UDC 519.6 10.23947/2587-8999-2018-2-1-9-16

On a computing test of an ideal non-interacting gas model *

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In the present paper the problem of non-interacting ideal gas kinetic model construction is considered. The direct simulation Monte Carlo method was used for the problem solution. Results of statistical estimates derived from numerical simulation were presented. These results were compared with the analytic solution. Numerical error depending on particles and computing experiments were researched.

Keywords: Monte Carlo method; Euler's gas; Liouville's equation

Introduction. The paper is devoted to the study of a numerical method related to modeling the features of gas flow in transport problems for dynamical systems consisting of noninteracting particles [1, 5]. Such problems include the description of focusing areas and cumulative phenomena in the dynamics of a photon gas, neutrons, and so on. [3].

The aim of the paper is to construct an ideal gas model using the Monte Carlo direct statistical simulation method and to study statistical estimates of macroscopic gas parameters in an elementary volume.

Kinetic model of gas dynamics. The basis of the kinetic model is a dynamical system consisting of a statistically large number of particles. The motion of noninteracting gas particles can be described using the Liouville's equation written in vector form:

$$\frac{\partial f_i(t,x)}{\partial t} + v_i \frac{\partial f_i(t,x)}{\partial x} = 0, \quad (1)$$

where $f(t,x)$ is the distribution function of *i*-th group of particles; v_i is the speed of *i*-th group of particles; *x* are the coordinates of the motion of particles; *t* is the time.

Since the initial state of the system is unknown, $f(t,x,v)$ is introduced *N* is a partial distribution function. Despite the fact that the state of such a system displays a curve in 6*N* is the dimensional phase of Γ-space, from the point of view of the study of the dynamic system as a whole or part of it, macroscopic parameters such as density, pressure, temperature are most interesting.

*The research is done with the financial support from Russian Foundation for Basic Research, the grants № 15-41-00013, № 15-41-00059

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Below is a description of the mean values of macroscopic parameters and statistical estimates of the density (2), the mass (hydrodynamic) velocity (3), and the internal energy of a unit of gas mass (4), temperature (5), and pressure (6).

$$\rho(t,x) = \int_{R_3} f dv, \hat{\rho}(t,x) = \frac{1}{NV} \sum_{j:x_j \in D(h)}^{N} m_j, \tag{2}$$

$$\bar{v}(t,x) = \frac{1}{\rho} \int_{R_3} v f dv, \bar{v}(t,x) \cong \begin{cases} 1/(\hat{\rho} NV) \sum_{j:x_j \in D(h)}^{N} v_j, & \hat{\rho} > 0, \\ 0, & \hat{\rho} = 0, \end{cases} \tag{3}$$

$$e(t,x) = \frac{1}{2\rho} \int_{R_3} (v - \bar{v})^2 f dv, \; e(t,x) = \frac{1}{2N} \sum_{k=1}^{3} \left[\sum_{j:x_j \in D(h)}^{N} (v_j^k)^2 - \frac{1}{N} \left(\sum_{j:x_j \in D(h)}^{N} v_j^k \right)^2 \right], \tag{4}$$

$$T(t,x) = \frac{2}{3R} e, \tag{5}$$

$$p(t,x) = \frac{1}{3} \int_{R_3} (v - \bar{v})^2 f dv, \; p(t,x) = \frac{2}{3} \hat{\rho} e, \tag{6}$$

where V is a measure of elementary volume; $D(h)$ is an elementary volume; m_j is a mass of j-th particle; v_j is a speed of j-th particle; $R=8,314459(84)$ is s the universal gas constant. From equations (2)-(6) follows the standard Clapeyron-Mendeleev relation for an ideal gas ($p = R\rho T$).

Estimation of errors in macroscopic parameters. One of the main advantages of stochastic calculation methods is due to the fact that it is possible to estimate the statistical error, i.e. In the course of the calculation, it is possible to calculate not only the average values, but also the variance. The statistical error decreases very slowly in comparison with other numerical methods. At the same time, it is impossible to compare certain influences of small effects on two reports [2, 4]. The error in the obtained statistical estimates of macroscopic parameters (hereinafter macroscopic parameters) can be estimated in the following ways.

