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RESEARCH ARTICLE

The modeling of two-dimensional vortex flows in a cylindrical channel using parallel calculations on a supercomputer

Ivan G. Lebo @,
Ivan V. Obruchev

MIREA – Russian Technological University, Moscow, 119454 Russia
@ Corresponding author, e-mail: lebo@mirea.ru

Abstract
Objectives. The study aimed to examine vortex structures formed during the interaction of incident and reflected shock waves in a cylindrical channel. The shock wave was described by the Hugoniot relations, which make it possible to determine the parameters of the gas behind the shock front by a given Mach number and the values of the gas-dynamic parameters ahead of the pressure jump. The propagation of a strong shock wave (Mach number was 20) in argon was simulated.
Methods. The methods of mathematical modeling were used. A parallel algorithm for solving two-dimensional equations of gas dynamics in cylindrical coordinates (r, z, t) was developed and a new version of the *NUTCY_ps* program created. The calculations were performed on an MVS-100K supercomputer.
Results. Two methods of parallelization when solving a system of equations were considered. Using a specific task as an example, a comparison of the effectiveness of these methods was conducted. A parallel algorithm was developed and a program was upgraded for solving two-dimensional equations of gas dynamics in cylindrical coordinates (r, z are spatial coordinates, t is time). Numerical calculations were performed to simulate: 1) the shock wave incidence to and reflection from a metal screen; 2) the propagation of the shock wave through a hole in the screen; 3) the propagation of the shock wave through a cylindrical channel and its reflection from the bottom of the channel and interaction with the incident wave.
The results obtained by the parallel supercomputer with different numbers of processors are presented. It is shown that using 16 processors, it is possible to reduce the computation time for getting a solution for the test problem by approximately 12 times.
Conclusions. It is shown that the interaction of incident shock wave and the one reflected at an angle leads to the formation of regions with low and high gas densities, as well as vortex flows. The vortex interaction area (turbulence zone) gets a complex shape. The article discusses the possibility of carrying out full-scale experiments in shock tubes or using a laser shock tube. Such studies would make it possible to compare experimental data with the results of numerical simulation and, on their basis, to develop more advanced models of turbulent motions.

Keywords: numerical simulation, supersonic flows, vortices, two-dimensional gas dynamics in cylindrical coordinates

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НАУЧНАЯ СТАТЬЯ

Моделирование двумерных вихревых течений в цилиндрическом канале с помощью параллельных вычислений на суперкомпьютере

И.Г. Лебо @,
И.В. Обручев

МИРЭА – Российский технологический университет, Москва, 119454 Россия
@ *Автор для переписки, e-mail: lebo@mirea.ru*

Резюме

Цели. Изучается эволюция вихревых структур, формирующихся при взаимодействии падающей и отраженной под углом ударных волн в цилиндрическом канале. Сама ударная волна задается с помощью соотношений Гюгонио, позволяющих определить параметры газа за фронтом ударной волны по заданному числу Маха и значениям газодинамических параметров перед скачком давления. Моделировалось распространение сильной ударной волны (число Маха равнялось 20) в инертном газе аргоне.

Методы. Используются методы математического моделирования. Разработан параллельный алгоритм решения двумерных уравнений газовой динамики в цилиндрических координатах (r, z, t) и создана новая версия программы *NUTCY_ps*. Расчеты выполнены на суперкомпьютере МВС-100K.

Результаты. Рассмотрены две методики распараллеливания процессов при решении системы уравнений. На примере конкретной задачи проведено сравнение эффективности этих методик. Развит параллельный алгоритм и модернизирована программа для решения двумерных уравнений газовой динамики в цилиндрических координатах (r, z – пространственные координаты, t – время). Проведены численные расчеты, моделирующие: 1) падение и отражение ударной волны от металлического экрана; 2) прохождение ударной волны через отверстие в экране; 3) прохождение ударной волны через цилиндрический канал и ее отражение от дна канала, взаимодействие с падающей волной. Представлены результаты тестовых решений на параллельном суперкомпьютере с использованием различного числа процессоров. Показано, что при использовании 16 процессоров удается приблизительно в 12 раз сократить время расчета тестовой задачи.

