO AN SSSR 154-60.

[6] Khisamutdinov A I 2000 On connection between “Continuous time” and “Direct simulation” Monte Carlo methods for Boltzmann equation and on some new approximate methods Monte Carlo Meth. and Appl. 6 No.4 323-40.

[7] Khisamutdinov A I and Velker N N 2012 On Reduction of Computational Cost of Imitation Monte Carlo Algorithms for Modeling Rarefied Gas Flows Math. Mod. and Comp. Simul. 4 No.2 187-202.

[8] Bird G A 1994 Molecular gas dynamics and the Direct Simulation of Gas Flows (Oxford: Clarendon Press).

[9] Belotserkovskii O M and Yanitskii V E 1975 The statistical method of particles in cells for the solution of problems of the dynamics of a rarefied gas Zh. Vychisl. Mat. Mat. Fiz. 15 No.5 1195-08 No.6 1553-67

[10] Koura K 1986 Null-collision technique in the direct-simulation Monte Carlo method Phys. Fluids. 29, No.11 3509-11.

[11] Khisamutdinov A I 2007 Statisticheskoe modelirovanie odnogo tipa par sluchainykh velichin s ispolzovaniem fiktivnykh skachkov (Statistic Simulation of Single Type of Pairs of Arbitrary Quantities Using Fictive Jumps) ZhVM i MF, 47 No.1 162-73.

[12] Aoki K, Sone Y, Nishino K and Sugimoto H 1991 Numerical Analysis of unsteady motion of a rarefied gas caused by sudden changes of wall temperature with special interest in the propagation of a discontinuity in the velocity distribution function Raref. Gas Dynam. 222-31.