Supercomputer Calculation of Gas Flow in Metal Microchannel Using Multiscale QGD-MD Approach

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***Abstract*–An important factor in modern development are promising nanotechnologies. One of the most popular areas of research in this field is modeling the nonlinear gas-dynamic processes in micro- and nanochannels. This problem is relevant for many applications on introducing and using the nanotechnology in various industries. A feature of mathematical problems in this area is the simultaneous study of processes at many scales, including micro- and nanoscales. In this paper, technology of the supercomputer realization of multiscale two-level approach to modeling the gas flow in microchannel is presented. The approach is based on combining the models of continuum mechanics and the Newton's dynamics for single particles. Two scale levels are considered: macroscopic and microscopic. The quasigasdynamic equations system is used as a mathematical model at the macrolevel. The molecular dynamics method is used as a mathematical model at microlevel. Numerical implementation of approach is based on the method of splitting into physical processes. The quasigasdynamic equations are solved by finite volume method on grids of different types. The Newton's equations of motion are solved by Verlet integration in each cell of grid independently or in groups of connected cells. Within the framework of common methodology, the four classes of algorithms and methods of their parallelization are offered. Parallelization technology is based on the principles of geometric parallelism and efficient partitioning the computational domain. Special dynamic algorithm is used for load balancing the computational units. The approach testing was made by the example of the nitrogen flow in the nickel microchannel. Obtained results confirmed the high efficiency of the developed methodology.**

Keywords-multiscale mathematical models; parallel algorithms; multiscale computing; gas dynamics

I. INTRODUCTION

Modern computer technology allows modeling very large technical systems and complex physical processes at the level of detailing that was previously not available. In computer models of past years, the lack of detail was often compensated by introducing the correction coefficients in the model that reflected the data obtained experimentally. This approach is still being applied, but with the development of massively parallel computing systems, it becomes possible to get rid of many limitations inherent in simplified models and perform direct predictive modeling of a large set of interacting nonlinear and multiscale processes. The foregoing is relevant to the study of complex gas-dynamic processes in technical micro- and nanosystems, developed with the aim of introducing the nanotechnology in industry. A feature of mathematical problems in this area is the simultaneous study of processes on many scales, including micro- and nanoscale. One of the modern and actively developing approaches to solving such problems is a multiscale approach that combines the methods of continuum mechanics and particle methods. This combination allows you to replace an expensive and difficult realized physical experiment with computer calculations.

In the paper, the problem of gas flow through a microchannel is considered as an example. A multiscale approach [1][2] is used for modeling the process, which has two levels of detail related to the dimensions of the specific geometry of the problem (tens of mean free paths of gas molecules and more) and the distance between interacting particles (on the order of 1 nm). The implementation of the approach is based on splitting by physical processes. At the macrolevel of detail, a description of the flow of gas media occurs. At the microlevel, the interactions are calculated for: 1) gas molecules among themselves (forming the equation of state, determining transport coefficients); 2) gas molecules and atoms of solid surfaces (describing phenomena in boundary layers). The system of QuasiGasDynamic (QGD) [3] equations is used as the macrolevel model, the Molecular Dynamics (MD) [4] method is used as the microlevel model.

Modeling of tasks with many scales should occur according to certain rules. In the approach used, these rules also apply. The MD calculations can be carried out in a direct way, combining QGD and MD in one implementation, and indirectly, by accumulating a corresponding database, calculated in advance. It is also possible to use partially the MD database and partial direct MD modeling in conjunction with the QGD calculations. As a result, computational technology contains four main classes of algorithms.

The main goal of the work is to describe the details of algorithms in which the QGD and MD models are used directly, alternating at each step, and the results of calculations for these algorithms and analysis of the calculated data obtained will also be presented.

This paper is organized as follows. Section II describes the state of the art. Section III states the problem and the mathematical model. Section IV describes what methods and computing algorithms are used in the research. Section V presents the results of the current research.

 ISBN: 978-1-61208-668-2

II. STATE OF ART

The computing complexity of modeling the gas flows in microchannels is associated with the violation of continuity hypothesis in some parts of the computational domain. The physics for functioning of the similar systems is usually described by whole hierarchy of mathematical models up to the atomic level. The difference in the scales of the computational domain and near-surface interaction of the gas with the metal lead to the necessity to take into account the relief and the properties of the microchannel at the molecular level. As a result, the mathematical model of the research flow can not be fully formulated within the framework of the macroscopic approach.

