VNIIEF Methods of Numerical Simulation for Multi-Dimensional Gas Dynamic Flows

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The Introduction presents a brief review of the approaches to the development of mathematical simulation methods for 2D and 3D gas dynamic flows, used by VNIIEF. In the main part of the Report the development principles of the regular Lagrangian-Eulerian technique (LEGAK), based on the application of the concentration method for computation of gas dynamic flows with big contact boundaries deformations, are presented in detail. The examples of several problem computations are presented.

Introduction

The application area of developed in VNIIEF gas dynamic techniques is computation of multi-dimensional non-stationary flows of inhomogeneous continuum with consideration of different physical phenomena, such as: gas dynamics, elastoplasticity viscosity, detonation of explosives, radiant heat conductivity, etc.

The special features of simulated problems are the existence of several physical substances in studied systems and big deformations of contact boundaries.

As we know, numerical simulation of such flows, especially in the 3D case, is followed by many troubles. These troubles come from two contradictory requirements to numerical techniques: the possibility of computation of flows with big deformations of contact boundaries in the “crash-proof/hand-off” mode (which is especially important at parallel computations on cluster systems) and the necessity of high computation precision (required by certain applications). Various approaches to these troubles, based on the compromise between the precision and “crash-proofness”, led to the development of a row of finite-difference methods and techniques, which differ from each other in the

types of used computation grids (regular, non-regular, Lagrangian, Lagrangian-Eulerian and Eulerian ones) and the methods of detachment of contact boundaries.

The DMK (Sofronov et al., 1984) and MEDUZA (Glagoleva et al., 1972) techniques are based on the application of Lagrangian grids. In MEDUZA there is the possibility of grid topology variation in the course of problem solution (including variation in the vicinity of contact boundaries) and appropriate recalculation of values in accordance with convection flows.

In the regular Lagrangian technique D (Dmitriev et al., 1979, Artem'ev et al, 1989) local correction of fragments of the Lagrangian grid at big deformations by means of automatic improvement of "bad" points of the 3D Lagrangian grid and recalculation of grid values for the improved grid is used. At point improvement the technique of "mixed" cell computation is used on the interface of different substances, which is based on the introduction of adaptive grids in the cells with several substances.

In some VNIIEF techniques, which use regular computation grids, a part of (or all) the contact surfaces with complicated topologies or seriously deformed during computation, are computed on a grid, which lines do not coincide with them. It is carried out by means of the concentration method developed in VNIIEV (Bakhrakh et al., 1981) for computation of so called "mixed" cells occurring in this case. Such approach is used in the EGAK (Bakhrakh et al., 1981) and TREK (Yanilkin at al., 1997) Eulerian techniques, the LEGAK Eulerian-Lagrangian technique (Bakhrakh et al., 1984, Bakhrakh et al., 1999, Bakhrakh et al., 2003) and LEGAK-3D (Bakhrakh et al., 2004), MIMOZA (Sofronov et al., 1989, Zmushko et al., 1988), RAMZES-KP (Voronin et al., 1988, Sofronov et al., 1999). Realizations of the concentration method in the techniques specified above differ from each other in the models and computation algorithms for "mixed" cells on the Lagrangian and Eulerian (calculation of convection flow values) stages. Thus, for example, in the RAMZES-KP technique the algorithm of contact boundary localization inside the computational cell, proposed by Youngs (1982), is used. The algorithms, resident in the concentration method, are also used in the MEDUZA non-regular technique. Apart from this, the specified methods are characterized by the topology of used regular grids and finite-difference schemes.

To improve the quality of difference approximation of homogeneous substance convective flows on the Eulerian computation stage in the techniques, which use the regular computational grid, the PPM method (Wodward and Colella, 1984) and its modifications have been widely used. Such approach combined with the concentration method in "mixed" cells, is used in the EGAK, TREK, LEGAK, RAMZES-KP techniques. In MIMOZA the modified method of finite linear reconstruction is used.

