Kinetic Methods for Solving Unsteady Problems with Jet Flows

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The article presents a comparison of numerical solutions obtained by the model equations (S-model and ES-model) and the complete Boltzmann equation for the unsteady problem of gas flow in a low-pressure tank after reflection from the wall. The weak influence of the collision operator on the solution in the rarefied domain and the need to use a detailed velocity grid due to the presence of the "ray effect" are shown on the basis of numerical analysis of auxiliary problems. To reduce computational costs, a hybrid method based on the synthesis of the model and Boltzmann equations is proposed.

**Keywords:** rarefied gas, Boltzmann equation, model equations, Ellipsoidal Statistical model, Shakhov model

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**Introduction**

At present there is a large number of studies devoted to the jet flows. The development of micro and nano-electromechanical systems (MEMS / NEMS), the creation of installations for pulsed jets used in the application of thin films and special coatings on solid surfaces increase interest to this problem. The results of numerical calculations of stationary jet flows in various formulations and rarefaction regimes are fairly fully represented in the literature, for example, in [1–7].

The problems of unsteady gas outflow into the region of strong rarefaction are characterized by both a variety of flow geometry and the large computational complexity. Numerical solutions associated with unsteady gas outflow from microchannels into vacuum are presented in [8-10]. The laser ablation problems were studied in [11] and other publications by A. Morozov.

The present article is a supplement to the study [12], devoted to the research of unsteady gas flow, reflected from the wall and flowing through a suddenly formed gap. The physical aspects
of this formulation were considered in [12], and the effect of gas outflow into a vacuum tank on the velocity of a shock wave front through a channel is shown.

The purpose of this article is to analyze possible numerical approaches for solving such non-stationary problems and identify the difficulties encountered in their calculations.

Since it is necessary to use the Boltzmann kinetic equation (BE) for modeling strongly nonequilibrium processes, the numerical implementation of which is quite time-consuming, it is important to have alternative more economical approaches, for example, using model kinetic equations. Thus, we estimate the difference between the numerical solutions of the model equations and the BE. To reduce the computational cost, we propose a hybrid method based on the synthesis of a model equation and the Boltzmann one, which makes it possible to reduce the computational domain of the complete collision integral. The results presented in this paper were obtained using two different software packages Unified Flow Solver (UFS) [13] and Nesvetay 3D [14-15]. Note that UFS uses the discrete ordinate method with uniform grid in velocity space and a hierarchical adaptive refinement grid in physical space. The possibilities of calculating both the complete Boltzmann equation and the model equations are realized. The Nesvetay3D complex was created to solve the model equation of E.M. Shakhov (S-model) and allows to perform calculations on unstructured non-uniform grids, both in velocity and physical spaces.

1. Statement of the problem

The problem is considered in 2D geometry, representing a long flat channel and a reservoir of infinite capacity, separated from the channel by a thin vertical plate (Fig. 1).

It is assumed that gas enters the channel from the left with the specified macroparameters: pressure $p_0$, density $\rho_0$ and velocity vector $\mathbf{u}_0 = (u_{0x}, 0)$. Initially gas at rest ($\mathbf{u}_1 = 0, p_1 \ll p_0$) is to the right of the plate and it is assumed that the gas temperatures in both regions are equal $T_0 = T_1$.

At the moment $t = 0$, the diaphragm opens, forming a hole of width $2d$, and the gas begins to flow into the rarefied domain. In this case, the gas moving in the channel is mixed with the reflected gas from the channel end (vertical wall).

![Fig. 1. The geometry of the flow (the upper half-plane)](image)
The channel and the tank with a rarefied gas are assumed to be symmetrical with respect to the \(x\)-axis, therefore the problem is considered only in the upper half-plane with symmetry conditions.

The laws of reflection from a vertical plate, both in the channel (left) and in the tank (right), are completely diffuse with the Maxwell distribution function.

At the upper boundary of the channel the mirror reflection condition is set. The velocity distribution functions of particles entering into the tank at the upper and right boundaries are Maxwellian distributions with the parameters of the background gas. The unsteady flow, obtained as a result of the discontinuity of the initial gas states, the reflection from the channel end and the gas outflow through the slit are investigated. The gas is assumed to be monatomic with particle interaction law according to the model of hard spheres.