Estimation of errors in modeling independent stories. The confidence interval is $(\hat{\mu} - \delta, \hat{\mu} + \delta)$, in which the true value is found μ random variable ξ , distributed according to the normal law, with a given probability P, is defined as follows:

$$P\left\{ \left| \frac{1}{n} \sum_{i=1}^{n} x_i - \mu \right|, \leq \frac{3\hat{s}}{\sqrt{n}} \right\} \approx 0,9975, \tag{7}$$

$$\hat{\mu} = \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i, \tag{8}$$

$$\hat{s}^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left(x_i - \bar{x} \right)^2, \tag{9}$$

where $\hat{\mu}$ is the expected value $M\xi$; n is the independent stories (number of tests); x_i is an unknown values obtained as a result of testing; $\hat{S}$ is the unbiased variance estimate $D\xi$. Thus, it can be argued that a random variable ξ will not deviate from the mathematical expectation $\hat{\mu}$ in absolute value more than 3σ with probability 0,9975 (the rule of three sigma).

Statistical fluctuation is the estimation of the error in the oscillation of macroscopic parameters, which is determined by the following expression:

$$\frac{\sqrt{\langle (\Delta F)^2 \rangle}}{\langle F \rangle} \sim \frac{1}{\sqrt{L}}, \tag{10}$$

where F is a macroscopic quantity; L *i*s the number of particles in an elementary volume.

Comparison of numerical results with analytical ones. In the case when there is an analytical solution for the problem, the accuracy of the numerical solution of macroscopic parameters, one can estimate the maximum absolute ΔF and relative δF error:

$$\Delta F = \max_t |F_{num} - F_{an}| \qquad \delta F = \frac{\Delta F}{|F_{an}|} \cdot 100\% \tag{11}$$

where F_{num} is the numerical value; F_{an} is the analytical value; $t \in [0;T]$ is the time interval.

The dynamic model of the Euler's gas motion. Let us consider an example of particles moving in opposite directions, in which the distributional density functions are determined by the following relations [3]:

$$\begin{cases} f_1(x,t) = \rho_0(1-\theta(x-v_1 t)) \\ f_2(x,t) = \rho_0\theta(x-v_2 t) \end{cases}, \tag{12}$$

where $p_0 = const > 0$ is the initial density; $\theta(x)$ is the Heaviside's function; $v_1 = v_0 \geq 0$ is the velocity of the particle; $v_2 = -v_0 \leq 0$ is the velocity of the particle.

Then the macroscopic quantities of the analytical solution for the Euler's model have the following form:

$$v(x,t) = \begin{cases} 0, & |x| \leq v_0 t, \\ -v_0, & x > v_0 t, \\ v_0, & x < -v_0 t, \end{cases} \tag{13}$$

$$\rho(x,t) = \begin{cases} 2\rho_0, & |x| \leq v_0 t, \\ \rho_0, & |x| > v_0 t, \end{cases} \tag{14}$$

$$T(x,t) = \begin{cases} v_0^2/(3R), & |x| \leq v_0 t, \\ 0, & |x| > v_0 t. \end{cases} \tag{15}$$

The numerical model. An algorithm designed to simulate the dynamics of an ideal gas consists of the following steps: 1) setting the initial conditions; 2) calculation of the new particle

location; 3) calculation of macroscopic parameters; 4) preservation of intermediate results; 5) check the exit condition.

Step 1. Initialization of the initial conditions (figure 1) includes specifying the parameters of particles, elementary volume and time step Δt. The initial location of the particles is determined randomly with a uniform distribution law on the interval $(-5;5)$. The particle velocity modulus is 1, the direction vector is determined by formula (12). Elementary volume is installed in the center, its size is equal to $[1;1]$.