Выводы. Показано, что при взаимодействии падающей и отраженной под углом ударными волнами формируются области с пониженной и повышенной плотностью газа, а также вихревые течения. Область взаимодействия вихрей (зона турбулентности) приобретает сложную форму. В статье обсуждается возможность проведения натурных экспериментов на ударных трубах или с помощью лазерной ударной трубы. Такие исследования позволили бы сравнить экспериментальные данные с результатами численных расчетов и на их основе развить более совершенные модели турбулентных движений.

Ключевые слова: численное моделирование, сверхзвуковые течения, вихри, двумерная газовая динамика в цилиндрических координатах

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INTRODUCTION

The study of complex turbulence in supersonic gas flows is a demanding problem of modern gas dynamics and high energy density physics. Such phenomena occur when flying vehicles enter the Earth's atmosphere, in astrophysics, when analyzing the consequences of collisions of our planet with space objects, and in researches in the field of laser thermonuclear fusion.

Methods of mathematical modeling are used for the numerical solution of such problems [1−4].

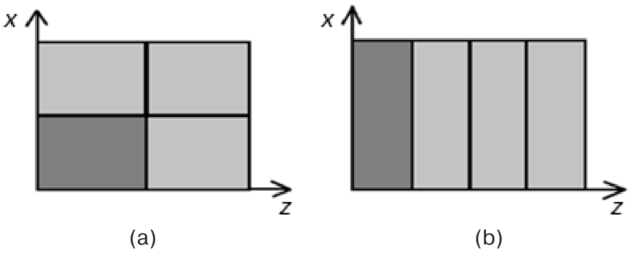
In [5], the peculiarities of the interaction of two vortices in a gaseous medium were studied. To simulate this phenomenon, a parallel algorithm and a 2D program *NUT_2D* were developed to solve the equations of dynamics of a two-component gas in Cartesian coordinate system on MVS-100K supercomputer at the Joint Supercomputer Center of the Russian Academy of Sciences (JSCC RAS)[1]. To solve the equations, TVD-difference schemes of a higher order of approximation are used [6, 7].

The next step is the development of a 2D program for solving the equations of gas dynamics in cylindrical coordinates and an algorithm for solving problems using a parallel supercomputer MVS-100K.

In this article we present the results of calculations performed using the advanced 2D *NUTCY* program in cylindrical coordinates (r, z are spatial coordinates, t is time) [8]. The mathematical model of the program is based on the equations of gas dynamics along with the Hugoniot conditions, which make it possible to set the parameters of the gas behind the shock front [9].

An algorithm for parallel computations was developed and a new version of the *NUTCY_ps* program was created to find the solution to two-dimensional equations of gas dynamics in cylindrical coordinates. The calculations were conducted on the MVS-100K complex using a large number of processors.

There are two main types of parallelization: algorithmic (through control) and geometric (through data). Due to significant potential of the *NUTCY* program in data parallelization, a geometric method was chosen to solve the problem: 1) to be computed region in the form of a cylinder in the section orthogonal to the cylinder's axis was divided by planes perpendicular to the axis into subregions of equal linear dimensions; 2) the division was conducted in two directions—along the Oz axis and into cylindrical layers of equal thickness along the Or^1 axis ($x = r$, Fig. 1). The boundaries and locations of the subregions computed by the processor were calculated using their indexes, which were assigned by the MPI communicator during initialization. Each processor stores in memory the values of only those cells that are included in its subregion; the control processor has additional buffers for data input and output. At each computational node, the calculation was conducted according to the same scheme. In the course of the calculations, we used both variants of partitioning the region: along two axes (Fig. 1a) and along one axis (Fig. 1b).