Despite the rather simple geometry of the problem, the numerical implementation by the method of discrete ordinates turns out to be rather laborious. This is because of the need to use a very detailed grid in velocity space. It should be noted that a small velocity step is necessary to obtain smooth macroparameters in the region of strong rarefaction, where the flow is close to the free molecular. Such a flow regime is realized if the Knudsen number of the gas, entering the channel, is not very small. The insufficiently detailed velocity grid leads to nonphysical oscillations of macroparameters due to the "ray effect"[16, 17] caused by the discontinuity of the distribution function at the reservoir inlet. Carrying out numerical calculations of the complete BE on a very fine velocity grid is quite time consuming, so, the application of the model equations and the estimation of the possible errors of model equations are important.

2. Kinetic equations

In the numerical implementation the Boltzmann kinetic equation is used without taking into account the action of the force in the form [18]:

\[
\frac{\partial f}{\partial t} + \nabla_r \cdot (\xi f) = I(f, f),
\]

where \(f(r, \xi, t)\) is the velocity distribution function, depending on the spatial vector \(r = (x, y, z)\), velocity vector \(\xi = (\xi_x, \xi_y, \xi_z)\) and time \(t\). The collision integral \(I(f, f)\) for elastic collisions of a monatomic one component gas in the classical formulation is written as follows (the dependence on \(r\) and \(t\) is omitted):

\[
I(f, f) = \int_{\mathbb{R}^3} \int_0^\infty \int_0^{2\pi} \left( f(\xi_1) f(\xi') - f(\xi) f(\bar{\xi}) \right) |g| \cdot d\rho d\delta d\xi_1.
\]

Here \((\xi, \xi_1)\) are the velocities of the particles before the collisions, \((\xi', \xi_1)\) are the velocities past the collisions, related by the conservation laws of momentum and energy, \(g = \xi - \xi_1\) is the vector of the relative velocity of the colliding particles, \(b\) and \(\varepsilon\) are the parameters of the collisions. For the model of hard spheres, the parameter \(b\) is related to the particle scattering angle \(\chi\) by the formula \(b = d_M \cos(\chi/2)\), where \(d_M\) is the diameter of the molecules.
Using the distribution function the macroscopic variables such as particle number density $n$, average velocity $\mathbf{u}$, temperature $T$, stress tensor components $P_{ij}$, heat flux vector $\mathbf{q}$, pressure $p$ and nonequilibrium stress tensor components $p_{ij}$ are defined as follows:

$$
n = \int f d\xi, \quad \mathbf{u} = \frac{1}{n} \int \xi f d\xi, \quad T = \frac{m}{3k_B n} \int c^2 f d\xi,$$

$$
P_{ij} = m \int c_i c_j f d\xi, \quad \mathbf{q} = \frac{m}{2} \int c^2 c f d\xi, \quad p = \frac{1}{3} (P_{11} + P_{22} + P_{33}),$$

$$
p_{ij} = P_{ij} - p,$$

where $c = \xi - \mathbf{u}$, $m$, $k_B$ are the vector of relative velocity of the particles, molecular mass, and the Boltzmann constant, respectively. The subscripts $i$ and $j$ take values from 1 to 3 and denote the corresponding components along the $x$, $y$, $z$ axes.

Along with the full BE, model equations are used, the general form of which is

$$
\frac{\partial f}{\partial t} + \nabla_r \cdot (\xi f) = \nu (F^+ - f).
$$

In the case of the Shakhov model (S-models) [19]

$$
F^+ = F_M(n, \mathbf{u}, T) (1 + \frac{2m}{5pk_BT} (1 - Pr) \mathbf{q} \cdot \mathbf{c} \frac{mc^2}{2k_BT} \frac{5}{2}),
$$

where $F_M(n, \mathbf{u}, T) = n \left( m/(2\pi k_BT) \right)^{3/2} \exp(-mc^2/2k_BT)$ is Maxwellian, $Pr$ is Prandtl number and $\nu = p/\mu$ is collision frequency depending on viscosity $\mu$ and pressure $p$. In the case of ellipsoidal statistical model (ES-model) [20] $F^+$ and collision frequency $\nu$ are as follows:

$$
F^+ = \frac{n}{\sqrt{\det(2\pi \mathbf{T})}} \exp\left(-\frac{1}{2} \mathbf{c} \mathbf{T}^{-1} \mathbf{c} \right), \nu = \frac{p}{(1 - \lambda_{ES}) \mu}.
$$