Speaking about "subgrid" approaches to the description of contact boundaries, developed in VNIIEF, we should mention the method of adaptive refined grids, used, for example, in the EGAK++ technique (Yanilkin et al., 2000), and the method of explicit detachment of contact boundaries, which do not coincide with the grid lines, that is the method of contact line detachment (CLD, Stenin et al., 1998), developed in the frames of the LEGAK technique. In the method of adaptively refined grids a more refined (than the basic one) computational grid is introduced in the vicinity of contact boundaries. The method of contact line detachment (CLD) as the lines, which motion is calculated in a

certain way, traces back to Nokh's work (1964). The points, describing contact boundaries, are located independently of the nodes of the computational grid.

Another VNIIEF approach to the development of numerical algorithms is the realization of the discrete method of smoothed particles (the SPH technique by Bashurov and Potyanhina, 1998).

The main part of the Report contains a more detailed description of the Regular Lagrangian-Eulerian technique LEGAK-2D (Bakhrakh, 2004), based on the application of the concentration method for the computations of gas dynamic flows with big deformations of contact boundaries. Some examples of problem computations are presented.

LEGAK-3D Method for Computation of 3D Non-Stationary Flows of Multi-Component Continuum and Principles of Its Realization on Multiprocessor Computers with Distributed Memory

Principles of the LEGAK technique

The LEGAK technique (Bakhrakh, 1984) is the fininte-difference Lagrangiean-Eulerian technique, which uses a regular grid. In the 3D geometry it is the grid, made of prominent hexahedrons.

In the LEGAK technique the following is applied:

- The Lagrangian-Eulerian computational grid, which is partially carried along by the substance; at that it is admitted that the surfaces of the computational grid may both coincide and not coincide with the boundaries of the substances; in the latter case cells with several substances appear and concentrations are introduced for consideration (Bakhrakh, 1999);
- Continuous concordant representation (Bakhrakh, 1988) of the flows of mass, energy, momentum and other values at the approximation of convective terms of the initial system of equations;
- Donor-acceptor algorithm (Bakhrakh, 1981, Bakhrakh, 1999) of convective flow computation to avoid computation diffusion; basing on the fields of substance concentrations in the vicinity of a donor cell the algorithm determines which substances and in what ratio flow out from the cell containing several substances.

When the difference scheme is being built, the system of conservation laws, written for an arbitrary element of the space **Ω,** limited by the surface **S**, is used:

$$\frac{dF}{dt} + \int_S G(\overline{u} - \overline{u}^{\times})\, d\overline{s} = -\int_\Omega H\, dv, \qquad (1)$$

where vectors *F, G, H* have the following components:

$$F(M, M\bar{u}, Me);\ G(\rho, \rho\bar{u}, \rho e);$$
$$H\left\{o, grad\, p + div\, \hat{k}, p\, div\, \bar{u} + sp(\hat{k}\hat{D})\right\};$$

$M=\rho v$ is the mass, comprised by an element of the space , **Ω**;,
P is the pressure determined by the equation of state of the medium, $p(\rho, e)$;
$\hat{D}$ is the deviator of the deformation velocity tensor;
$\hat{k}$ is the strain deviator, determined by Hooke's law and Mises' yield condition;
$\bar{u}^{\times}$ is determined by the law of motion of the surface S.
Other denotations are conventional.

Solution of the system of equations 1 is carried out by integration over time with the application of the splitting method (by Koven'a and Yanenko, 1981).

For this purpose the initial system of equations 1 is split into two subsidiary ones.

The first system – the Lagrangian stage – is obtained out of the supposition, that the surface ***S*** moves with the same velocity as the substance, that is at the first stage the following system of equations is solved:

$$\frac{dF^{(1)}}{dt} = -\int_{\omega} H\, dV\ . \tag{2}$$

At the second (Eulerian) stage it is supposed, that the substance is at rest, while the surface ***S*** is moving. Thus, the system of equations to be solved at the second stage, has the following view:

$$\frac{dF}{dt} + \int_{S} G^{(1)}(u^{(1)} - u^{*})\, dS = 0. \tag{3}$$

In its turn when the system of equations 2 is solved, the method of splitting over physical processes is used.

Difference formulae for the system of equations 2 and equation 3 are the generalization for the 3D case of corresponding correlations, accepted at the computation of axially symmetrical flows (Bakhrakh et al., 1984). At that the experience of building difference formulae for the computation of 3D non-stationary flows, accumulated during the development of other techniques in VNIIEF (Artem'ev et al, 1989, Yanilkin et al., 1997, Zmushko et al, 1988, Sofronov et al., 1999) was used.