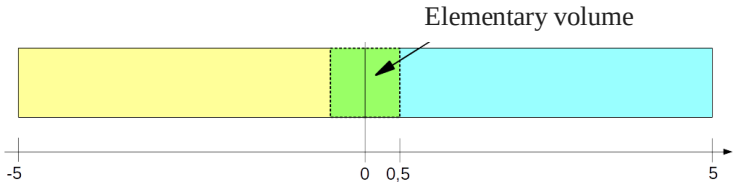

Fig. 1. Computational scheme

Step 2: Calculate a new location *i*-th particle is determined by the following iteration formula written in the vector form:

$$q_i^{(k+1)} = q_i^{(k)} + v_i^{(k)} \Delta t, \tag{16}$$

where *k* is the iteration number; $q_i^{(k)}$ is the coordinates *i*-th in the previous step; $v_i^{(k)}$ is the speed *i*-th particle; Δt is the time step.

For this task, setting boundaries and boundary conditions is not required.

Step 3. Calculation of macroscopic parameters in an elementary volume is based on formulas (2)-(6). The size of the elementary volume must be chosen in accordance with the distance that the particle overcomes in one iteration ($\Delta x \leq | v_0 | \Delta t$).

Step 4. Save the intermediate results. In order to save computing resources, writing to a file is carried out through a special accumulation buffer, which allows you to write in large blocks at a time, while saving space in RAM during long calculations.

Step 5. At the last step, the exit condition is checked. Steps 2-4 are one step in time Δt. Before the end of the program, the accumulated information is written from the buffer to the file for further processing.

In order to improve efficiency, the sequential algorithm written in C language has been adapted with OpenMP and MPI technologies for high-performance computing systems with traditional architecture. Computational calculations were carried out on a single computing node with a classic processor Intel XEON CPU E5-2690 V2 and 32 GB of RAM.

The results of modeling. Fig. 2 and 3 show the comparison of the numerical simulation results with the analytical solution. It can be seen from the graphs that the statistical estimates of the

macroscopic parameters of a gas approach the analytic values with an increase in the number of particles (velocity $v_0 = 1$, the density $\rho_0 = 0{,}1$ and temperature $\tau \approx 0,0400908$).

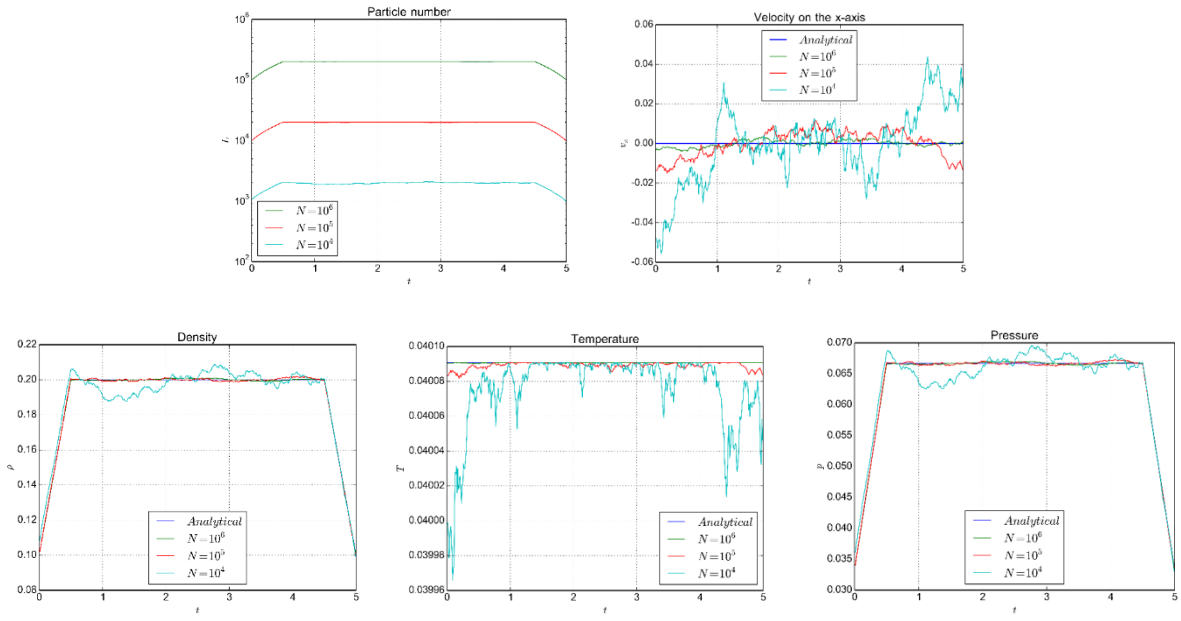

Fig. 2. Comparison of the macroscopic parameters of the Euler's gas model of numerical simulation at $\Delta t = 0{,}01$ with analytical solutions for a different number of particles