Here $\mathbf{T}$ is the tensor expressed in terms of temperature $T$ and pressure tensor $\mathbf{P}$ according to the formula,

$$
\mathbf{T} = (1 - \lambda_{ES})RTI + \lambda_{ES} \mathbf{P}/\rho,
$$

where $\rho$ is density, $R$ is gas constant, $I$ is unit tensor, and parameter $\lambda_{ES} = \frac{Pr - 1}{Pr}$ takes values from -0.5 to 1.

Dimensionless quantities are normalized to a characteristic scale of length, temperature, density and velocity, which respectively are slit half-width $d$, temperature $T_\infty$, density $\rho_\infty$, and the maximum possible molecular velocity $u_p = \sqrt{2k_BT_\infty/m}$. Heat flux, pressure and viscosity coefficient are normalized on $\rho_\infty u_p^3/2$, $\rho_\infty u_p^2/2$ and $\mu_\infty = \mu(T_\infty)$, respectively. The characteristic time scale is assumed to be equal $d/u_p$. The introduction of dimensionless parameters into model equations and to the BE leads to the parameter $\delta = p_\infty d/(u_p \mu_\infty)$, and the Knudsen number $Kn = \frac{\lambda_\infty}{d} = \frac{8}{5\sqrt{\pi}\delta}$, respectively. Where the free path length $\lambda_\infty$ and viscosity are related by the law of the hard sphere model $\mu_\infty = \frac{5}{16} mn_\infty \sqrt{2\pi k_BT_\infty/m \lambda_\infty}$.  

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In the numerical implementation a velocity grid bounded by a sphere is introduced. The radius of the sphere is defined as \( r = \max(|u| \pm 3\sqrt{T}) \), where \( u \) and \( T \) are the dimensionless values of the velocity vector and temperature in the flow. Since the problem under consideration is two-dimensional, the velocity grid for calculations based on BE is set on half the sphere. The model equations in the UFS are replaced by a system of reduced equations for functions averaged on \( \xi_z \),

\[
  f_0(\xi_x, \xi_y) = \int f(\xi_x, \xi_y, \xi_z)d\xi_z, \quad f_1(\xi_x, \xi_y) = \int \xi_z^2 f(\xi_x, \xi_y, \xi_z)d\xi_z.
\]

When calculating the software complex Nesvetay 3D a three-dimensional velocity grid is used.

### 3. Numerical analysis of auxiliary problems

Initially, two auxiliary simpler problems are considered: the flow of reflected gas from the vertical wall and gas outflow from the slit into the rarefied domain.

In the first problem, the channel is assumed to be closed from one (right) end. The gas enters the channel with given flow parameters \( p_0 = 1, \rho_0 = 1, u_{x0} = 2, u_{y0} = 0 \). The reflection of the gas from the wall (the law of reflection is considered to be completely diffuse with the temperature of the wall \( T_w = 1 \)) leads to the formation of a shock wave moving through the channel. The velocity of propagation of a shock wave and its structure are investigated in the flow regimes with the parameters of rarefaction \( \delta = 1 \) and \( \delta = 10 \). The uniform velocity grid and the grid with a condensation near the wall in physical space are used in calculations. The calculations using both the UFS and Nesvetay 3D are carried out with the second order of accuracy in physical space and time.

Figures 2–3 show the profiles of macroparameters obtained as a result of calculations using the model equations and the BE. The radius of the velocity sphere \( R_s = 9 \), the step of the velocity grid \( h_x = 0.5 \), and the minimum steps of the spatial grid \( h_r = 0.125, h_r = 0.0625 \) at \( \delta = 1 \) and \( \delta = 10 \), respectively. To control the accuracy, the calculations were carried out with a decrease in the grid step in both the velocity and physical spaces.

