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Simulation of Unstable Rarefied Gas Flow in a Channel in Transition from Continuum to Free-Molecular Regime

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Abstract
Numerical study of gas flow in a channel is difficult for rarefied gas (i.e. for high Kn) because this flow could not be described by differential equations: the solution of Boltzmann equation or numerical DSMC methods are required. The problem becomes even more complex for unstable rarefied gas flow. Analytic model of rarefied gas flow in a channel for high Knudsen number can be represented as nonlinear dynamic system based on iterative equations. However, the flow in transitional regime between free-molecular and continuum flow could not be described by iterative scheme. To minimize calculation time we apply artificial neuron network (ANN) in its basic form – multilayer perceptron.

1. Introduction

Numerical simulation of rarefied gas flows in channels applying artificial neuron network (ANN) is the main purpose of this paper. If Knudsen number is high enough, ordinary grid methods become inaccurate, and DSMC methods are preferred. However, often DSMC procedure must be repeated many times, so that powerful high-efficiency computers and much computation time are necessary. Therefore, difficult time consuming computation requires here computer time economy methods like ANN. For testing ANN in rarefied gas we consider one of the most complex type of rarefied gas flows – unstable (relative to a variation of the parameters) flows. Such flows (including the flows in micro- channels) are described by nonlinear dynamic systems with attractors and bifurcations, and has been investigated in our previous papers [1]–[7].
The learning and training of ANN is based here on relative simple test flows, on analytic solutions in limit cases and on comparatively few Monte Carlo simulations. Rarefied gas flows in channels are discrete dynamic systems (unlike continuous dynamic systems specified by differential equations), because they are described by the laws of mutual interactions of gas particles and of collisions with the surface. Thus, these systems can exhibit strange attractors whatever their dimensionality, whereas in a continuous dynamical system according to the Poincaré-Bendixson theorem a strange attractor can only arise if the system has three or more dimensions. The cascade of bifurcations in rarefied gas flow in a channel has been studied in [1]–[7] for the ray model of scattering function V of gas atoms from channel walls.
Simulated unstable states of the system are close to physical situations observed in experiments. Under certain conditions corresponding iterative equations may have unstable solutions in some regions of the values of gas-surface interaction parameters. Numerical study of unstable flow in this regime is especially difficult because to construct the bifurcation diagram we need to repeat the DSMC procedure many times (at least 10^4) for different values of the parameters. The main purpose of ANN procedure in its basic form (multilayer perceptron –MLP) is to find the regions where the flow becomes unstable. To analyze the bifurcations near these regions the Monte Carlo simulation is applied. The results of numerical calculations have demonstrated that the effect of substantial change in a gas flow in a channel by negligible deviation of one of the parameters of scattering function near the bifurcation points becomes less considerable in transitional regime in comparison with free-molecular analytic results. In numerical calculations the same ray model of scattering function V is applied.

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2. Description of rarefied gas – surface interaction

The ray model, as well as the specular reflection, determines only one velocity of reflected from the surface gas atoms by given incident velocity. However, the angles of incident and of reflected gas atoms for the ray model could be different. So the ray model defined by the expression $V(\vec{u},\vec{u}') = \delta(\vec{u}' - \vec{u}_*(\vec{u}))$ [4] could be regarded as the generalized specular reflection. Here δ is Dirac delta function and $\vec{u}_*$ is some specified velocity of reflected from the surface gas atoms that is in general different from the specular velocity. The function $\vec{u}_*(\vec{u})$ is not arbitrary – some restrictions are required to ensure that $V(\vec{u},\vec{u}')$ satisfies the known criteria on wall collision kernels. For example, if the distribution of the velocities $\vec{u}$ of incoming gas atoms is Maxwellian, then corresponding distribution of the velocities $\vec{u}_*(\vec{u})$ of reflected from the surface gas atoms must be the same. In this case the function $\vec{u}_*(\vec{u})$ transforms Maxwellian distribution into itself. More general restrictions to the function $\vec{u}_*(\vec{u})$ can be represented as the principle of detailed balance in gas-surface interactions [8]. However, it is known from the papers of Barantsev and Miroshin (who considered the ray reflection originally) that the class of such functions $\vec{u}_*(\vec{u})$ is wide enough [4]. In our calculations only the functions $\vec{u}_*(\vec{u})$ are applied satisfying these restrictions. In spite of this, various analytical expressions of momentum exchange coefficients (depending on the angles of the incidence and of the reflection) can be obtained in the context. Correspondingly many different shapes of limit gas atoms trajectories are the advantages of the ray model. The diffuse addition (multiplied by the coefficient σ, $0 \le \sigma \le 1$) to the ray model gives us the more general ray-diffuse scattering function

