Problems of coordinating the solutions of quasigasdynamic equations with results of molecular-dynamic calculations in analysis of real gas flows

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Abstract. This paper is devoted to the numerical study of complex gas -dynamic processes in microchannels of technical systems. The analysis is carried out on the basis of the equations of quasigasdynamics, taking into account the real dependences of the equation of state and kinetic coefficients on temperature and pressure, as well as the realistic description of the channel walls. As an example, the flow of nitrogen in the nickel channel of the actual structure is selected. The task is considered in the context of a multiscale approach. The main idea of this approach is to combine models of continuum with models of particles. Combining models is implemented in the framework of the method of splitting by physical processes. The correctness of this approach is ensured by the selection of suitable time intervals and the conjugation of scale levels. The goal is to develop a numerical algorithm that integrates grid methods for solving quasigasdynamic equations and molecular dynamics method, allowing to take into account the properties of real substances in the general model. In work the method of coordination of numerical solutions at different scale levels in time and space is investigated. Based on the proposed methodology, direct molecular modeling of the flow in the channel was carried out and data were prepared for calculating such a flow using the equations of quasigasdynamics. The study confirmed the possibility of synthesizing these two numerical methods.

1. Introduction

The system of quasigasdynamics (QGD) equations [1-3] is now widely used due to its useful kinetic properties, which allow to calculate the flow of gas and mixtures for large Mach and Knudsen numbers. However, there are still questions about the numerical implementation of this system of equations in case of the real equation of state, which is given by complex formulas or in a tabular way. It also raises the question of the coordination of all kinetic coefficients characterizing the gaseous medium, as well as the addition of bulk viscosity. When calculating the flows in the microchannels, a realistic description of their walls is also required.

In this paper, using the example of calculating the flow in a channel, the above range of questions is studied. Pure nitrogen is considered as a gaseous medium. Nickel is considered as the material of the walls. This problem is regarded in the context of the multiscale approach developed in [5, 6]. The
main goal is to develop such a numerical algorithm, which combines the grid methods for solving quasigasdynamic equations and molecular dynamics (MD) methods [4], allowing to take into account the properties of real substances in the general model.

To date, based on the technology [5-8], direct numerical molecular modeling of the flow in the channel has been carried out and data have been prepared for calculating such a flow using the equations of quasigasdynamics. Preliminary studies confirmed the possibility of synthesizing these two numerical methods.

2. Numerical algorithm and model coordinating technique
As indicated above, the method for calculating complex gas-dynamic processes in the case of many scales has already been presented by authors in set of papers (for example, [7, 9]). The main idea of the proposed approach is to unite models of a continuous medium with models of particles. A similar symbiosis of models is realized in the framework of the splitting method by physical processes. The splitting method assumes that when studying complex non-linear multiscale processes, it is possible to consider each physical process independently of the others. The correctness of this approach is ensured by the selection of suitable time intervals and the conjugation of scale levels.

In the framework of the proposed approach, the system of QGD equations and the MD equations were used together. The main area of the approach application is the solution of gas-dynamic problems of nanotechnology. A feature of such tasks is the presence of at least two characteristic scales - macroscopic and microscopic. The first scale refers to the size of individual structural elements or components of technical systems, which are hundreds of microns or more and can reach the centimeter range. The second scale relates to objects of micron, submicron and nanometer dimensions, which are the subject of study and/or synthesis.

In [5-7], 4 classes of algorithms were proposed that implement a multiscale approach. The first two assumed the solution of gas-dynamic problems either only within the framework of MD methods (1st class) or only on the basis of the QGD model (2nd class). Approach of many scales within these algorithms was taken into account by coordinating the parameters of the gaseous medium at the macroscopic and microscopic levels. In particular, when using algorithms of the 1st class, standard macroparameters of the gaseous medium (density, velocity, pressure and temperature) were calculated statistically. When using algorithms of the 2nd class, data on the parameters of the equation of state and the dependence of the kinetic coefficients of the gaseous medium on temperature and pressure, obtained in the framework of MD calculations, as well as the parameters of the boundary conditions were taken into account. The implementation of MD computation is performed using the well-known Verlet scheme. The implementation of QGD calculations uses the grid method of control volumes (Cartesian or unstructured grids of various types can be used as grids).

Algorithms of the 3rd and 4th classes imply joint integration of QGD and MD equations. In this case, the 3rd class algorithms use local application of MD calculations in individual cells of the computational grid. Algorithms of the 4th class can operate with sufficiently large subdomains (subzones) of the application of MD computations, significantly exceeding the size of individual grid cells. In this sense, the 4th class algorithms are non-local.

The essence of the 3rd and 4th class algorithms is that when solving a dynamic problem, at each time step the equations of quasigasdynamics and molecular dynamics are solved either alternately or in parallel.

The general algorithm of the 3rd class consists of the following four stages.