![Figure](image-url)
As can be seen from the results of the solution (Fig. 2), the model equations give the correct velocity of the wave. The extreme values of the heat flux and the nonequilibrium stress tensor are close to the values obtained using the BE. In the region of the shock-wave front, parameters of temperature, velocity, heat flux, and longitudinal component of the nonequilibrium stress tensor have characteristic differences from the BE solution, which are a consequence of the constant collision frequency.

When the rarefied parameter \( \delta = 10 \), the solutions according to the model equations and the full BE almost coincide (more precisely, the differences between the macroparameters are localized in a narrower region of physical space), and the profiles of the macroparameters approach the Navier-Stokes solution. Fig. 3 shows the profiles of velocity and temperature at the same times as in Fig. 2.
In the second problem, the free flow of gas from the slit is investigated. Despite the presence of a large number of publications on jet flows, let us consider the solution of this problem in more detail.

It should be noted that the outflow of gas at moderate Knudsen numbers from an aperture into a vacuum or into a very rarefied space is a flow close to the free-molecular regime.

In [21-22] a stationary solution of the problem of free molecular gas outflow from a slit with constant parameters at the inlet is analytically obtained. Comparison of the analytical solution and the numerical one obtained by direct Monte Carlo simulation (DSMC) showed the coincidence of the results. The calculations of this problem by discrete ordinate method cause certain difficulties due to the “ray effect” [16-17], which leads to nonphysical (non-monotonic) behavior of macroparameters at a large distance from the source. This effect is a consequence of a discrete set of velocities and the ratio

\[ \frac{y - d}{x} < \frac{\xi}{x} < \frac{y + d}{x} , \]

that determines the slope (angle) of the velocity vector of particles emitted from the slit and reaching the point of physical space \((x, y)\) [21]. The distribution function of the velocity vectors located outside this angle is zero.

If the velocity values are discrete, then the fulfillment of this condition for points far from the slit (when the angle becomes small), depends on the velocity step. The small changes in the coordinates in the physical space can lead to significant changes in the velocity distribution function due to its discontinuity. Note that there is no “ray effect” in the DSMC, since a sufficiently large number of particles (about 1 million [21]) are emitted from a slit with different random velocities (no discreteness), and the resulting stochastic noise is suppressed by the averaging procedure. As is known in the discrete ordinate method, the problem of the “ray effect” can be solved by using a detailed grid in the velocity space.

Fig. 4 presents a comparison of the analytical and numerical solutions obtained by the discrete ordinate method for the problem of jet outflow into a vacuum with a sound velocity at the inlet \(u_0 = \sqrt{5/6}\). The step of the uniform velocity grid \(h_\xi = 0.04\), the radius of the velocity sphere \(R_\xi = 6\), and the number of velocity nodes of the two-dimensional grid are \(N_\xi \sim 70.E+3\). The figure shows a good agreement of the results.

**Fig. 4.** Analytical (top) and numerical (bottom) solution of the problem of the free jet flow from the slit into vacuum at \(u_0 = \sqrt{5/6}\), a) density isolines, b) isolines of longitudinal velocity component
However, as the step of velocity grid increases, deformations and fluctuations of macroparameter profiles appear. Reducing the amount of computation gives rise to the use of a non-uniform velocity grid with a condensation in the vicinity of the jet flow velocity. The use of such an approach is effective for model equations, but it is rather laborious for BE, despite the development of numerical algorithms for solving kinetic equations on adaptive velocity grids [23-24].

As the initial Knudsen number decreases, the “ray effect” weakens due to maxwellization of the distribution function and smoothing its discontinuities. The correct behavior of macroparameters is achieved with a larger velocity step, but the number of velocity nodes still remains quite large. The Fig. 5 shows the results of calculations using S-model at $\delta = 10$ and time $t = 10$ with input parameters $p_0 = 1, \rho_0 = 1, u_{x0} = \sqrt{5}/6, u_{y0} = 0$ and pressure in rarefied domain $p_1 = 1.E-12$ (variant 1). The velocity step of both velocity components $h_{\xi} = 0.09$, the radius of velocity sphere $R_S = 6$ and the number of velocity nodes $N_c \sim 13.E+3$.