As it has been indicated above, in the LEGAK technique the edges of computational cells (hexahedrons) may not coincide with the contact boundaries of substances.

In this case the cells containing several substances (mixed cells) occur. Additionally to quantities $\vec{r}, \vec{u}$, ρ, e, g, P the following ones are introduced:

$a_i = M_i / M$ is mass and $\beta_i = V_i / V$ is volume concentrations of components; $\boldsymbol{e}_i$ is the specific (for the unit mass of the given substance) intrinsic energy, where , M_i, V_i are the mass and the volume of the substance number i, contained inside the computational cell ω. Each substance has its own equation of state $P_i = P_i\ (\rho_i, e_i)$.

It is supposed, that for each substance, contained inside a mixed cell, the variation of values is described by equations, analogous to those of the system 2 at the Lagrangian stage and the system 3 at the Eulerian stage.

To determine the variation of densities of the components at the Lagrangian stage, it is supposed, that:

$$div\overline{u}_i = div\overline{u}. \tag{4}$$

In the 1D case this supposition is equivalent to the supposition, that the velocity of the contact boundary inside one computational cell is determined with the linear interpolation over velocities in the grid nodes.

Thus, the rule of pressure ***P*** computation in a mixed cell follows from the condition of the additivity of unit energies and the accepted method of approximation of the equations of energies of components:

$$\rho_i = \alpha_i \rho / \beta_i \qquad P = \sum_{i=1}^{N} \beta_i P_i(\rho_i, e_i), \tag{5}$$

where N is the number of substances in a mixed cell, ρ_i is the density of the substance number i.

At the Eulerian stage the introduction of a special donor-acceptor computation algorithm for the flows from the cells with several substances (Bakhrakh et al., 1981) constrains the computation diffusion and allows localizing contact boundaries, not detached explicitly, with the precision of up to one computational cell. The idea of the algorithm, limiting the computation diffusion, can be explained by the following simple example: first, a substance, contained by a clean cell, is flowing away from a mixed cell into that clean one. In the general case the field of concentrations around the donor cell, containing several substances, is analyzed, and basing on this analysis we determine, which substance, in what proportion and with what velocities flows out of the given cell.

The difference scheme (the two-layer explicit one) has the first order of strength and is conditionally stable with the limitation of the step of integration over time: $\tau(\tilde{u} + c) < kh$, where h is the distinctive linear dimension of a computational cell, c is the sonic speed, $\tilde{u}$ is the velocity of grid motion in respect of the substance, $k = 0.5$.

Program realization of the LEGAK-3D technique

The basic principles of program realization of the LEGAK-3D technique coincide with the principles of realization of LEGAK (Avdeev et al., 2001), made for the computation of axially symmetrical flows.

In the LEGAK-3D technique the sheet-by-sheet data organization is made. One of the families of computational grid surfaces represents either planes intersecting over one line (system axis), or parallel planes.This family is the Eulerian one, the planes of the sheets are fixed. In the sheets the grids are built following the rules, accepted in the LEGAK technique (Avdeev et al., 2001).

The flat structure of the sheets can be affected by the module of Lagrangian gas dynamics computation. The flat structure of the sheets is restored by grid correction and value recalculation modules. Owing to this these modules operate in two phases.

At the first phase points are projected on the sheets and due to this changes of the grid values are recalculated (convection flows through “intersheet” edges of the hexahedrons.

At the second phase the computational grid on the sheets is corrected and the corresponding recalculation of the values is made (convection flows though “intrasheet” edges of hexahedrons).

The types of computational grids in the sheets are the same as in the LEGAK technique.

The LEGAK-3D technique allows to compute non-stationary flows of continuum in Lagrangian-Eulerian variables, which includes:

- Computation of non-stationary gas dynamic flows;
- Computation of elastoplastic flows;
- Computation of detonation wave distribution with constant velocity and taking into account the kinetics of the explosive break-up;
- Consideration of material destruction.

Codes for the computations of the above specified processes are realized as separate computation modules.

The software realization of the LEGAK-3D technique, as well as the LEGAK program realization, consists of the computational and service parts.

The computational part is written in Fortran-90. It can operate on both PC and other computation complexes, which support Fortran-90 and the data transfer standard MPI (MPI, 1994).

