Investigation of gas-dynamic processes in a boundary layer on a basis of molecular dynamics simulation

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Abstract. The work is devoted to numerical simulation of the nonlinear gas dynamic processes in technical systems of micron sizes. This problem is relevant for many applications related to the implementation and the use of nanotechnology in various industries. As an example, a gas flow in micro channel with metal walls is considered. Within this problem, we are interested in a calculation of the boundary layer parameters from first principles. The numerical analyses are carried out according to the Newton’s equations of classical dynamics. The model under consideration takes into account the molecular composition of the gas, the atomic structure of the metal surfaces, and heat exchange of the gas with the metal. Computer implementation is focused on using high-performance systems with hybrid architecture. The calculations are performed on the example of a nitrogen flow into a nickel micro channel for several micro channel lengths. The flow velocity varied over a wide range. It is considered in the subsonic, transonic, and supersonic ranges. In numerical experiments, macro parameters of gas flow in the boundary layer are obtained and the corresponding near-wall model is formed. It can be used for the calculation of flows in micro channels using continuum mechanics methods.

1. Introduction

Technical (applied) gas dynamics [1] emerged as an independent science in the 30 s of the last century. It received a powerful theoretical and practical impetus in the 40 s-60 s in connection with the development of aviation and rocket technology, nuclear energetics and other industries. The central place in technical gas dynamics is occupied by boundary layer theory [2]. The development of mathematical modeling methods [3] and the use of high-performance computing enable us to study complex gas-dynamic processes without the application of expensive field experiments. It is become necessary to study gas dynamic processes at the atomic-molecular level due to the massive introduction of nanotechnology in industry. Such detailed study is carried out for cases where the similarity theory and/or the continuity hypothesis are violated. The most significant deviations from theoretical estimates are observed on micro and nano scales, taking into account the specific composition of the gaseous medium and structure of real surfaces, streamlined by supersonic gas flows. Up to a certain point in these cases, methods for calculating free-molecular flows have been successfully applied [4]. However, due to increasing the complexity of technical gas dynamics problems, the methods based on the Boltzmann kinetic equation (see, for example, [5]) and the
molecular dynamics methods (see, for example, [6,7]) are increasingly used in specific applications. In this paper, the molecular dynamics (MD) approach [8-18] is chosen. A number of computational experiments on interaction of the nitrogen stream with the nickel surface is carried out. A preliminary model of the boundary layer is formulated. This model can be used at various levels of detail analysis of the flow in the near-wall layer.

2. Mathematical model and numerical technique

The approach based on models and methods of molecular dynamics [8-18] is used to describe the processes in gas-metal micro systems. It is assumed that there are mainly molecules of the gas mixture \( N_{\text{gas}} \) (total kinds) in the gas part of the micro system. On solid surfaces and in their vicinity, atoms or metal molecules \( N_{\text{met}} \) (total kinds) are added to them. They constitute surface material and are potentially able to break away from it. The evolution of the micro particle system under study is described by the Newton's equations [15-18]. The system of equations for moving the particles of \( l \) kind has the following form. The particles can be both gas and metal.

\[
m_i \frac{d\mathbf{r}_{i,l}}{dt} = \mathbf{F}_{i,l}, \quad \mathbf{v}_{i,l} = \frac{d\mathbf{r}_{i,l}}{dt}, \quad i = 1, \ldots, N_i, \quad l = 1, \ldots, N_{\text{tot}} \left( N_{\text{tot}} \equiv N_{\text{gas}} + N_{\text{met}} \right),
\]

where \( i \) is the particle number, \( l \) is the particle kind, \( N_i \) is the total number of particles of \( l \) kind. The particle of \( l \) kind with \( i \) number has its own mass \( m_i \), \( \mathbf{r}_{i,l} = (r_{x,i,l}, r_{y,i,l}, r_{z,i,l}) \) is particle displacement vector, \( \mathbf{v}_{i,l} = (v_{x,i,l}, v_{y,i,l}, v_{z,i,l}) \) is velocity vector and \( \mathbf{F}_{i,l} = (F_{x,i,l}, F_{y,i,l}, F_{z,i,l}) \) is total force acting on this particle.