The results of calculations at $\delta = 1, t = 10$ with the parameters at the inlet $p_0 = 1, \rho_0 = 1, u_{x0} = 2, u_{y0} = 0, p_1 = 1.E - 3$ (variant 2) are presented in Fig. 6. The step of velocity grid $h_{\xi} = 0.1, R_S = 8$, and $N_c \sim 20E+3$. Note that these calculations use reduced equations and a two-dimensional velocity grid. In calculations using BE on 3D uniform velocity grid $N_c \sim 200E+3$.

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**Note**: The diagrams in the text are not provided here, but they likely depict the flow of a free jet from a slit to background gas at different time steps and initial conditions.
Thus, to obtain the correct behavior of macroparameters in the region of strong rarefaction even in the presence of collisions ($\delta \leq 10$), the use of the BE leads to large numerical costs. However, as the calculations show, the type of collision integral has little effect on the behavior of gas macroparameters in the rarefied domain.

**Fig. 7.** Macroparameters along the symmetry axis of the free jet outflow from the slit for different moments of time, $\delta = 10$, variant 1, a) density, b) longitudinal velocity component

**Fig. 8.** Macroparameters along the symmetry axis of the free jet outflow from the slit for different moments of time, $\delta = 1$, variant 2, a) longitudinal velocity component, b) temperature, c) longitudinal component of the heat flux vector, d) transverse temperatures
The behavior of macroparameters on the symmetry axis obtained using the BE and the S-model for different times is shown for $\delta = 10$ (variant 1) and $\delta = 1$ (variant 2) on Figs. 7 and 8, respectively. Figs 8(c,d) show the most sensitive macroparameters of flow, heat flux and transverse temperatures, $T_x$ and $T_y$ at $t = 20$ for variant 2.

The relative deviations of the macroparameters for the S-model and the BE in the flow field are summarized in table 1. From where it can be seen that the values of density and velocity are almost the same. A large relative difference is given by the heat flux for variant 2, but the $q_x$ values are close to zero.

\[
\begin{array}{|c|c|c|c|c|}
\hline
\text{Variant No} & \text{T (time)} & \Delta n / n(\%) & \Delta u / u(\%) & \Delta T / T(\%) & \Delta q_x / q_{x\text{max}} (\%) \\
\hline
1 & 5,0 & 0,5 & 0,4 & 4,0 & 3,7 \\
& 10,0 & 0,9 & 0,6 & 1,3 & 3,6 \\
& 30,0 & 0,5 & 0,2 & 1,0 & 2,6 \\
2 & 5,0 & 0,4 & 0,3 & 2,0 & 6,0 \\
& 20,0 & 1,0 & 0,6 & 3,0 & 6,0 \\
\hline
\end{array}
\]

We emphasize that the distribution function in the rarefaction domain is essentially nonequilibrium, as evidenced by different values of transverse temperatures (Fig.8d), however, the solutions obtained using the model equations and the BE are similar. Such coincidence of the solutions is connected both with small value of the collision frequency (especially at $\delta \sim 1$) and with decrease in gradients of macroparameters in the far region from the slit. This fact makes it possible to use model equations in a rarefied domain without a large loss of the accuracy of the solution.

4. Numerical analysis of the problem of gas reflection from the wall and flowing into the tank

The results obtained for solving the initial problem (Fig. 1) with the reflection of the shock wave from the wall and the outflow into the tank with a rarefied gas, similar to those discussed above. Calculations using the S-model were carried out by both the UFS and the Nesvetay3D complex on a nonuniform velocity grid with condensation in the vicinity of zero velocity and showed good agreement. In this case, the number of velocity nodes for a nonuniform grid $N_c = 40.E+3$, and when using UFS, $N_c = 100.E + 3$.

The behavior of macroparameters along the axis of symmetry at $\delta = 1$ (variant 2), obtained from the solution of model equations (S-model, ES-model) and BE, are shown in Fig.9.

Since the main difference of solutions at $\delta \sim 1$ is manifested in the channel (this region is $x<0$ in Fig.9), efficiently to perform splitting of the solutions of model equations and the BE at the inlet to the tank. For other rarefied parameters the value of local Kn can be used as a decomposition criterion. Such splitting without additional restrictions on the distribution function can be easily implemented for the ES model, which guarantees the positivity of the velocity distribu-
tion function throughout the velocity space. It is more difficult to use the S-model, since the distribution function in this case can take negative values, which are transfer to the domain of the solution. The BE numerical algorithm relies heavily on the positivity of the distribution function, so additional constraints on the distribution function and a more complex domain decomposition are needed to synthesize these equations.