At the first stage, the next step is carried out in a finite volume scheme.

At the second stage, in the required subzones, a transition takes place from the macroscopic parameters of the gaseous medium to the microscopic distributions of the properties of individual particles, preserving the basic balance ratios (mass, momentum, energy) in the grid cells or entire subzones.

At the third stage, MD computations are performed using a significantly smaller time step.
At the fourth stage, macroscopic gas-dynamic parameters (density, velocity, pressure, temperature) are corrected on the basis of MD calculations in the corresponding subzones.

In the algorithms of the 4th class, MD calculations in non-intersecting subzones proceed simultaneously with QGD calculations, and the transition between the macroscopic and microscopic levels takes place at the boundaries of the subzones, and in the intersecting subzones the calculation algorithm is similar to the 3rd class algorithm.

The coordination of models in the algorithms of the 3rd and 4th class is made in space and in time. Spatial coordination consists in choosing the size of the grid cells on which the QGD equations are solved. The main requirement is that the linear cell size should be at least half (a quarter) of the mean free path of the molecules of the gaseous medium. The upper limit of the linear size of the grid cells is usually determined by the computational capacity of the MD computation. In the case of a highly rarefied gas, it can be tens and hundreds of free paths of molecules. In the case of dense gas, the linear size can be up to ten free paths. Also, in order to save computing resources, the dummy cells can be used, that are significantly smaller than the cells of the computational grid. However, in this case, problems may arise in extrapolating the gas-dynamic parameters to the cell or subzone.

Time coordination is the selection of macroscopic and microscopic integration steps. A macroscopic time step is usually determined by the velocity mode of the flow and in dimensional units can be in the range from milliseconds to nanoseconds. The microscopic time step ranges from fractions of a femtosecond to several picoseconds. The microscopic time step is determined by the parameters of the interaction potentials of the particles. The most correct results are obtained when using the lower edges of the specified time ranges. However, to increase the speed of calculations, often these parameters increase tenfold.

The main criterion for the selection of the integration step over time $\Delta t$ is the condition $l = \langle v \rangle \Delta t \leq l_{\text{max}}$, where $\langle v \rangle$ is the average velocity of the particles. At the macroscopic level, it means that the value $l$ should not exceed the linear size of the grid cell ($l_{\text{max}} - h$, where $h$ is the size of the grid cell for solving the QGD equations). At the microscopic level, a special scale $l_{\text{max}}$ is selected, usually associated with the cutting radius of the interaction potentials of the particles ($l_{\text{max}} - r_{\text{cut}}$).

In conclusion of section, we emphasize that when modeling complex gas-dynamic processes, it is first necessary to carry out calculations using algorithms of 1st and 2nd classes. Then, based on the data obtained, algorithms of 3rd and 4th classes can be applied.

3. Calculation results
This section shows the use of calculation according to the 1st class of algorithms for carrying out the calculations based on algorithms of 2nd and 4th classes. For this, the flow of nitrogen in the nickel microchannel was considered. The model geometry contained two nickel plates (top and bottom) with layers of adsorbed nitrogen adhered to them and a free layer of nitrogen between them (see Fig. 1). To accelerate the calculations in the second direction (y), a thin layer was taken (on the order of the mean free path of nitrogen molecules under normal conditions).

The geometrical parameters of the considered microsystem were as follows:
1) the sizes of the top and bottom nickel plates in nanometers $1017 \times 101.7 \times 8.5$;
2) the size of the gas medium between the plates in nanometers $1017 \times 101.7 \times 614.5$;
3) the number of nickel atoms in both plates was 162.57 millions;
4) the number of nitrogen molecules on the plates and between them was 2.68 millions.
At the beginning of the calculation, an equilibrium fixed gas-metal system was prepared corresponding to normal conditions ($p = 101325$ Pa, $T = 273.15$ K) and taking into account the effect of adsorption on the walls of the microchannel (see Fig. 1).

Then the gas in the middle part of the region (total height $H_z = 406.8$ nm) was accelerated to supersonic velocity ($0.4$ nm/ps) using a Langevin thermostat. After a short time (about 5 ps) the thermostat was turned off, and the gas subsystem evolved freely to an equilibrium state. In this case, the boundary conditions in the x and y coordinates were periodic, and in the z coordinate, rigid fixation of the microchannel walls was used.

The calculation results showed that at the level of the MD model, a flow is formed over time, whose longitudinal velocity profile has a Gaussian or hyper-Gaussian shape (depending on the height $H_z$ of the accelerated layer). However, the flow parameters near the wall are more interesting. To clarify this issue, Fig. 2 shows the dynamics of the main gas-dynamic parameters in several sections of $z$: a gas layer adsorbed on a metal ($z = 11.12$ nm), a moving layer nearest to it ($z = 12.18$ nm), an average section of the Knudsen layer ($z = 25.43 \sim 1/3$ of average free path length $\lambda$ in nitrogen under normal conditions), as well as in the center of the channel ($z = 305.11$ nm).