The forces are the sum of two terms. The first term is connected with the interaction of the \( i \)-th particle with the surrounding particles. It depends on the potential energy. The second term is responsible for external influence. The potential energy of the system is represented as a sum of partial energies. It is calculated according to the formula of the selected interaction potential.

\[
F_{i,l} = -\frac{\partial U}{\partial \mathbf{r}_{i,l}} + F_{i,l}'', \quad U = \sum U_{i,l''}, \quad i = 1, \ldots, N_i, \quad l = 1, \ldots, N_{\text{tot}},
\]

where \( U = U \left( \mathbf{r}_{i,1}, \ldots, \mathbf{r}_{i,N_i}; \ldots; \mathbf{r}_{N_{\text{tot}},1}, \ldots, \mathbf{r}_{N_{\text{tot}},N_{\text{tot}}} \right) \) is the total potential energy, \( U_{i,l''} \) is the potential of interaction of \( l \) kind particles with \( l'' \) kind particles, \( F_{i,l''} \) is the force of interaction with the external environment.

The choice of interaction potentials is based on a comparison of the mechanical properties of the computer model and the real material. At the same time, it is necessary to consider all variants of gas-gas, metal-metal and gas-metal interactions. Only the pair interactions of particles are taken into account. Each type of interaction is described by its potential. For gas mixtures, the Mie potential in the form of "n-6" [9] is usually used. For the interaction of metal atoms, the EAM [13] potential is used, which takes into account the pair interactions of atoms, as well as the effect of collective electron density in the conduction band. To account gas-metal interactions, the Morse [10] or Lennard-Jones [11] potentials are used with parameters calculated on the Lorentz-Berthelot formulas [8].

The initial conditions at the micro level are determined by the equilibrium or quasi equilibrium thermodynamic state of the particle system at a given temperature, pressure, and average momentum. The boundary conditions at the molecular level depend on the modeled situation. To determine the general properties of a medium, it is enough to consider the selected three-dimensional volume with periodic boundary conditions in all coordinates. When studying micro systems of real geometry, such as a micro channel, one or several directions have a finite size. And the preservation of the shape of an object is achieved by selecting a potential or fixing the system. In this case, we consider two variants: either the mirror boundary conditions can be used as boundary conditions, when the particles interact...
with their mirror reflection and do not consequently leave the boundary; or the condition is applied of the disappearance of a particle at the boundary and its appearance elsewhere in the micro system (so that the equilibrium of the system is not broken). It can also be defined for an input stream of particles on one side of the selected volume and the free exit of the particles on the other side. Monitoring the temperature of the system and its total momentum is carried out using thermostatic methods [14,15].

3. Numerical technique

The system of equations (1) and (2) is solved using the Velocity Verlet integration [12]. At first time step we calculate start forces:

$$F_{i,j}^0 = F_{i,j} \left( r_{i,1}^0, ..., r_{i,N_i}^0; ..., r_{N_{tot},1}^0, ..., r_{N_{tot},N_{tot}}^0 \right), \quad i = 1, ..., N_I, \quad l = 1, ..., N_{tot};$$  (3)

Further, for $n = 0, 1, 2, ...$, we calculate new positions of particles, new forces and velocities:

$$r_{i,j}^{n+1} = r_{i,j}^n + v_{i,j}^n \Delta t + \frac{F_{i,j}^n}{m_i} \frac{(\Delta t)^2}{2}, \quad i = 1, ..., N_I, \quad l = 1, ..., N_{tot};$$  (4)

$$F_{i,j}^{n+1} = F_{i,j} \left( r_{i,1}^{n+1}, ..., r_{i,N_i}^{n+1}; ..., r_{N_{tot},1}^{n+1}, ..., r_{N_{tot},N_{tot}}^{n+1} \right), \quad i = 1, ..., N_I, \quad l = 1, ..., N_{tot};$$  (5)

$$v_{i,j}^{n+1} = v_{i,j}^n + \frac{F_{i,j}^{n+1} + F_{i,j}^n}{2m_i} \Delta t, \quad i = 1, ..., N_I, \quad l = 1, ..., N_{tot}.\)  (6)