The results of the calculation using the hybrid approach of the BE and ES-model are shown in Fig. 10 at time $t=20$, $\delta = 1$, (variant 2). The upper part of the figure shows the profiles obtained by the hybrid method, and the lower one by using the BE. It can be seen that the velocity isolines coincide, and the temperature has a slight difference (2-4%) in the far region from the entrance to the tank.
When $\delta = 0.1$, the whole problem can be solved using model equations. It should be noted that the hybrid methods developed at present [13,25] allow to reduce the domain of solution of the complete BE, using the connection of the kinetic solution with the solution of the Euler or Navier-Stokes equations. The decomposition criterion is a small value of the collision integral (or its approximation by a model operator) for small Knudsen numbers, which is equivalent to the distribution function being close to the equilibrium one. However, as shown by the above calculations, a small value of the collision integral can be also at a strongly non-equilibrium distribution function, if the local Knudsen number $Kn >> 1$. In this case, the hybrid methods can be supplemented by coupling of the solutions the BE and model equations, which further reduces the domain needed to use the full BE.

Conclusion

We numerically compare the solutions obtained by the model equations (S-model and ES-model) with the solution by the BE for the non-stationary problem of reflecting the flow from the wall and flowing to a tank filled with a rarefied gas. Analysis of auxiliary problems showed that a detailed velocity grid is necessary for obtain the correct behavior of macroparameters by the discrete ordinate method. The use of a detailed velocity grid makes it difficult to calculate the BE. However, the weak influence of the type of the collision integral on the solution in rarefied domain allows to use a hybrid method based on the synthesis of model equations and the BE. This approach is more economical, and the calculations showed the correct results.

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Кинетические методы решения нестационарных задач со струйными течениями

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Изучению нестационарных течений разреженного газа в настоящее время уделяется большое внимание. Такой интерес к этим задачам вызван созданием импульсных струй, используемых при нанесении тонких пленок и специальных покрытий на твердые поверхности. Однако проблемы, связанные с нестационарным течением разреженного газа недостаточно изучены из-за их большой вычислительной сложности. В этой статье рассматриваются вычислительные аспекты исследования нестационарного движения отраженного потока газа от стенки и вытекающего через внезапно образованную щель. Целью этого исследования является анализ возможных численных кинетических подходов для решения таких нестационарных задач и выявление трудностей, возникающих при их решении.

При моделировании процессов, происходящих при сильном разрежении необходимо использовать кинетическое уравнение Больцмана, численная реализация которого, как правило, достаточно трудоемка. Чтобы использовать более простые подходы, основанные, например, на аппроксимирующих кинетических уравнениях (Эллипсоидально-статистической модели, модели Шахова), важно оценить отличие решений модельных уравнений от решения уравнения Больцмана. Для этого рассматривается две вспомога-
тельные задачи: отражение потока газа от стенки и истечение свободной струи в разреженный фоновый газ.

Численное решение этих задач показывает слабую зависимость решения от типа оператора столкновения в разреженной области, но при этом сильную зависимость поведения макропараметров от шага скоростной сетки. Детальная скоростная сетка необходима, чтобы избежать немонотонного поведения макропараметров, вызванных так называемым “эффектом луча”. Для уменьшения вычислительных затрат решения на детальной скоростной сетке предлагается гибридный метод, основанный на синтезе модельных уравнений и уравнения Больцмана. Такой подход может быть перспективным, поскольку уменьшает область применения интеграла столкновений Больцмана.

Результаты, представленные в этой статье, получены использованием двух различных программных комплексов Unified Flow Solver (UFS) [13] и Несветай-3Д [14-15]. Отметим, что в UFS реализован метод дискретных ординат для скоростного пространства на равномерной сетке и иерархическая адаптивная сетка в физическом пространстве как для уравнения Больцмана, так и модельных уравнений. Программный комплекс Несветай-3Д создан для решения модельного уравнения Шахова на неструктурированных неравномерных сетках, как в скоростном, так и в физическом пространствах.

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