The way to overcome the problem of boundary processes is molecular modeling of flow-wall interactions [5][6]. In the proposed approach, a joint solution of the gas-metal problem taking into account the wall structure is carried out within the framework of direct MD simulation. Previously, the structure of the walls was not taken into account due to the complexity of the calculations and the lack of computing power.

The way to overcome the problem of discontinuity is using a multiscale approach [7]-[12]. Multiscale approaches have become popular, but existing combinations have many limitations on the type of problems, the size of systems, on taking into account the real boundary conditions, and so on. Most often within the framework of the multiscale approach, the Navier-Stokes equations with a continuous model of the boundary layer are used without taking into account the real structure of the walls. In the proposed approach, there is a combination of two models (QGD, MD) and various methods of this combination (4 classes of algorithms) are presented, and a database calculated by the first class of algorithms is also created. Such an integrated approach did not exist before.

Why and when it is necessary to choose the proposed approach: when precision calculation is needed; when the simulated process is not represented enough and a detailed picture of what is happening is necessary; there is computing power to apply the approach.

Advantages of the developed approach are the possibility of calculations from the first principles; the ability to vary the different parameters of the technique in order to obtain acceptable accuracy results within a reasonable time.

The motivation for a particular study of this work is to show that in reality a continuous boundary layer model can not give an accurate picture of the flow, since all important factors are not known, especially in the case of microflows. In this situation, algorithms of class 4 or direct MD modeling can give an adequate result to reality.

III. STATEMENT OF THE PROBLEM

The mathematical model includes two components corresponding to the scale levels.

At the macroscopic level, the QGD equations are used. In the case of a pure gas of one kind, the system of QGD equations in the three-dimensional case in a form invariant with respect to the coordinate system in dimensional variables, together with the equations of state is written as:

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \mathbf{W}^{(\rho)} = 0, \ \frac{\partial E}{\partial t} + \operatorname{div} \mathbf{W}^{(E)} = 0, \quad \frac{\partial (\rho u_k)}{\partial t} + \operatorname{div} \mathbf{W}^{(\rho u_k)} = 0, \ k = x, y, z, \tag{1}$$

$$E = \frac{1}{2}\rho |\mathbf{u}|^2 + \rho\varepsilon, \ \ \varepsilon = c_V T, \ p = Z\rho\Re T. \tag{2}$$

Here $\rho = mn$ is the mass density (m is the mass of molecule of gas, n is the concentration), T is the temperature and $\mathbf{u}$ is the macroscopic velocity. Other parameters: p is the partial pressure of gas; E and ε are the total energy density and internal energy. Variables $Z = Z(T, \rho)$, $c_V = c_V(T)$ and $\Re = k_B / m$ are the compressibility coefficient, specific heat capacity and individual gas constant (k_B is the Boltzmann constant); vectors $\mathbf{W}^{(\rho)}$, $\mathbf{W}^{(\rho u_k)}$, $\mathbf{W}^{(E)}$ coincide, up to sign, with the fluxes of mass density, momentum density of the corresponding components, and energy density.

The system of equations (1)-(2) is closed by the corresponding initial and boundary conditions. The initial conditions are taken in accordance with the equilibrium state of the gas medium in the absence of interaction with external factors. The boundary conditions for the QGD equations on the microchannel walls can be specified by determining the fluxes of mass density, momentum density and energy density across the boundary using Newton's conditions, or by the normal components of them near the walls by the MD method. On the free surfaces of the computational domain, the so-called "soft" boundary conditions [3] are given.

Near the walls, the particles (atoms or molecules) that make up the material of the walls and are potentially capable of detaching from the microchannel surface should be added to the consideration. The evolution of the investigated system of particles is described by Newton's equations [4]. The equations system describing the motion of particles of l kind (gas or metal) has the following form:

$$m_l \frac{d\mathbf{v}_{l,i}}{dt} = \mathbf{F}_{l,i}, \quad \frac{d\mathbf{r}_{l,i}}{dt} = \mathbf{v}_{l,i}, \quad i = 1, ..., N_l, \ \ l = a, b, \tag{3}$$

where i is the particle number, l is the particle type (a – molecules of gas, b – atoms of metal in the microchannel), N_l is the total number of particles of type l , m_l is the mass of particle, $\mathbf{r}_{l,i} = (r_{x,l,i}, r_{y,l,i}, r_{z,l,i})$ and $\mathbf{v}_{l,i} = (v_{x,l,i}, v_{y,l,i}, v_{z,l,i})$ are the position vector and the velocity vector of the i -th particle of type l , $\mathbf{F}_{l,i} = (F_{x,l,i}, F_{y,l,i}, F_{z,l,i})$ is the resultant force acting on this particle.