The service part, made to prepare problems and process the results, is realized as a Windows-application, written in C++; it functions on PC.

Parallelization of the LEGAK-3D technique

When the principles and schemes of the LEGAK-3D technique parallelization were being developed the experience of the LEGAK (Avdeev et al, 2001) parallelization was used. At that the main principles of parallelization remained unchanged:

- No software limitations of the number of used computers (the limitation may arise out of the size of solved problem only);
- Possibility to change the numbers of processors in the course of problem solving;
- Physical computation results do not depend on the numbers of used processors (including one computer when the computations are held in the scalar mode);
- The main load, connected with the computations in the multiprocessor mode, is put on the complex of support subprograms;
- Portability of program complex to different computation systems with distributed memory, which support the MPI data transfer standard;

- Parallelization of computation programs is provided by means of minimum alterations of their texts; operation in the multiprocessor mode is organized analogously to one-processor mode.

The scheme applied for LEGAK-3D parallelization is partially similar to that applied for 2D technique parallelization; still it has several noticeable differences.

For LEGAK-3D parallelization the *matrix* geometrical problem decomposition over processors is used (with overlaps). At that the computation portion for one processor is several adjacent cells (in rows and columns) of the computational grid with complete data over all sheets. Fig.1 represents problem fragmentation into 9 fragments (3×3 per sheet).

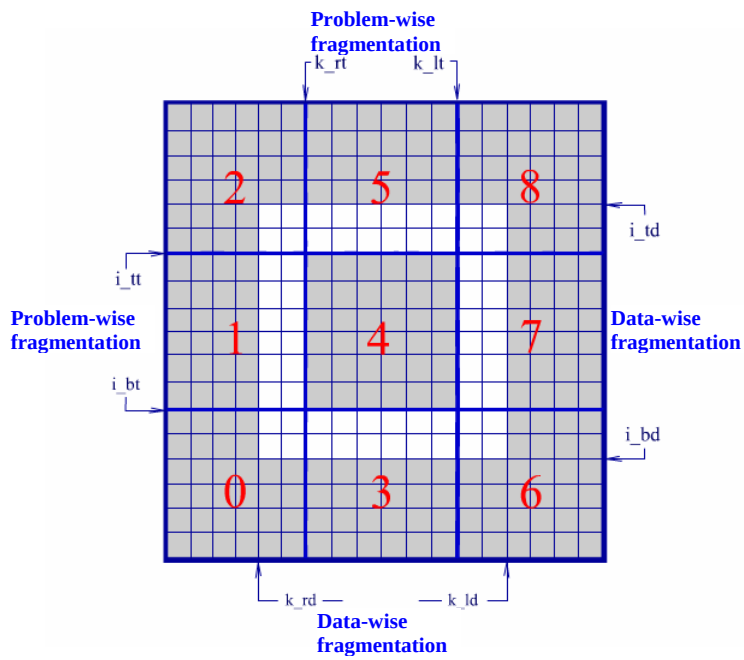


Fig.1. Example of problem fragmentation into 9 fragments (3×3 per sheet).

Thin lines indicate rows and columns of data overlaps. Decomposition for fragment 4 is indicated with brackets. .

Each processor computes its problem fragment, at that one processor is in charge of the computation control and synchronization.

Groups of values, which depend on the number of rows and/or columns in the problem are subject to decomposition and in the operative memory of each processor only important for this process cross-sections of these groups are stored.

In the LEGAK-3D technique for the majority of physical processes, which are taken into account explicit finite-difference schemes are mainly used. At that to find new values of quantities in a cell the values of several cells in three dimensions are needed. To compute the values in fragment boundary points the values of the adjacent cells are needed. The *overlap* (by data) in rows and columns in the LEGAK-3D technique equals 2. To provide adequate data decomposition over overlaps in the neighboring fragments after the computation programs are over the interprocessor data exchange in the overlapping cells is executed.

To realize these principles data structures and a package of service subprograms have been created.

Examples of computations with the LEGAK-2D technique

Several test and methodical computations were carried out to prove the LEGAK-3D ability to compute non-stationary continuum flows. Below the examples of some computations are presented.

Problem 1. Adiabatic expansion of a gas ellipsoid. The analytical solution of this problem was obtained in the work (Nemchinov, 1965).