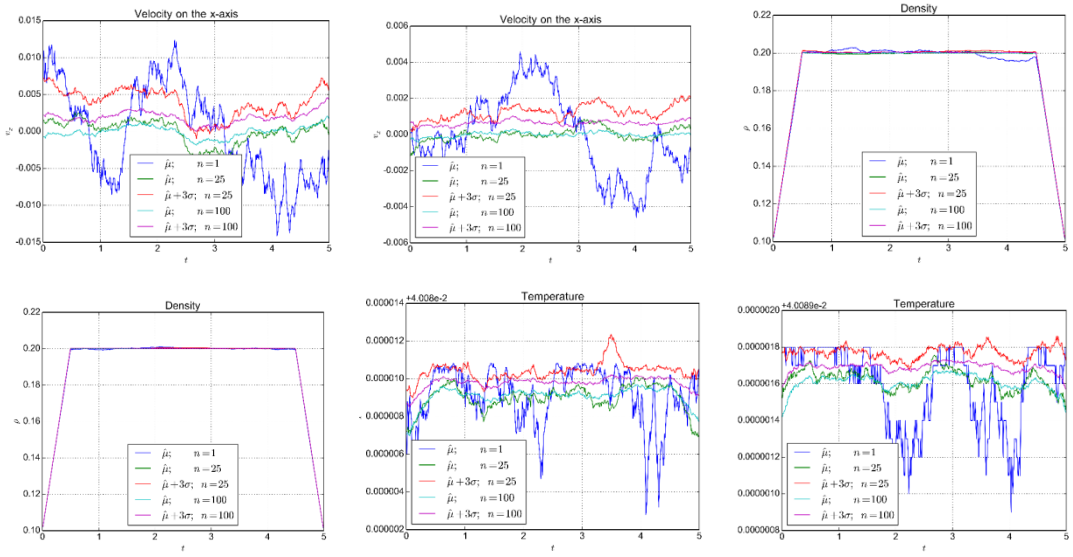

Fig. 3. Comparison of the macroscopic parameters of the Euler'sgas model of numerical simulation for Δt=0,01 with analytical solutions for a different number of stories: on the left $N=10^5$; on the right $N=10^6$.

Table 1 shows the errors of macroscopic parameters obtained as a result of modeling for a different number of particles.

Table 1. Maximum absolute and relative errors for a different number of particles

N	Δv	$\Delta\rho$	ΔT	Δp	$\delta\rho$	δT	δp
10^3	$1{,}89\cdot10^{-1}$	$3{,}20\cdot10^{-2}$	$1{,}44\cdot10^{-3}$	$1{,}01\cdot10^{-2}$	$1{,}60\cdot10^{1}$	3,59	$1{,}51\cdot10^{1}$
10^4	$5{,}58\cdot10^{-2}$	$1{,}22\cdot10^{-2}$	$1{,}25\cdot10^{-4}$	$4{,}10\cdot10^{-3}$	7,27	$3{,}12\cdot10^{-1}$	7,01
10^5	$1{,}50\cdot10^{-2}$	$1{,}98\cdot10^{-3}$	$9{,}00\cdot10^{-6}$	$6{,}60\cdot10^{-4}$	1,38	$2{,}24\cdot10^{-2}$	1,40
10^6	$3{,}91\cdot10^{-3}$	$1{,}00\cdot10^{-3}$	$5{,}98\cdot10^{-7}$	$3{,}34\cdot10^{-4}$	$5{,}01\cdot10^{-1}$	$1{,}49\cdot10^{-3}$	$5{,}01\cdot10^{-1}$

To compare the accuracy of macroscopic parameters based on $\hat{\mu}$ and $\hat{s}$, i.e. c with a different number of tests n, with the analytical solution, the formula (11) for the absolute error is modified as follows:

$$\Delta F' = \max_t[|\hat{\mu} - F_{an}| + \delta], \tag{17}$$

where $\delta = 3\hat{s}/\sqrt{n}$ is the error, depending on the number of tests.