The forces include the component of i -th particle interaction with the surrounding particles and the component responsible for external action:

$$\mathbf{F}_{l,i} = -\nabla_{\mathbf{r}_{l,i}} U + \mathbf{F}_{l,i}^{ext}, \quad i = 1, ..., N_l, \ \ l = a, b. \tag{4}$$

 ISBN: 978-1-61208-668-2

Here, $\mathbf{F}_{l,i}^{ext}$ is the force of interaction with the environment, U is the total potential energy and it depends on choosing the interaction potential of molecules. The potential energy of the system is represented as a function that depends on the coordinates of considered particles and describes the interaction between the particles of the system.

The initial conditions at the microlevel are determined by the equilibrium or quasiequilibrium thermodynamic state of the particle system at a given temperature, pressure, and average momentum. The boundary conditions at the molecular level depend on the simulated situation.

In the presented technique, there is a choice between the accuracy of the result and arithmetic complexity in combination with a large amount of computation. The compromise is to get the solution with the required accuracy in the minimum time. What parameters can we control: the size of the grid cells at the macrolevel. If the size is large, then QGD is considered fast, the MD is considered very slow; if the size is small, then a statistics for MD calculations is not very representative. In addition, there is a technique for allocating a virtual volume within a cell (see [2]). Also, the database, accumulated from the first principles, makes it possible to reduce the amount of computation in those flow zones where there are no strongly nonequilibrium processes. In particular, most of the metal can be frozen.

A set of benchmarking tests was carried out. For example, the calculations of kinetic coefficients were carried out according to the algorithms of class 1 [13], calculations of gas flows by algorithms 2-4 were carried out in [14][15].

IV. COMPUTING ALGORITHMS

The calculation of the macroparameters according to the QGD equations (1) is carried out using an explicit on time grid numerical algorithm, which is based on the finite volume method on grids of arbitrary type [16][17]. For the convenience of solving the problem in areas of complex geometry, the hybrid block meshes consisting of cells of various shapes and sizes can be used.

In the presented variant of computational technology, a hybrid spatial grid is introduced in the computational domain at the macrolevel. All parameters of gas components (density, pressure, temperature, velocity vector components, etc.) refer to the mass centers of the cells. Flux variables refer to the faces centers of the cells. Spatial approximations of the basic terms of the QGD equations are performed by standard methods (see, for example, [18][19]). The computing scheme on time is chosen explicit and two-stage (predictor-corrector) and is integrated with the variable step.

The system of MD equations (3), (4) is used in additional calculations independently, or as a subgrid algorithm applied within each control volume. To integrate the equations of motion (3), (4), the Verlet integration [20] is used.

To carry out a correct calculation of the QGD, the model is supplemented by real gas equations of state, transport coefficients and other accompanying parameters (enthalpies, average mean free paths, etc.), as well as real boundary conditions. Calculation of these dependencies, coefficients, and conditions is made using MD methods.

Modeling of problems on the basis of the multiscale approach under consideration with two levels of detail is carried out with the help of special algorithms that in general, depending on the degree of microlevel use, are divided into four classes [15].

Algorithms of class 1 suggest the study of the properties of gas medium and the properties of solid surfaces with which the gas medium contacts in technical applications. As a numerical implementation of the approach in this case, the Velocity Verlet scheme acts. With the help of 1 class algorithms, a DataBase of Molecular dynamic Calculations (DBMC) is accumulated for the properties of gases and solid materials, which can be used in the framework of other algorithms.

Algorithms of class 2 assume the solution of problems only at macrolevel based on QGD system of equations. In this case, the properties of the gas (the equations of state by pressure and energy, the kinetic coefficients such as viscosity and thermal conductivity, the parameters of the boundary conditions) are determined from the above-mentioned DBMC accumulated in advance for the desired temperature and pressure range.