The initial problem geometry is 1/8 of a three-axis ellipsoid ($x \geq 0$, $y \geq 0$, $z \geq 0$) with half-axes: $a_x = 3$, $a_y = 2$, $a_z = 1$ (Fig. 2).

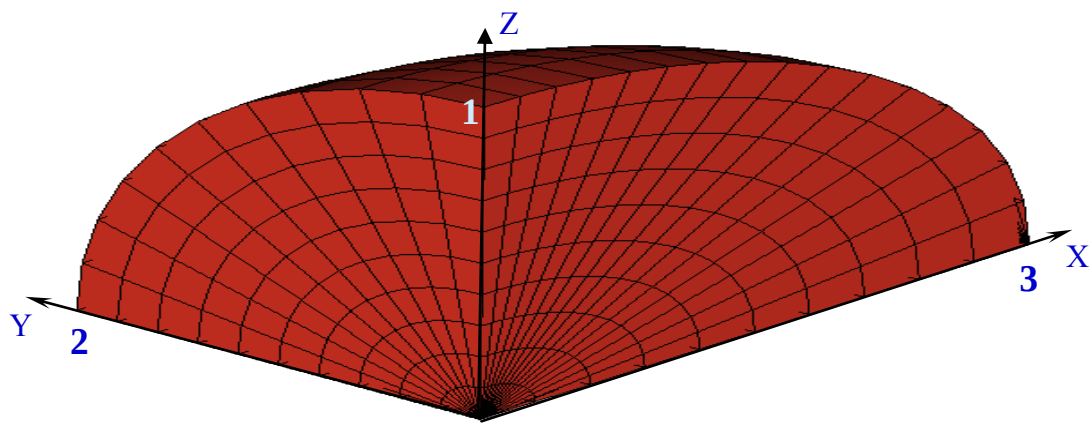


Fig. 2. Three-axis ellipsoid. The domain is filled with an ideal gas $(\gamma = 7/5)$.

The initial density and pressure distribution is determined with the following correlations:

$$P_0 = (1-\eta^2)^{\frac{\gamma}{\gamma-1}},\ \rho_0 = (1-\eta^2)^{\frac{1}{\gamma-1}}.\ \text{Here}\ \eta^2 = \frac{x^2}{a_x^2} + \frac{y^2}{a_y^2} + \frac{z^2}{a_z^2}.$$

The boundaries, coinciding with coordinate planes, are “rigid” walls. The pressure on the outer boundary is given as zero.

In Table 1 the computation results for different numbers of points are presented.

Table 1. Problem 1 computation results.

Grid	*Ux*	*Uy*	*Uz*	$S_1 = \frac{a_y}{a_x}$	$S_2 = \frac{a_z}{a_y}$	$S_3 = \frac{a_z}{a_x}$
16×10×16	2.33	2.89	3.8	1.225	1.32	1.616
16×20×16	2.43	3.02	3.92	1.233	1.3	1.605
16×30×16	2.46	3.07	3.97	1.236	1.3	1.607
Asymp. solution	2.56	3.17	4.27	1.23	1.35	1.66

Here 16×10×16 means problem fragmentation into 16 columns, 10 rows and 16 sheets, etc.

Basing on the computation results we can see the satisfactory agreement between the obtained values and the asymptotic solution. At that, the more the fragmentation is in the direction of the expansion, the closer the numerical solution to the asymptotic value.