$$V(\vec{u},\vec{u}') = (1-\sigma)\delta(\vec{u}' - \vec{u}_*(\vec{u})) + \sigma \frac{2h_d^2}{\pi} u_n' \exp(-h_d u'^2). \quad \textbf{(1)}$$

depending on the velocities $\vec{u}$ of incident upon the channel wall and $\vec{u}'$ of reflected from the surface gas atoms.
This addition causes a randomization and changes fundamentally the limit behavior of the studied dynamic system [1], [2]. The ray model has better experimental confirmation (especially combined with diffuse scattering) in comparison with other surface interaction models widely applied in practical DSMC calculations, in particular with the specular-diffuse model [4]. The approximation of real gas-surface characteristics by the ray model is good enough for different physical conditions. Therefore we assume the ray model to be valid also in considered flows.
By investigating analytically and numerically the limit behavior of this nonlinear dynamic system most interesting is not a strange attractor which can be observed in rarefied gas flows as a cascade of bifurcations (unlike usual applications of the chaos theory, where the corresponding chaotic behavior is the case of most interest). However, in a rarefied gas flow especially interesting is the transition from regular to chaotic behavior of the system, because such transition indicates in practice the values of the parameters where the solution changes substantially by a very small deviation of these parameters. Our problem is to study it not only for different values of the parameters, but also for different analytical approximations of momentum exchange coefficients. From the point of view of nonlinear dynamics it corresponds to different iterative equations describing the trajectory of a gas atom.
Studying the transition from regular to chaotic behavior of the system requires multiple computations by small deviation of initial conditions, i.e. in rarefied gas we need to repeat DSMC procedure many times. For example, to construct the bifurcation diagram the whole DSMC computation of the flow must me repeated at least 10^4 – 10^5 times. Applying ANN to minimize calculation time enables us to reduce repetitive computation time significantly.
The rarefied gas flow is detected becoming unstable in our previous analytical and numerical investigations [1]–[7] in long enough channels or nozzles for some transition parameter values of the scattering function $V(\vec{u},\vec{u}')$ under some specified conditions. Analytic results for unstable rarefied gas flows are obtained in free-molecular flow [3]–[7]. Similar analytical study of unstable dynamic systems can be found in different applications (for example, in [9]–[10]). The local interaction approximations we need to apply in rarefied gas flow to take into account that Knudsen number is finite [4], i.e. the flow is not free-molecular, but in transition regime from continuum to free-molecular flow. The local interaction theory, being exact for free-molecular flow, gives confirmed by experiment approximations of momentum and energy exchange coefficients for this transition regime. Meanwhile we detect the bifurcations, the attractors and corresponding physical values in the flows. However, the problem of the empirical confirmation of the obtained numerically effect is still difficult, because the scattering conditions, as well as the regions of corresponding empirical parameters, are narrow enough. Therefore these scattering conditions are hardly reproducible in the experiments, and no experimentally observed unstable flows of this type are known yet: the experiments are expensive enough. But it does not mean that it does not correspond to a real physical problem: numerical calculations indicate all the required physical values (scattering function, Knudsen number etc.), so the

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discussed unstable flows will be certainly confirmed experimentally in the future. Considered bifurcations can essentially affect different gas flows applied in practice, such as flows in propulsion systems and in microelectronic vacuum devices. Moreover, the effect of increasing conductivity of the channel because of flow instability under specific conditions can have important practical application.

The parameters of rarefied gas flow in a channel are naturally connected with the parameters of the scattering function $V(\vec{u},\vec{u}')$. This function V determines entirely the parameters of a rarefied gas flow in a channel (if the geometric shape is known) in a near free-molecular flow (Kn→∞). The basic condition for appearing the attractors and the bifurcations is that the model describing scattering function V is close to the ray reflection. Corresponding momentum exchange coefficients for the ray scattering function V are expressed by $p = 2\cos\theta(\cos\theta + u'\cos\theta')$, $\tau = 2\cos\theta(\sin\theta - u'\sin\theta')$, where u and u' are absolute values of the velocities $\vec{u}$ and $\vec{u}'$, θ and θ' are corresponding angles for incident and reflected gas atoms [4]. In numerical calculations for finite Knudsen number we apply the same boundary conditions as in a free-molecular flow (Kn→∞): it gives the possibility to find the regions of flow instability and to compare obtained results.