(a) (b)

Fig. 1. Schemes of parallelization in the new version of *NUTCY_ps*: (a) along two axes, (b) along one axis. In Fig. 1, $x = r$

To keep the uniformity of the computational scheme for each new subregion, two layers of fictitious cells were introduced on each of the four (two in the case of a one-dimensional distribution) boundaries. The values in these cells were determined in two ways, depending on the position in the grid:

1) based on the boundary conditions (if the boundary of the new subregion coincided with the boundary of the entire computational region);
2) data were transferred to the boundary of the next subdivision from the processor that processes the previous subregion (for internal subregions).

A special procedure has been written for data exchange. Each processor maintains indexes of its "neighbour processors." The procedure implements the transfer of the values of the gas-dynamic values

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[1] www.jscc.ru

of the boundary cells to the "processors–neighbours" and the receipt of the values of the fictitious cells from the neighbours. If we consider the "left" boundary of the subregion, then the values of cells with indices 1 and 2 will be transferred to the neighbour "on its left," the values of cells 0 and −1 will be received from the latter. For non-uniform operations (for example, data input and output) the processor with index zero acts as the manager and exchanges data with the rest of the processors. All data transfer operations between computational nodes are implemented using MPI tools.

TASK STATEMENT

The *NUTCY* program enables to numerically solve the equation of gas dynamics in a 2D cylindrical configuration in the Euler coordinate system:

$$\begin{aligned}
&\frac{\partial\rho}{\partial t}+\frac{1}{r}\frac{\partial r\rho u}{\partial r}+\frac{\partial r\rho\omega}{\partial z}=0,\\
&\frac{\partial\rho u}{\partial t}+\frac{1}{r}\frac{\partial r\rho u^2}{\partial r}+\frac{\partial\rho u\omega}{\partial z}+\frac{\partial\rho}{\partial r}=0,\\
&\frac{\partial\rho\omega}{\partial t}+\frac{1}{r}\frac{\partial ru\omega}{\partial r}+\frac{\partial\rho u\omega}{\partial z}+\frac{\partial\rho}{\partial z}=0,\\
&\frac{\partial e}{\partial t}+\frac{1}{r}\frac{\partial ru(e+p)}{\partial r}+\frac{\partial(e+p)\omega}{\partial z}=0.
\end{aligned}\qquad(1)$$

Here ρ is the density; p is the pressure; $V_r = u$, $V_z = \omega$ are the components of the velocity vector, **V**; $e=\rho\left(\varepsilon+\frac{V^2}{2}\right)$ is total energy. In addition, the following equations are added to (1):

1) gas law:

$$p=(\gamma-1)\rho\varepsilon,$$

where, ε is specific internal energy, γ is adiabatic gas constant.

2) the continuity equation for each gas component (total number of components is n):

$$\frac{\partial\rho_i}{\partial t}=\operatorname{div}\rho_i V=0,\ \text{где}\ i=\overline{1,n-1}.\qquad(2)$$

If the gas contains two components, then it is convenient to solve the continuity equation for the mixture (the upper equation of system (1)) and the equation for one of the components (2). Next, the concentration of the first component C is determined, and the concentration of the second component is found as $1 - C$.

The shock wave (SW) was given by the Hugoniot relations:

$$\begin{aligned}
&P_1=P_0\frac{2\gamma M_x^2-(\gamma-1)}{\gamma+1},\quad ZP=\frac{P_1}{P_0},\\
&C_s^2=\gamma\frac{P_0}{\rho_0},\qquad D=M_xC_s,\\
&\rho_1=\rho_0\frac{\gamma+1+(\gamma-1)/ZP}{\gamma-1+(\gamma+1)/ZP},\\
&u_1^2=\left(\gamma\frac{P_1}{\rho_1}\right)\frac{\gamma-1+(\gamma+1)/ZP}{2\gamma}.
\end{aligned}\qquad(3)$$

Here $P_1(0)$, $\rho_1(0)$ are the pressure and density behind the shock front (ahead of the shock front) of the SW; C_s is the speed of sound; D is the velocity of the shock front in the laboratory frame of reference. It is sufficiently to set the Mach number (M_x) and the thermodynamic parameters of the gas ahead of the shock front to determine the corresponding parameters behind the shock front. The gas velocity behind the shock front in the laboratory frame of reference is determined by the formula $w_1 = D - u_1$.