Here $\Delta t$ is the integration step, $n$ is the step number, $F_{i,j}^n$ is the force value at the $n$ step, $F$ is the procedure for calculating the forces. The thermostating procedure [14,15] is added to formulas (3)-(6) to achieve the desired parameters of gas and metal in the state of thermodynamic equilibrium. The Berendsen thermostat [14] is used to achieve a given temperature by the micro system. The Langevin thermostat [15] is used to achieve the given temperature and momentum.

4. Parallel implementation

A parallel implementation of the MD algorithm assumes the use of a cluster (supercomputer) with central or hybrid architecture. Each node has several multicore central processor units (CPU) and several vector or graphic processors units (VPU or GPU). Parallelization of the algorithm is based on the principles of geometric and functional parallelism. The computational domain is divided into sub-domains of the same power. The power of a domain is measured by the number of elementary boxes where all molecules interact with each other. The domain partitioning is performed within the three-dimensional lattice topology. Each calculated domain is directed to a cluster or supercomputer (SC) node. The distribution of domains on SC nodes is implemented using the MPI library.

There is a certain set of elementary boxes grouped into a three-dimensional sublattice inside the computational domain. This set is distributed among the cores and threads of the computational devices of the SC node. Such decision takes place because of the calculations inside the boxes have a higher intensity than among the boxes. As a result, intermolecular interactions in boxes are realized in parallel mode by using OpenMP technology for CPU or VPU. When using graphic accelerators, a copy of the boxes is created in the memory of the GPU. The necessary data to calculate the interactions of the particles are transferred there. The implementation of such mechanism uses CUDA technology.

The basic computational algorithm is as follows. The 1st stage is reading the source data by an MPI application and initializing the data structures on each computational unit. The 2nd stage is basic calculations in a time cycle based on the formulas (4)-(6). The 3rd stage is performing the resulting
calculations and finalization.
At the first stage, in particular, the number of particles in the computational domain is determined, generation of their placement, generation of uniform on angles and Maxwellian on modulus distribution of their momentum distribution, and the calculation of starting forces is performed.

The following sequence of actions is implemented within the time cycle.

First, new coordinate values are calculated. Then, they are corrected using periodic boundary conditions. After that, particles are exchanged among specific boxes and that is carried out both within the calculated domains and among the calculated domains using MPI functions.

Further, the forces are calculated, on the basis of which the particle velocities are corrected and all the necessary integral characteristics are computed. When the control time points are reached, the necessary data are stored in files.

The difference of the proposed approach from others is the use of data structures based on elementary boxes. The dimensions of the boxes are related to the cutoff radius of the interaction potentials and the lattice parameters of the metal. Such solution is rather costly in terms of the size of RAM needed, but it greatly saves time of calculations. The processing of a small number of particles in several adjacent boxes, located practically in one or several adjacent pages of RAM, is performed as quickly as possible and is well cached. In fact, we implement a RAM localization mechanism. During intensive calculations, the processor does not need to be switched among far-spaced pages of memory.

Also, in the proposed algorithm, we managed to avoid the expensive procedure for determining the belonging of various particles to specific boxes. The other codes perform this procedure at each time step. Another advantage of using the box structure is the transfer of particles among nodes of MVS that associated with the movement of particles over the computational domain, integrated both with the implementation of the periodic boundary conditions and with the exchange of information among MPI processes adjacent in the cubic lattice. This exchange is achieved by using shadow (virtual) boxes with fictitious particles. The interaction of the main particles and the fictitious particles must be taken into account in the potential energy of the system. A more detailed parallel technology is described in [19].