3. Analytic models of unstable rarefied gas flows as test examples

Simulation of successive gas atoms reflections from channel walls in a free-molecular flow produces the nonlinear dynamic system. Denoting $x_m = \tan\theta_m$, $x_{m+1} = \tan\theta_{m+1}$ (x_m and x_{m+1} are successive values defining the trajectory of a gas particle in the channel, subscript m indicates the number of reflections), and expressing θ' from presented formulae of momentum exchange coefficients p and τ, we obtain iterative equation

$$x_{m+1} = \tan\left[\psi\left(l_m, \arctan\frac{2x_m - \tau(1+x_m^2)}{p(1+x_m^2)-2}\right)\right], \qquad \textbf{(2)}$$

where the function ψ and the variable l_m are determined by the geometrical shape of the channel (Fig. 1), and the momentum exchange coefficients p and τ are assigned by local approximations.

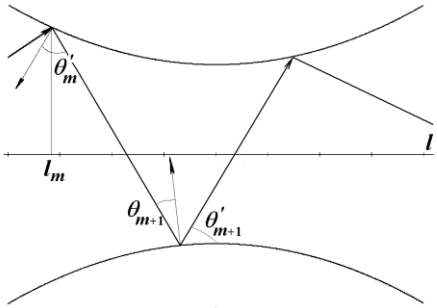

Figure 1: The iterative scheme of successive reflections of a gas atom from the walls in a channel.

If the solutions of the equation (2) become unstable, considered nonlinear dynamic system has many different limit solutions – attractors [1]–[7]. In this case system parameters lie in some small regions, and corresponding parameters of the scattering function V represent the values of singularity. Numerical calculations of the trajectories of gas atoms in a channel demonstrate significant changes of the aerodynamic characteristics of the flow near considered values of system parameters. The investigation of the behavior of nonlinear dynamic system in these regions is very difficult because the describing it iterative equation (2) is more complicated than well-known equation for logistic map $x_{m+1} = rx_m(1-x_m)$. Therefore additional restrictions are taken into account to construct simple analytical solutions applied as test examples.

First, we consider (following our previous papers [1]–[7]) two-dimensional flow, i. e. flat or cylindrical channel (Fig. 1). Then the function ψ in the equality (2) is identical, and the connection between the angles θ'_m and θ_{m+1} in successive m-th and $(m+1)$-th points of collisions of a gas atom with the surface becomes simple: $\theta'_m = \theta_{m+1}$.

Second, only three following most applied in practice local approximations are examined.

DOI: 10.13009/EUCASS2019-650

1. Depending on three parameters approximation [1]–[2] based on the expansion of p and $\frac{\tau}{\sin\theta}$ in terms of $\cos^n\theta$, $n = 1, 2, \ldots$ This model has been confirmed by experiment in many papers (cited in [4]) from St.-Petersburg State University and Central Aviation Institute (TSAGI, Moscow) and can be described by the equations $p = p_1\cos\theta + p_2\cos^2\theta$, $\tau = \tau_0\sin\theta\cos\theta$. Special cases of this approximation have been examined by Miroshin [4], [11]: $p_2 = \tau_0$ ("model A") and $p_2 = 2$ ("model Z"). The coefficients p_1, p_2, τ_0 can be expressed in terms of aerodynamic values, such as Kn, Mach number, temperature factor etc. Substitution into (2) permits to reduce three coefficients p_1, p_2, τ_0 to two parameters a and b transforming iterative equation (2) to

$$x_{m+1} = \frac{x_m}{a\sqrt{1+x_m^2} - b}, \text{ where } a = \frac{p_1}{2-\tau_0}, \quad b = \frac{2-p_2}{2-\tau_0}. \tag{3}$$

2. Another approximation suggested also by Miroshin [11] ("model B") reduces three coefficients p_2, p_4, τ_0 (p_2 and τ_0 remain the same, p_4 is corresponds to higher power $\cos^4\theta$) to two parameters a_1 and b_1 transforming iterative equation (1) to

$$x_{m+1} = \frac{x_m\left[1 - a_1 + (1-b_1)x_m^2\right]}{a_1 + b_1 x_m^2}, \text{ where } a_1 = \frac{p_2 + p_4 - 2}{p_2 - \tau_0}, \quad b_1 = \frac{p_2 - 2}{p_2 - \tau_0}. \tag{4}$$