Algorithms of class 3 imply the simultaneous use of QGD equations in the calculations and equations of Newtonian mechanics for molecules of a gaseous medium. Algorithms of class 3 are realized within the framework of the method of splitting into physical processes. It is assumed here that in the gaseous medium and on its boundaries it is possible to confine ourselves to a local consideration of the processes of the gases and gases with a solid wall.

Algorithms of class 4 also imply the simultaneous use in the calculation of QGD equations and equations of Newtonian mechanics for molecules of the gaseous medium and atoms of the surface layer of the wall. The difference of this case from the previous one is that in some areas of the medium (usually at the boundary and in the zones of a strong drop of the gas parameters), molecular dynamics calculations are carried out continuously without going to the macrolevel. In the same areas, the principle of locality of molecular interactions is not used, that is, in the general case, the algorithms of class 4 are nonlocal at the molecular level.

Direct MD calculation in the framework of algorithms of 3 and 4 classes seems to be the most justified, since it allows to coordinate the interaction processes at micro- and macrolevels. Also, a direct MD calculation can be performed for a specific set of physical conditions that are not present in the DBMC and appear in it as a result of this calculation.

In this work, the algorithms of class 4 are used for calculation the gas flow in microchannel. The resulting grid equations in the framework of the algorithms of class 4 at the predictor stage are solved not on the whole grid, but on its subset.

In algorithms of class 4, some of the cells are permanently assigned to molecular computations (produced in parallel with the QGD computations at each time step using (1)) and are not considered at the macroscopic level. As a rule, these are grid boundary cells. In some cases, internal cells are added to them, where highly nonequilibrium processes occur, characterized by large

 ISBN: 978-1-61208-668-2

gradients of gas-dynamic parameters. Denote the set of all such cells as Ω_B (QGD equations in these cells are not used). The remaining cells of the grid will be denoted by Ω_V (in these cells, both QGD and MD calculations are realized). As a result, the grid is represented as a union of two disjoint sets: $\Omega_V \cup \Omega_B$. The transition to the MD calculations in the cells of the set Ω_B is carried out once at the beginning of the general calculation. In cells from the set Ω_V the transition to MD calculations is performed at each step in time.

The corrector stage includes the use of MD calculations and is associated with obtaining corrective values of the main gas-dynamic parameters. In algorithms of class 4, this correction is used only in cells of the set Ω_V.

Before the calculation begins, a grid is constructed that is split into sets of cells Ω_V and Ω_B. Then in the cells of the set Ω_V, the equilibrium state of the macrosystem is set; in the cells of the set Ω_B, the equilibrium state of the microsystem, corresponding to the equilibrium state of the macrosystem, is given.

Then, at each step in time, a two-stage procedure is carried out. A two-level calculation is carried out in the cells of the set Ω_V, presupposing first the solution of the QGD equations, and then the correction of the obtained gas dynamic characteristics by means of MD calculations. In the cells of the set Ω_B, a one-level two-stage calculation is performed on the basis of the equations of molecular dynamics.

At the first stage, gas-dynamic variables are calculated in the cells of the set Ω_V according to the QGD equations. Variables are transferred to the MD unit to recalculate the parameters of the conditions at the boundaries of the sets Ω_V and Ω_B. In the cells of the set Ω_B, the evolution of the boundary microsystems is calculated, the data of which will then form the parameters of the conditions on the boundaries of the sets Ω_B and Ω_V.

At the second stage, in cell sets Ω_V and Ω_B the direct calculations are made, which allow obtaining all gas-dynamic variables at the macrolevel taking into account all physical processes.

The calculation step is completed by testing the breakdown criterion, which consists in determining the relative time derivatives of the mass density and the energy density of the gas.

Parallel implementation of algorithms of classes 1-4 is considered in detail in [15] and earlier works. Here, however, it should be noted that the parallel decomposition at the macrolevel is based on the method of static decomposition of the calculated grid into microdomains. Such a partitioning, even with large configurations of computers, is deliberately redundant. It allows to equalize the load of processors and/or special calculators at various stages of calculations by "transferring" a part of microdomains from one calculator to another. In the implementation of MD calculations, in addition to geometric decomposition, the particle partitioning and dynamic load balancing are used.

The developed approach can be generalized and applied to different types of flows, but additional calibration calculations and the addition of a database for specific gases and metals are needed. The algorithm itself will not change.