The propagation of a SW in a region filled with gas and its interaction with an aluminum screen (density ρ = 2.7 g/cm^3) located in this region were simulated. The computational region ($0 < r < R$, $0 < z < L_z$, where R, L_z are the sizes of the region) is filled with an inert gas—argon; adiabatic exponent $\gamma = 5/3$; initial pressure P_0 = 0.5 atm; density ρ_0 = 0.804 mg/cm^3.[2] The task statement is illustrated by Fig. 2a. The SW specified by the Hugoniot relations in the region $0 < z < b_0$ (the initial boundary of the subregion, disturbed SW, Mach number M_x = 20) propagates from the top to bottom. The gas velocity behind the shock of the incident SW is V_z = −4.817 km/s.

TASK 1:
SW REFLECTION FROM THE SCREEN

In Task 1, an aluminum screen with the initial density ρ = 2.7 mg/cm^3 is placed in the computational region. In the first run of calculations, the solution to the quasi-one-dimensional problem was checked, and the propagation of the SW along the channel and its reflection from the screen were simulated. The parameters used in Task 1: R = 0.25 cm, L_z = 0.5 cm, gas velocity behind the shock front v_z = –4817 m/s.

The calculations were performed on a difference grid (250 × 500 nodes) on a personal computer. Below are the results of the calculations.

The shock wave has reached the screen and reflected off. By the time t = 0.0005 ms, the reflected wave propagates towards the upper end of the shock

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[2] The *NUTCY* program uses the CGS system to operate, however, here the time scale is given in milliseconds.

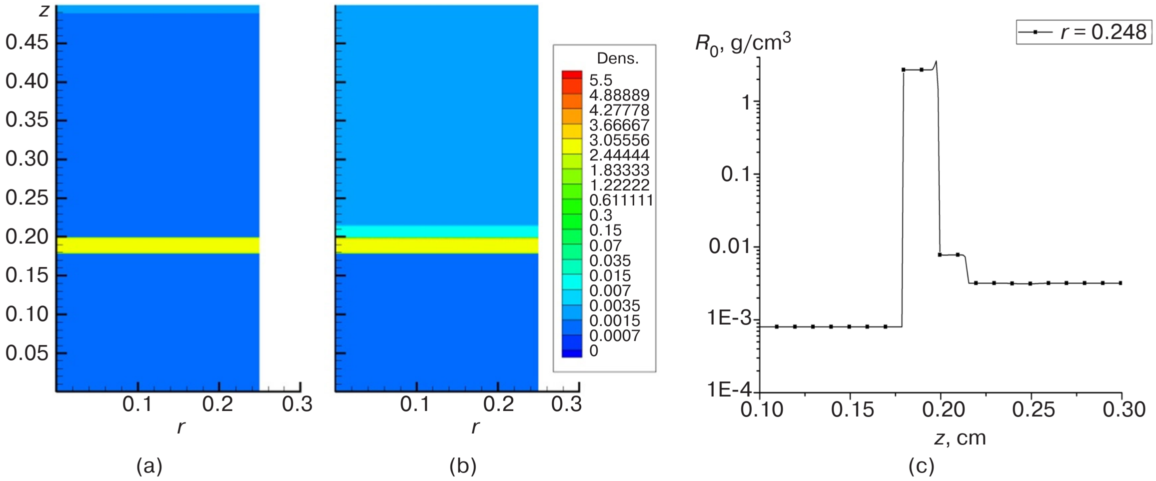


Fig. 2. Density distributions at (a) $t = 0$; (b) $t = 0.0005$ ms, (c) instantaneous density distribution along axis Oz at $t = 0.0005$ ms; $r = 0.248$ cm is the radius value for which the "density profile" is plotted along axis Oz ($R_0 = \rho(z)$ [g/cm^3])