5. Simulation results
As an example, the flow of nitrogen into a nickel micro channel with a length of 1 to 3 microns and a thickness of about 600 nm is considered. The computational geometry contains two nickel plates (top and bottom) with layers of adsorbed nitrogen adhered to them and a free layer of nitrogen between them (see figure 1). In this case, the real structure of the nickel base of the micro channel, the effect of the initial adsorption of nitrogen molecules on the walls of the micro channel, and the energy discharge of the microchannel walls into the environment are taken into account. The calculations are performed with using the hybrid supercomputer K60 of Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences.

![Figure 1. Geometry of simulated micro system.](image-url)
The calculations are carried out for several widths of the nitrogen jet and several values of velocity. The velocity is considered to exceed the speed of sound in nitrogen, and for significantly smaller values. To accelerate the calculations on the second direction (y), a thin layer and periodic boundary conditions are taken. The general parameters of the gas-metal micro system are proposed in table 1.

| Physical parameters of the gas-metal micro system. |
|--------------------------------------------------|
| Parameter                             | Value                                      |
| Length, mm                            | $L_x = 1017, n = 1,2,3$                     |
| Width, mm                             | $L_y = 101.7$                              |
| Height, mm                            | $L_z = 8.5$                                |
| Temperature, K                        | $T = 273.15$                               |
| Pressure, MPa                         | $P = 0.101325$                             |
| Longitudinal velocity, nm/ps          | $v_x = 0 \rightarrow v_{x,max} = 0.4$ (is varied*) |
| Transversal velocity, nm/ps           | $v_y = 0$                                  |
| Vertical velocity, nm/ps              | $v_z = 0$                                  |
| Particle number, $\times 10^6$        | $162.57 \cdot n, n = 1,2,3$                |

*Note that the speed of sound in nitrogen under the normal conditions is 350.6 m/s i.e. 0.3506 nm/ps. Transition from the subsonic range to the supersonic one occurs when a stationary gas is accelerating to a speed of 0.4 nm/ps.

The parameters of the Ni–Ni interaction (it is based on EAM model) were taken from [13]. Our preliminary results show that the equilibrium value of lattice parameter for the normal conditions is $a_{Ni} = 0.35314$ nm. The parameters of the $N_2–N_2$ interaction (it is based on Lennard-Jones "n-m" model [11]) are $n = 11.5$, $m = 6$, $\epsilon / k_B = 97.78$ K, $\sigma = 0.3649$ nm. The parameters of Ni–N$_2$ interaction (it is based on Lennard-Jones "12-6" model [11] with the Lorentz-Berthelot correction [8]) are $\epsilon / k_B = 343.59$ K, $\sigma = 0.2795$ nm. The cutoff radius of the interaction potentials is 0.9 nm. Numerical integration by the Verlet scheme are carried out with time step $\Delta t = 0.002$ ps.

The boundary conditions are periodic along the x(I) and y (II) coordinates. The first (I) allowed us to escape from the problem of the correct numerical implementation of the incoming gas flow using the molecular dynamics method. The second (II) allowed to reduce the computational capacity of the problem.

Along the z (III) coordinate, the region does not have certain boundary conditions because of external walls of the channel border the vacuum. At the same time, the backs of the metal plates are controlled by a thermostat in order to simulate heat removal to the environment.

Let's consider some calculation results. In the process of evolution, the average (on x and y coordinates) transverse profile of the longitudinal velocity component $\langle v_x \rangle$ gradually turns into a Gaussian profile (see figure 2). At the same time, there are small beats of velocity near the channel walls. They associated with nonlinear gas interaction not so much with the metal, as with the gas adsorbed on its surface.
Figure 2. Evolution of the averaged transverse profile of the longitudinal velocity component.

Note that the chaotic behavior of the longitudinal velocity profiles near the walls is associated with two factors. On the one hand, the calculation of gas macro parameters near the wall with a small number of molecules is not very correct. So we suggest adjusting these results below when macro models are using. On the other hand, the presence of a gas layer adsorbed on the metal affects the rest of the gas nonlinear and non-stationary. This is an objective process and it takes into account below when boundary layer model is formulating. The periodic appearance and disappearance of the longitudinal velocity peak near the walls is apparently associated with both of these factors.