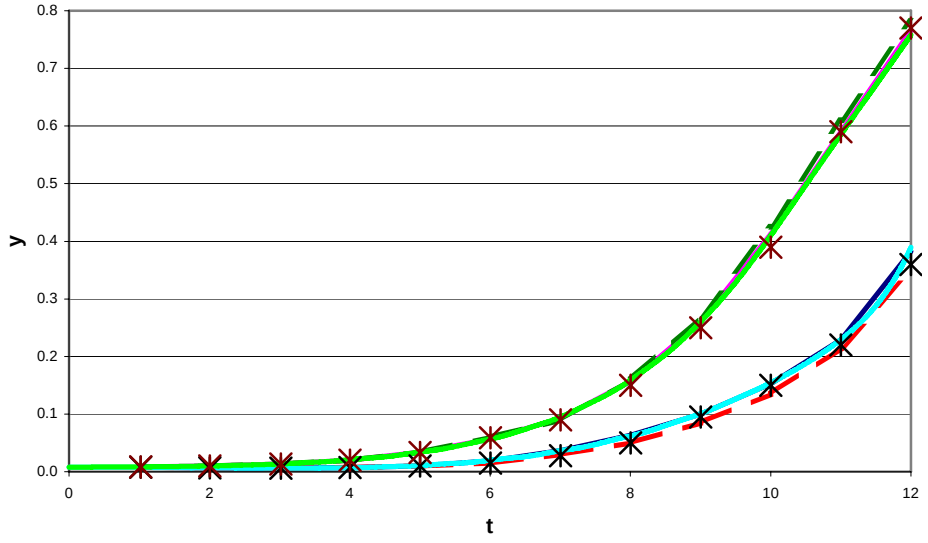
Problem 2. Development of Richtmyer-Mechkov's 3D instability. The problem set-up is taken from (Zmushko et al., 1988). The initial domain is a parallelepiped 0.4 cm high with the sides 1.5 cm long filled with gas with the equation of state $p = c_{sonic}^2 \left(\rho - \rho_0 \right)$. On the upper edge the given pressure P=1 is constant, the lower edge is a free surface, lateral edges are "rigid" walls.

At the initial moment for the whole domain a perturbation is determined as

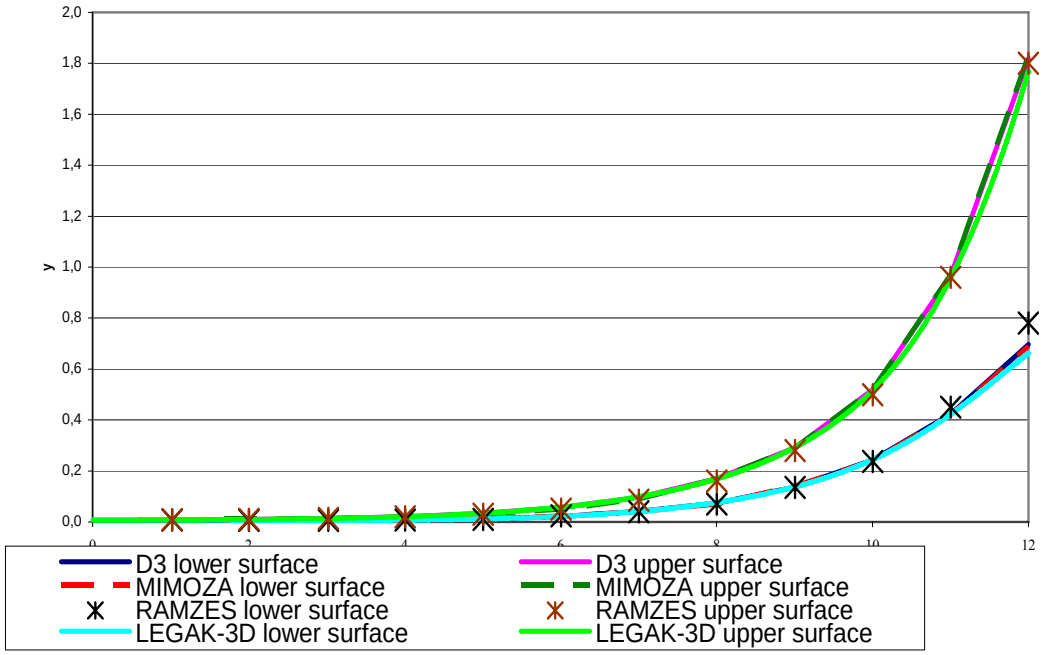
$$y = y_0 - A_0 \left(\cos \frac{\pi x}{l_1} + \cos \frac{\pi z}{l_2} \right).$$

The initial parameters are as follows: $c_{sonic} = 1 km/s$, $l_1 = l_2 = 1.5 cm$, $\rho_0 = 20 g/cm^3$, $A_0 = 0.004 cm$.