tube. Figure 2c shows the "density profile" near the outer boundary of the cylinder $r = 0.248$ cm. The gas velocity behind the shock front of the reflected SW is $V_z = -0.198$ km/s at time $t = 0.0005$ ms, that is, the shock front of the reflected SW propagates upward towards the incident shock, and the gas keeps compressing.

TASK 2: SW PROPAGATION THROUGH A HOLE OF THE SCREEN

In the second run of calculations, a hole was added to the aluminum screen located in the computational region. Partial propagation of a SW through the hole and its diffraction at the edge of the hole were simulated. Because of complex physical phenomena involved in this process, it was necessary to use high-resolution grids. The calculations were carried out in two stages: on a personal computer with a grid of 250 × 500 nodes and on one processor of the MVS-100K complex with a grid of 1000 × 2000 nodes. The obtained data showed similar results for both cases.

A diffraction region of the SW appears in the vicinity of the "hole-screen" boundary. Refraction of the wave leads to the formation of vortices. Note that the gas velocity behind the shock front of the SW reflected from the screen (red line in Fig. 3c) is $V_z = -0.198$ km/s, that is, equal to the gas velocity in the reflected wave in Task 1.

The increased number of grid nodes allows for, in principle, to study in more detail the processes occurring in the diffraction region. This, however, significantly increases the time required for these calculations. A version of the *NUTCY* program was developed for calculations on a multiprocessor supercomputer complex

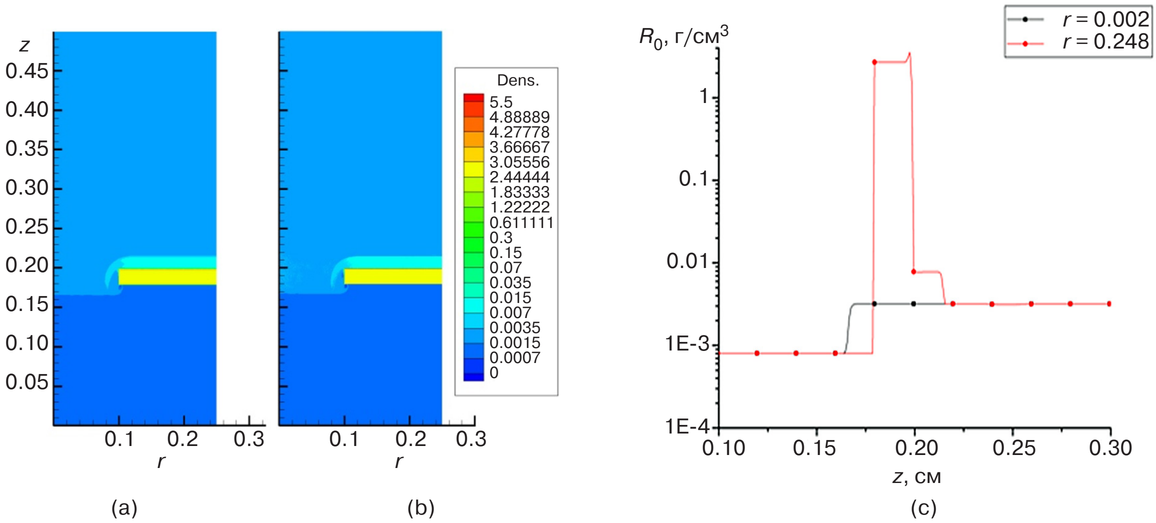
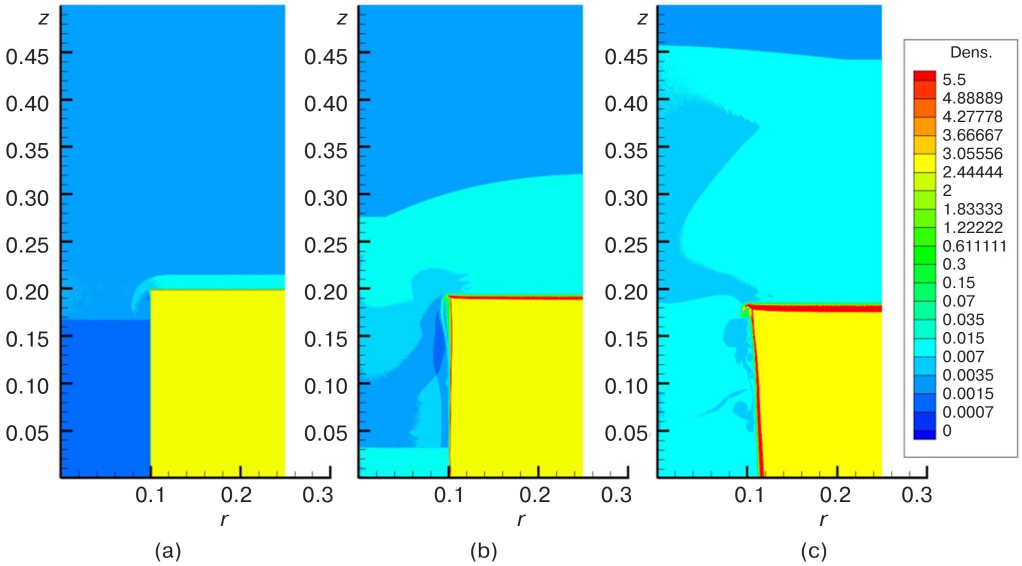