3. A more general approximation [1] containing four coefficients p_1, p_2, τ_0, τ_1 is corresponding to iterative equation with the same parameters a and b like in (3) and a new parameter d

$$x_{m+1} = \frac{x_m}{a\sqrt{1+x_m^2} - b}\left(1 - \frac{d}{1+x_m^2}\right), \text{ where } d = \frac{\tau_1}{2-\tau_0}. \tag{5}$$

For $d = 0$ the equation (5) coincides with (3). Hence the first approximation (3) is particular case of the third (5). However, the second model (4) cannot be represented in the form (5), but the main properties are similar by corresponding values of the parameters. Fig. 2 illustrates the graphs of the functions (2)–(4) for the values of variables a, b, c and d (and corresponding momentum exchange coefficients) observed in real physical conditions of gas-surface interaction (and in the experiments). In particular, $a = 2$, $b = 1.7$ for the approximation (2) (dashed line), $a = 0.2$, $b = 0.9$ for (3) (dotted line), $a = 2$, $b = 1.8$, $d = 0.3$ for (4) (solid line).

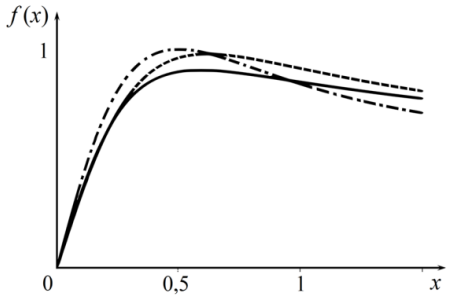

Figure 2: The functions in iterative equations (3)–(5) corresponding to successive reflections of a gas atom the walls in a channel.

Analytical and numerical investigation of limit solutions demonstrates, that all the three iterative equations (3)–(5) can have attractors of different types depending on the parameters a, b and d. Limit cycles corresponding to the roots of the equation $f(x) = x$ and stationary point $x = 0$ (indicating direct flow along the axis of the channel) are

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obligatory. Iterative equations (3)–(4) can also have stationary points $x_1 = \sqrt{\frac{(b+1)^2}{a^2} - 1}$, $x_2 = \sqrt{\frac{2a-1}{1-2b}}$ and $x_0 = \infty$ respectively. The last value has a physical meaning of locking the channel, i. e. its conductivity reduces significantly. The main conclusion from numerical study of the third model (4) is that the attractors and bifurcations in this case are noticeably more various than for the first two models (2)–(3). In particular, up to three attractors exist corresponding to the roots of the equation $at^3 - (b+1)t^2 + d = 0$. The attractors of higher degree could be obtained from the equation $f(...f(x)) = x$ (where $f(x)$ could be iterated many times) and the set of the solutions could be very rich for some values of *a*, *b* and *d*.

Under certain conditions iterative equations (3)–(5) may have unstable solutions in some regions of the values of gas-surface interaction parameters *a*, *b* and *d*. In these regions (which can be found analytically in described way) comparative small modification of the parameters *a*, *b* and *d* causes significant difference between corresponding limit values $x_m = \tan\theta_m$. From aerodynamic point of view it has following interpretation: macroscopic parameters of the flow may fluctuate unsteady while the difference in microscopic values describing gas-surface interaction remains negligible. However, the regions in which the flow becomes unstable are very narrow, therefore it is difficult to find them numerically or experimentally. In the coordinate system (*a*, *b*) the regions of instability obtained analytically are concentrated near the line $a = b$.

Real physical setup of considered rarefied gas flows has not yet detailed experimental confirmation because of technical difficulties in performing such experiments. However, these analytical evaluations are confirmed by numerical calculations. Considered analytical solutions we apply as test examples for ANN.

4. Numerical simulations with an application of artificial neuron network

To minimize calculation time in rarefied gas flow in a channel for finite Kn we apply artificial neuron network (ANN) in its basic form – multilayer perceptron (MLP). The learning and training of ANN is based on relative simple test flows, on described above analytic solutions in limit cases and on comparatively few Monte Carlo simulations.