Long-term calculations show that the final interaction of the flow with the walls of the micro channel is essentially non-linear and in some cases non-stationary. A particularly complex flow structure is observed at the initial stage of its evolution. The longitudinal velocity profile averaged over the transverse coordinate can have a Gaussian and hyper-Gaussian shape, which changes with time its characteristic features. In some cases, gas beats against the channel walls are observed. With increasing the channel length, the development of a turbulent flow is expected. However, this effect is realized at large times of the order of 20 ns or more (This corresponds to 10 million integration steps).

An analysis of the data obtained suggests that the structure shown in figure 3. It consists of four layers, between which there is an exchange of mass, momentum and energy (specific layer sizes will be obtained as a result of subsequent more accurate calculations). Taking into account this structure, we can say that under the conditions of the adsorption effect, the main gas flow actually interacts not with the metal wall, but with the buffer gas and the gas adsorbed on the surface.

Figure 3. Structure of boundary layers.
Therefore, at the macro level, the following multilayer boundary conditions should be considered:

\[
\frac{\partial \rho}{\partial n} = -\eta_1 (\rho - \rho_{bg}), \quad \frac{\partial \rho_{bg}}{\partial n} = -\eta_2 (\rho_{bg} - \rho_{ag}), \quad \frac{\partial \rho_{ag}}{\partial n} = -\eta_3 (\rho_{ag} - \rho^*_{ag});
\]

\[
W_{n,I}^{(I,-)} = W_{n,bg}^{(I,+)}; \quad W_{n,bg}^{(I,+)} = W_{n,ag}^{(I,-)}; \quad W_{n,ag}^{(I,+)} = W_{n,w}^{(I,-)}; \quad (7)
\]

\[
W_{n,E}^{(E,-)} = W_{n,bg}^{(E,+)}; \quad W_{n,bg}^{(E,+)} = W_{n,ag}^{(E,-)}; \quad W_{n,ag}^{(E,+)} = W_{n,w}^{(E,-)}; \quad (8)
\]

where \(\rho\), \(\rho_{bg}\), \(\rho_{ag}\) and \(\rho^*_{ag}\) are densities of gas in main flow, buffer layer, adsorbed gas layer and maximal density of gas on metallic surface; \(\eta_k\) are some coefficients; \(W_{n,I}^{(I,+)}\), \(W_{n,bg}^{(I,+)}\), \(W_{n,ag}^{(I,+)}\), \(W_{n,w}^{(I,+)}\) are normal components of pulse flows on corresponding boundaries, \(W_{n,E}^{(E,+)}\), \(W_{n,bg}^{(E,+)}\), \(W_{n,ag}^{(E,+)}\), \(W_{n,w}^{(E,+)}\) are normal components of energy flows.

In the layer of a buffer gas, it is necessary to solve the equations of multiphase hydrodynamics. In the layer of adsorbed gas, it is necessary to solve the two-dimensional diffusion convection equation. For the metal wall, it is necessary to consider the processes of heat conduction and dissipation of the normal component of the momentum. The formulation of these equations is the subject of a future analysis.

6. Conclusion

The use of the developed numerical technology enable us to calculate, from first principles, the process of nonlinear interaction of a nitrogen flow with the walls of a nickel channel. These calculations allow us to form the macroscopic model of the boundary layer. Within the model, three layers of gas are identified near the channel walls. These layers are clearly indicated when formulating the boundary conditions at the macro level. Firstly, it is the main moving gas layer. Secondly, it is a layer of low-mobility gas molecules adsorbed on the wall. Thirdly, it is a transitional layer in which heat exchange of gas and surface occurs and the flow velocity is lost due to friction against the gas adsorbed on the wall. The selection of specific parameters for this model shows that with certain restrictions on the velocity and density of the gas flow, this model can be used within traditional CFD modeling. However, in the general case, the multi scale modeling method should be used. We discussed it in [20]. This method uses a combination of mesh calculations and molecular dynamics.

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