Fig. 3. Density distributions (at $t = 0.0005$ ms), obtained on (a) personal computer with a grid of 250 × 500, (b) MVS-100K (8 processors, grid 1000 × 2000). (c) density profiles at $t = 0.0005$ ms near the axis ($r = 0.002$ cm) and near outer boundary ($r = 0.248$ cm)



(a) (b) (c)

Fig. 4. Density distributions at (a) $t = 0.0005$ ms, (b) $t = 0.00085$ ms, and (c) $t = 0.00135$ ms

(*NUTCY_ps* program). Using the multiprocessor version of the program, the calculations were performed for the previous task (Task 2); the obtained results were similar to those shown in Fig. 3a (see Fig. 3b). The calculations were performed on 8 processors. This computation served as an errors-free test for the new version of the *NUTCY_ps* program.

TASK 3:
SW PROPAGATING INTO A LONG CHANNEL

Calculations for the third task were conducted on a multiprocessor complex MVS-100K using the *NUTCY_ps* program.

As part of the third task, the aluminum screen was replaced by an aluminum wall with an extended channel. At its bottom end there was an absolutely elastic wall. We studied the propagation of the SW along the channel downward and reflected off—up to the time it escaped the channel. The density distribution across the computational region was studied. Due to the increased "time-consuming" calculations on the grid 1000 × 2000 nodes, the program was launched on 16 processors of the MVS-100K complex in two modes: distribution along one axis and along two axes.

The graphs illustrating the SW dynamics are shown below.

Figure 4a corresponds to the point in time when the SW enters the channel; Fig. 4b—the front of the SW reaches the bottom and is reflected off; Fig. 4c—the reflected SW escapes the channel.

The graphs show the appearance of zones of increased gas density and "bubbles" arising behind the refraction front of the SW when it enters the channel and escapes it.

The results obtained by this technique as well as the effectiveness of two approaches to geometric parallelization of computation are given in Table 1.