Preferred MLP has an important advantage over another type of ANN – Radial Basis Function (RBF) network: RBF network is better for interpolation between known solutions, and MLP gives better approximations for extrapolation problems and for solutions with steps and leaps (like shock waves) because it applies nonlinear activation function (usually a hyperbolic tangent). Moreover, MLP gives approximate solutions for very complex problems and allows solving problems stochastically [12].

The construction of ANN for rarefied gas flow in a channel can be described briefly as follows. The MLP consists of many layers (an input and an output layer with intermediate hidden layers) of nonlinearly-activating nodes. Each node in any layer connects with a certain weight w_{ij} to every node in the following layer.

Learning occurs in MLP by changing connection weights w_{ij} after each piece of data is processed. The output is compared to the expected result and connection weights w_{ij} are changed corresponding to the minimum value of error.

Repeated Monte Carlo simulation of the rarefied gas flow in the channel is applied to learn MLP under following conditions. In the initial section of the channel – uniform rarefied gas flow is assumed consisting of N_0 atoms, is considered from 40000 and above. The length of the channel varies from 20 to 100 (the channel must be long enough to produce attractors). Mutual collisions between gas atoms considered as hard spheres are simulated as usual in DSMC, while the trajectory of each gas atom is simulated applying MD approach. Scattering of gas atoms from channel walls is modeled by ray-diffuse scheme with parameters of gas-surface interaction (σ, *a* , *b* and *d*) chosen from the regions where unstable analytic solution obtained for free-molecular flow could be indicated. In the most part of our calculations the number of the layers was limited by 2 or 3 layers.

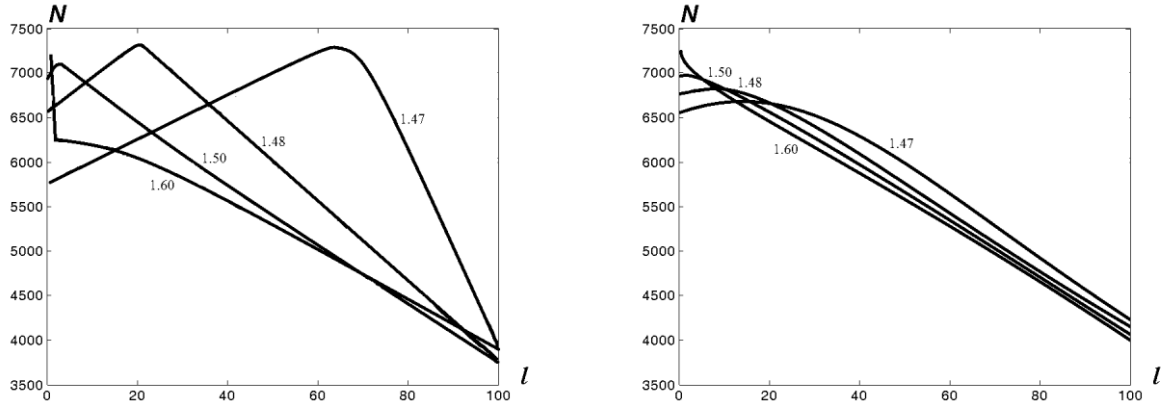
Calculated as a result of Monte Carlo and ANN simulation values are the distribution of average velocity inclination angles along the channel and the mean number of gas atoms in the sections of a channel.

To illustrate obtained results comparative graphs of the numerical density of gas atoms in some sections of a channel depending on the value *a* are presented (Fig. 3) for transitional regime between continuum and free-molecular flow, Kn = 1, compared to free-molecular flow.

The scattering function is assumed to be ray-diffuse with the identical value $\sigma = 0.05$. The parameters are changed gradually near the points of the instability to demonstrate the variation of the results. For instance, the variable *a* changes from 1.47 to 1.60 in four steps (Fig. 3). The largest difference between two graphs corresponding to nearest values $a = 1.47$ and $a = 1.48$ indicates the region of the instability in the segment $1.47 \le a \le 1.48$. Near the value $a = 1.47$ the conductivity of the channel reduces significantly – it has a physical meaning of locking the channel. Similar results have been obtained for other values of the parameters *a*, *b* and σ.