Table 2 presents the results of absolute and relative errors obtained by modeling a different number of particles and the number of stories. When comparing the number of particles with the number of histories, it is seen that with an increase in the number of particles by a factor of 10 in one test is equivalent to an increase in the number of stories by a factor of 100.

Table 2. Maximum absolute and relative errors for a different number of particles and stories

N	n	Δv	$\Delta\rho$	ΔT	Δp	$\delta\rho$	δT	δp
10^5	1	$1{,}41\cdot10^{-2}$	$4{,}56\cdot10^{-3}$	$8{,}00\cdot10^{-6}$	$1{,}52\cdot10^{-3}$	2,28	$2{,}00\cdot10^{-2}$	2,28
10^5	25	$4{,}01\cdot10^{-3}$	$6{,}72\cdot10^{-4}$	$3{,}89\cdot10^{-6}$	$2{,}21\cdot10^{-4}$	$5{,}03\cdot10^{-1}$	$9{,}69\cdot10^{-3}$	$4{,}93\cdot10^{-1}$
10^5	100	$2{,}09\cdot10^{-3}$	$4{,}00\cdot10^{-4}$	$3{,}82\cdot10^{-6}$	$1{,}31\cdot10^{-4}$	$2{,}82\cdot10^{-1}$	$9{,}53\cdot10^{-3}$	$2{,}73\cdot10^{-1}$
10^6	1	$4{,}60\cdot10^{-3}$	$1{,}01\cdot10^{-3}$	$8{,}98\cdot10^{-7}$	$3{,}37\cdot10^{-4}$	$5{,}07\cdot10^{-1}$	$2{,}24\cdot10^{-3}$	$5{,}06\cdot10^{-1}$
10^6	25	$1{,}16\cdot10^{-3}$	$3{,}46\cdot10^{-4}$	$3{,}38\cdot10^{-7}$	$1{,}16\cdot10^{-4}$	$2{,}25\cdot10^{-1}$	$8{,}44\cdot10^{-4}$	$2{,}26\cdot10^{-1}$
10^6	100	$4{,}19\cdot10^{-4}$	$2{,}32\cdot10^{-4}$	$3{,}77\cdot10^{-7}$	$7{,}71\cdot10^{-5}$	$2{,}08\cdot10^{-1}$	$9{,}41\cdot10^{-4}$	$2{,}07\cdot10^{-1}$

As a result, it turns out that it is more economical to build a model with a large number of particles than to conduct many repeated tests.

Conclusion. A detailed description of the construction of an ideal gas model consisting of noninteracting particles is presented. A software package was developed for numerical modeling of the dynamics of an ideal gas, which makes it possible to calculate statistical estimates of macroscopic parameters in elementary volumes. The implemented algorithm, which is the basis of the software package, allows to perform calculations on high-performance computing systems. A series of computational experiments was performed and an estimate of the accuracy of the results obtained was presented, while the numerical solution was compared with the known analytical solution.

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УДК 519.6

О вычислительном тесте для одной модели бесстолкновительного идеального газа *

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Рассматривается задача о построении кинетической модели идеального бесстолкновительного газа. Для решения задачи используется метод прямого статистического моделирования Монте-Карло. Представлены результаты статистических оценок макроскопических параметров, полученные в результате численного моделирования, проведено их сравнение с известным аналитическим решением. Исследована зависимость погрешности полученных результатов от числа частиц и количества испытаний

Ключевые слова: метод Монте-Карло; газ Эйлера; уравнение Лиувилля

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* Работа выполнена при поддержке РФФИ, гранты: № 15-41-00013, № 15-41-00059.

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