A comparison of these characteristics shows that a complex process is developing near the walls of the channel.

First, the gas adsorbed on the channel walls does not move; it has a very high density and does not satisfy the usual equation of state (the pressure in this layer is negative and close to the pressure in the metal). The temperature of the gas corresponds to the temperature of the metal.

Second, a strong instability develops in the gas layer near the wall, which is associated with the interaction of gas with the wall.

Thirdly, in the center of the Knudsen layer there is a strong influence of the total gas flow.

Thus, it is rather difficult to take into account all these processes within the framework of the classical boundary conditions for the QGD model. That is why, in such cases, instead of 2nd class algorithms, it is proposed to use the 4th class algorithms, in which the boundary layer is calculated on the base of the MD model, and the rest of the area is based on the QGD model.

**Figure 1.** Microchannel geometry in cross section.
Figure 2. Dynamics of flow parameters averaged over the x, y coordinates in different sections over z. Digit 1 corresponds to the layer of gas adsorbed on the metal; 2 corresponds to the layer of free-moving gas nearest to it; 3 corresponds to the Knudsen gas layer; 4 corresponds to the central layer of gas. Curves 1 of density and pressure are multiplied by the value of 0.001.

Let us now clarify the parameters of the coordinating the numerical models in the framework of the algorithm of the 4th class. It can be seen from the above calculations that the characteristic time for the MD to reach the regular mode is about 500 ps (250,000 MD steps, where one step is $\Delta t_{MD} = 0.002$ ps). The width of the boundary layer in this case is of the order $\lambda / 3$ for nitrogen under normal conditions (in fact, it determines the minimum cell size of the computational grid for QGD integration). The integration step of QGD equations $\Delta t_{QGD}$ should be 500 ps or more.

Let us now evaluate the possibility of practical implementation of the 4th class of algorithms. To do this, we note that the direct MD calculations were performed on the K60 supercomputer with the following parameters: the number of nodes with Intel Xeon E5-2690 v4 CPU is 78; the number of CPU on the node is 2; the number of trades on a node is 56; RAM on the node is 256 GB; total peak performance is 74.2 TFlops. The calculation time for one MD step at 10 nodes of K60 was 52.57 s. The calculations were significantly accelerated (up to approximately 0.003 seconds per MD step or up to 750 seconds for the entire calculation) by freezing the position of the metal particles. If we consider that outside the boundary layer, we can use the QGD equations calculated on a grid with cells with a linear size of $\lambda / 3$, then the calculated three-dimensional Cartesian grid required in this case will have a size of 43x4x26. This size is quite small and practically does not increase the total time for calculating one full time step. We also take into account that by increasing the number of K60 nodes used, the calculation time can be reduced up to 7 times. Finally, 250,000 MD calculation steps will be required only at the beginning of the calculation. In the future, MD computations will start from the
current state close to the equilibrium state. Therefore, the MD computation time will decrease significantly (up to 10 times or more). As a result, we can assume that on the K60 supercomputer in the full configuration, the average time for calculating one step for the QGD and MD models will be about 10 s. This value is quite acceptable for the calculation of stationary flow parameters (several thousand macroscopic time steps will be enough for this).

The prospect of the proposed technique is even more optimistic in the transition to calculations on new-generation graphics accelerators (for example, NVidia Tesla V100). In this new line of GPUs, each device has a fairly large RAM (up to 32 GB) and a peak performance of 8 TFlops for double-precision operations. If there is a modern interconnect (which is NVLink), the task based on the 4th class of algorithms will be solved only on the GPUs of the corresponding nodes and can be accelerated at least 25 times. This opens up great prospects for the transition to large particle systems (about 10 billion or more) and microsystems with linear sizes up to 100 microns.

4. Conclusions
The problem of numerical multiscale modeling of complex gas-dynamic processes in microchannels of technical systems is considered. To solve this problem, a multiscale approach based on the method of splitting by physical processes and the method of conjugation of a continuum model with a particle model was used. The equations of quasigas dynamics are used as a model of a continuous medium, and molecular dynamics is used as a model of particles. A feature of the problem was the consideration of the real dependences of the equation of state and kinetic coefficients on temperature and pressure, as well as the actual geometry of the microchannel walls. Research is performed on the example of the flow of nitrogen in the nickel microchannel. The paper considers the question of the methodology for coordinating the numerical solutions obtained in the framework of these models. As a result, the correctness of the multiscale approach was provided by the selection of suitable time intervals and grid sizes at the macrolevel. To support the proposed technique, direct molecular modeling of the flow in the channel was carried out and data were prepared for calculating such a flow using the equations of quasigas dynamics. The study confirmed the possibility of synthesizing these two numerical methods. The future of work is connected with the transfer of computer implementation to powerful graphics accelerators.

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