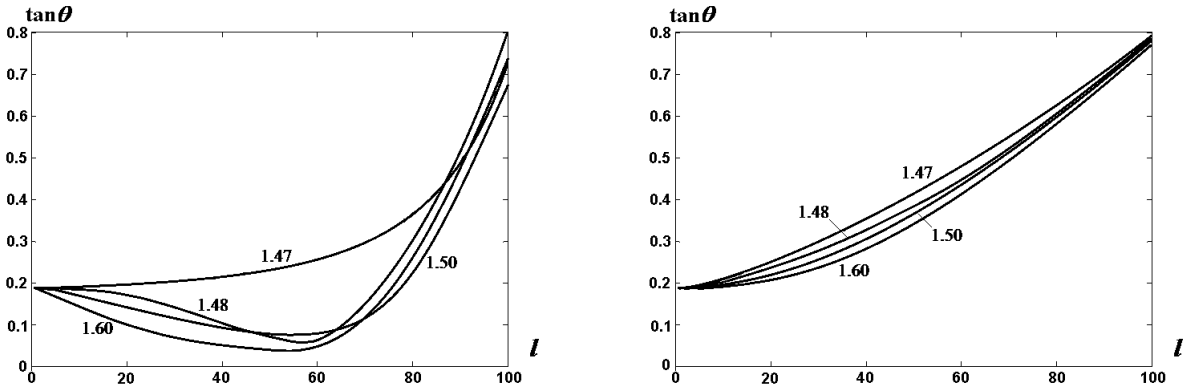
DOI: 10.13009/EUCASS2019-650

Corresponding results for the change of the average scattering angle θ of gas atoms along the channel are presented in Fig. 4.



(a) (b)

Figure 3: The change of the number N of gas atoms along the channel by the modification of the parameter from $a = 1.47$ to $a = 1.48$, $a = 1.50$ and $a = 1.60$ by constant $b = 1.7$, $\sigma = 0.05$, $N_0 = 40000$: (a) Kn = ∞, free-molecular flow; (b) Kn = 1, transitional regime between continuum and free-molecular flow.



(a) (b)

Figure 4: The change of the average scattering angle θ of gas atoms along the channel by the modification of the parameter from $a = 1.47$ to $a = 1.48$, $a = 1.50$ and $a = 1.60$ by constant $b = 1.7$, $\sigma = 0.05$, $N_0 = 40000$: (a) free-molecular flow; (b) Kn = 1, transitional regime between continuum and free-molecular flow.

The best way to study the limit behavior of unstable dynamic systems and their bifurcations is constructing the bifurcation diagrams presented in [1]–[2]. However, for increasing values of the coefficient σ, indicating the input of diffuse scattering into the function V, and for finite Kn (for instance, Kn=1) the bifurcation diagrams similar to presented in [1] become very dissolved because of the randomization. Hence the clearness in visualization is lost. The results of numerical calculations show that for relative small values of σ the effect of significant variation of flow parameters by a small modification of gas-surface interaction coefficients a and b remains qualitative the same as the effect for the ray scattering ($\sigma = 0$) and it can be observed by the same parameter values of a and b.
Near all the points of the bifurcation a negligible change of one of the parameters of the ray-diffuse model (less than 1%) causes also the substantial difference in gas flow in the channel.

5. Conclusion

Monte Carlo and ANN simulation of different nonlinear dynamic systems corresponding to rarefied gas flows in channels has indicated various developments of instability including cascades of period-doubling bifurcations. Several main conclusions follow from the analysis of the comparison.

DOI: 10.13009/EUCASS2019-650

- Proposed ANN procedure in its basic form – multilayer perceptron (MLP) allows computation time economy in rarefied gas flow simulation; analytic evaluations and comparatively few Monte Carlo simulations can be applied as a base for MLP learning. Studied algorithm could be applied to solve different problems, so the results are of interest for future ANN applications in rarefied gas.
- Substantial difference in the characteristics of gas flow in a channel by negligible change of the parameters of ray-diffuse model of gas atoms scattering from surface is confirmed analytically and numerically. Experimental confirmation for considered type of unstable flows will be certainly provided in the future.
- Numerical results allow finding the values of the parameters corresponding to possible unstable flows; the regions of instability are very small, therefore it is difficult to find them without special search. Simulated unstable states of the system are close to physical situations observed in experiments.
- The effect of substantial change in a gas flow in a channel by negligible deviation of one of the parameters of scattering function near the bifurcation points becomes less considerable in transitional regime in comparison with free-molecular analytic results.
- Obtained connection between the parameters of nonlinear dynamic system (a, b and θ_0) and momentum exchange coefficients (or accommodation coefficients) permits to express analytically the combinations of the gas dynamics characteristics (including Knudsen and Mach numbers, temperature factor etc.) specifying the unstable flows.

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