V. RESULTS AND DISSCUSSION

In this section, we will briefly present the results of testing the developed modeling technology. For this, we have chosen the problem of the nitrogen flow in a thin microchannel with a nickel coating of the inner walls. The scheme of the computational experiment consisted in calculating, on the basis of the algorithm of class 4, the interaction of a gas with a real crystal lattice of nickel. For simplicity, we chose a channel of rectangular shape, in the middle section of which the gas moves with supersonic speed (Mach is 14), and on the periphery the gas is strongly retarded by the wall. In this case, we took into account the effect of nitrogen adsorption on the nickel surface and heat exchange of the gas with the wall. The calculated region in one of the transverse directions (y) was considered extended and periodic boundary conditions were used along it. This approximation made it possible to reduce the amount of computation and take the following dimensions of the computational domain: $L_x = 3051\,nm$, $L_y = 101.7\,nm$, $L_z = 636\,nm$ (See Figure 1). Within this region, two boundary layers were identified, in which the interaction of the metal atoms of the walls and gas molecules was calculated by the MD method. The magnitude of these layers along the z coordinate was $L_{z1} = 86\,nm$. In the remaining middle layer with thickness of $L_{z2} = L_z - 2L_{z1}$ the gas flow was calculated on the basis of the QGD model. As a result, in the boundary layers, the total number of metal and gas atoms was approximately 488 million particles. In the middle part, a Cartesian mesh measuring 305x10x46 was used. With this size of the QGD grid, the computation takes up no more than 3% of the total computation. Therefore, the general time characteristics of the developed algorithm were analyzed below.

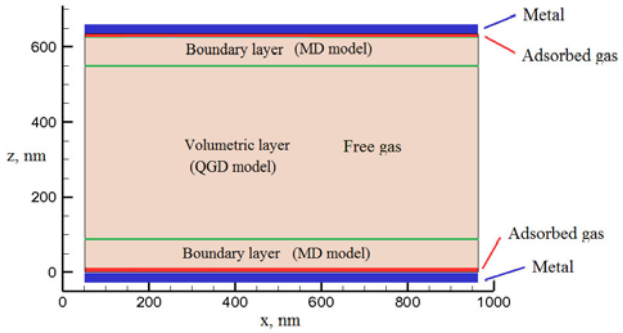

Figure 1. Computational domain. Section $y = 0$.

Test calculations of the flow in the microchannel of the indicated geometry were carried out on two computer systems with central and vector processors (see Table 1). The results of the acceleration and efficiency testing are presented in Figures 2 and 3.

TABLE 1. PARAMETERS OF USED COMPUTER SYSTEMS

Name	Node num-ber	Inter-connect type	Proc. type	Peak perfor-mance, TFlops	Proc. per node	Cores /Threads per proc.	Memo-ry per node, Gb
K60	78	Infini Band FDR	Intel Xeon E5-2690 v4	74,2	2	14/2	256
K48	16	Omni Path	Intel Xeon Phi 7250	48,7	1	68/4	96

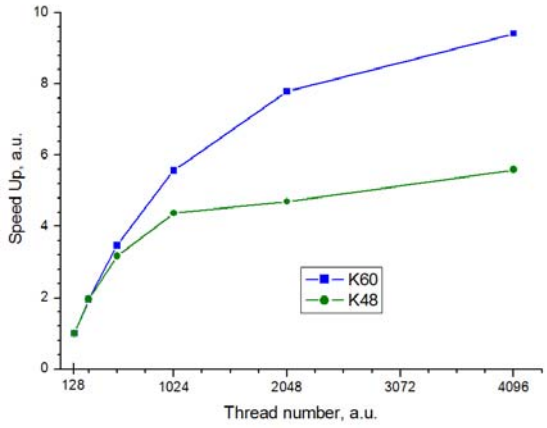

Figure 2. Speed up for the K60 and K48 systems.