Table 1. Comparison of consumed time for calculating one step and 6000 steps in different modes of parallelization

Calculation mode (grid 1000 × 2000 nodes)	Average time consumed for one step, s	Total time consumed by the program when calculating 6000 steps, s
Single processor	1.982	12462
Multi-processor in a configuration 4 × 4	0.155	1175
Multi-processor in a configuration 1 × 16	0.167	1234

It turns out that with the same number of processors, two-dimensional parallelization is more effective due to reduced total number of intra-processors' exchanges. The table shows that the computation time was decreased by about 10–13 times when switching from a single-processor program to a 16-processor one. With two-dimensional parallelization, a gain of 7–8% relative to the one-dimensional one is obtained. With an increase in the number of processors, this gain can be further increased; however technical and organizational disadvantages are possible.

DISCUSSION OF RESULTS AND CONCLUSION

Three runs of calculations were conducted.

In the first run, the numerical solution to the quasi-one-dimensional problem was verified. It is shown that the results agree with the analytical solution for the propagation of a SW in gas.

In the second run, two-dimensional phenomena associated with the refraction of a SW propagating through a hole in the screen were observed. It is shown that when developing a parallel computation algorithm (*NUTCY_ps* program) and switching to grids of increased resolution, the results of calculations for Task 2 are identical to the results obtained by the calculations when a single-processor version was used.

In the third run of calculations, the propagation of a SW along an extended channel and reflection from its bottom were studied. It was observed that the interaction of the incident and reflected waves leads to the appearance of zones with increased gas density and zones of low density. In this case, the vortex interaction region gets a complex shape.

Comparison of the two methods of geometric parallelization supported the theoretical assumptions about the greater efficiency of the two-dimensional computations. In conclusion, we note that further reduction of the computation time is possible by modifying the way of operation with data input and output (multiprocessor reading and writing to a file).

At the beginning of the article, it was noted that the study of the development of hydrodynamic instability and the transition to turbulence is of great importance for researches on laser thermonuclear fusion. In Russia [10] and overseas [11–13], high-power multichannel lasers are being built to initiate thermonuclear microexplosions. Along with the study of the compression of microtargets in such installations, it will be possible to perform research on the initiation and interaction of SWs and the development of substance mixing in a laser shock tube [14]. Compared to classical shock tubes, high gas flow velocities[3] (and high Mach numbers) are easily achieved in a laser shock tube, and it is possible to simulate these processes in complex chambers filled with various media. Laser shock tubes are promising for modeling in laboratories some astrophysical phenomena associated with the protection of the Earth from collisions with space objects, as well as other problems in high energy density physics.

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Authors’ contribution

I.G. Lebo—physicomathematical model and code development, problem statement, analysis of results (70%).

I.V. Obruchev—simulations and graphical treatment (30%).

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[3] Velocities are comparable to ones of space objects which can enter the Earth atmosphere (~10–20 km/s).

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About the authors

Ivan G. Lebo, Dr. Sci. (Phys.-Math.), Professor, Department of Higher Mathematics, Institute of Artificial Intelligence, MIREA – Russian Technological University (78, Vernadskogo pr., Moscow, 119454 Russia). E-mail: lebo@mirea.ru. https://orcid.org/0000-0001-8341-9453

Ivan V. Obruchev, Competitor of a Scientific Degree, Engineer, MIREA – Russian Technological University (78, Vernadskogo pr., Moscow, 119454 Russia). E-mail: ivan_obruchev97@mail.ru

Об авторах

Лебо Иван Германович, д.ф.-м.н., профессор кафедры высшей математики Института искусственного интеллекта ФГБОУ ВО «МИРЭА – Российский технологический университет» (119454, Россия, Москва, пр-т Вернадского, д. 78). E-mail: lebo@mirea.ru. https://orcid.org/0000-0001-8341-9453

Обручев Иван Владимирович, соискатель, инженер, ФГБОУ ВО «МИРЭА – Российский технологический университет» (119454, Россия, Москва, пр-т Вернадского, д. 78). E-mail: ivan_obruchev97@mail.ru

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