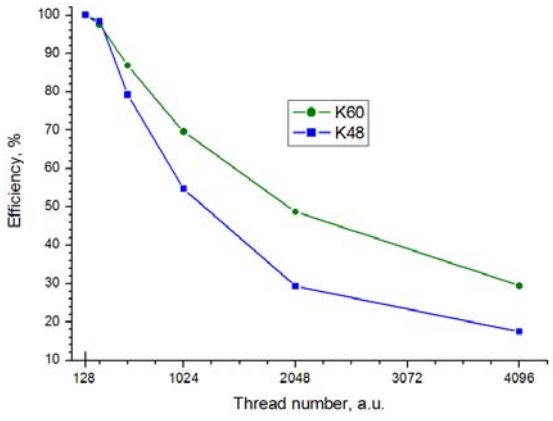

Figure 3. Efficiency of parallelization for the K60 and K48 systems.

Let us briefly discuss the results obtained. On the whole, it follows from the calculations carried out that the developed numerical approach and its parallel implementation make it possible to solve the chosen class of problems. A large amount of calculations in the MD block allows us to use rather large configurations of computer systems. However, the effective use of these systems lies in the ways of optimizing both the source algorithm and the developed code. In the case of using the CPU, the concurrency resource is not exhausted and the efficiency of the generated code is quite high. When using VPU of the specified type, there are 2 problems: 1) the cores of these processors are 10-15 times weaker than the CPU cores; 2) the fast VPU memory has a relatively small amount. As a result, in order to get the maximum effect from the VPU, you need to take order of magnitude larger configurations (in this example, containing about 160 nodes or more).

We also give some data on the simulated process. In accordance with the boundary value problem, the evolution of the jet is associated with the dissipative processes of the channel walls. They cause the jet to broaden with time, the flow rate decreases, the energy of the stream is transferred to the walls. This is illustrated by the distribution of the Mach number (Figure 4).

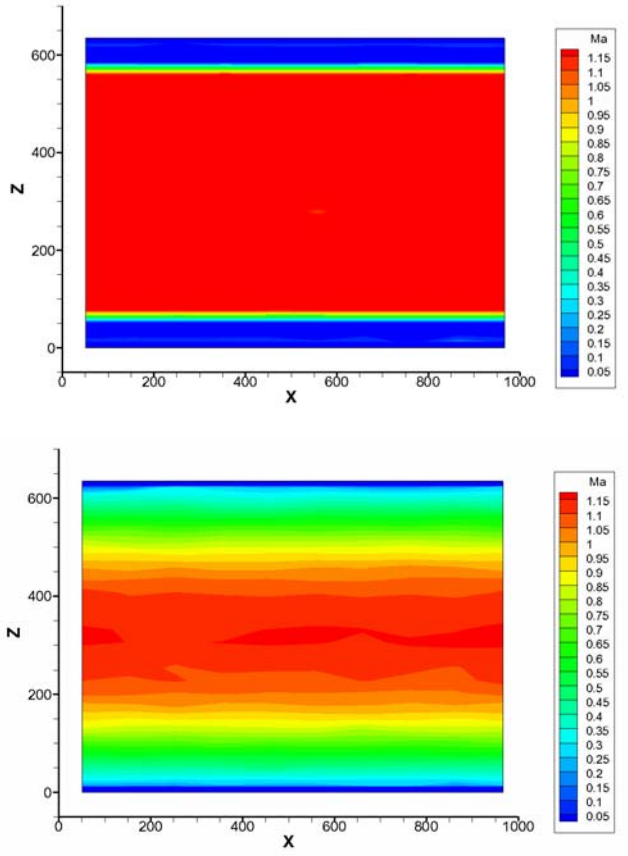

Figure 4: Initial (top) and steady state (bottom) distributions of Mach number averaged on y-coordinate.

 ISBN: 978-1-61208-668-2

VI. Conclusion and Further Work

The presented approach, computational algorithms and their program implementations work and allow specifying the flow parameters in the required place with the required accuracy.

The results are presented; they show the difference in performance between different computing systems when calculating the same problem. It should be noted that it is not possible to perform the calculation of one problem on one fixed computer system by other methods with the same or higher accuracy. Knowing the results of calculations for this approach, it is possible to form a QGD model or a Navier-Stokes model with a boundary layer and obtain the same result with the same accuracy in less time. However, "blindly" this can not be done.

The prospects of this work lie in further optimizing the code and adapting it to new generations of CPU, VPU and GPU and carrying out of detailed numerical experiments.

Future work involves expanding the database and analyzing the flows of various gases and liquids, as well as multiphase flows.

Acknowledgment

This work was supported by the Program of the Presidium of the Russian Academy of Sciences No. 26.

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 ISBN: 978-1-61208-668-2