The computation was carried out up to the moment of time t=12 mcs. The computational domain was decomposed into 21 points along OX and OZ and 6 points along OY. As the problem does not have the analytical solution, the computation was carried out under other techniques (Yanilkin at al., 1997, Bakhrakh et al., 1984, Bakhrakh et al., 1999, Bakhrakh et al., 1999, Bakhrakh et al., 2003, Bakhrakh et al., 2004). Computation results were compared among each other over the increase of the perturbation amplitude in the sections Z=0 and Z=1.5. These curves are presented in Fig.3. A good agreement between these data and the data, obtained with other techniques, is well seen.



a



b

Fig. 3. Problem 2. Computed dependences of perturbation amplitude on time: *a* –z=0; *b* – z=1.5.

In Fig.4 the computational domain is presented for the moments of time 10 mcs and 12 mcs.

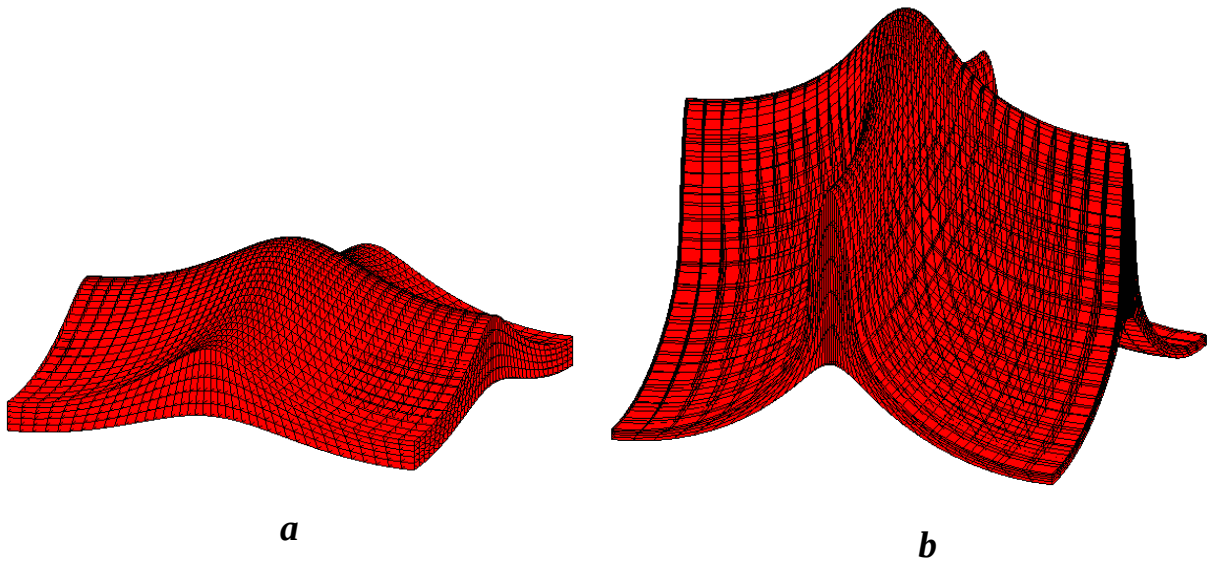


Fig. 4. Problem 2. Computational domain: *a* – t=10 mcs; *b* – t=12 mcs.

Problem 3. Computation of Richtmyer-Mechkov's instability. In the 3D set-up this problem was first computed under the MEDUZA technique (Barabanov et al., 2003).

In the domain $0 \le X \le 12\,cm,$ $0 \le Y \le 6\,cm,$ $0 \le Z \le 24\,cm$ two ideal gases are disposed: air with parameters $\rho = 0.001205\ g/cm^3$, $e = 0.2033195\ kJ/g$, $\gamma = 1.4$ and freon with parameters $\rho = 0.00513\ g/cm^3$, $e = 0.1374339\ kJ/g$, $\gamma = 1.139$. Freon occupies the domain with the dimensions $0 \le X \le 6$ cm, $0 \le Y \le 6$ cm, $0 \le Z \le 9$ cm. The initial problem geometry is presented in Fig.5. All the computational domain boundaries, except the upper one, are rigid walls. On the upper domain boundary (*z=24 cm*) the given pressure was $P = 2.2148 \cdot 10^{-4}$ GPa. The initial grid was fragmented into 101 rows, 101 columns and 101 sheets in the directions Z, X, Y respectively. The sheets of the computational grid were parallel to plane XOZ. The grid in the sheets was as follows: in the interval $0 \le Z \le 9$ cm it contained 90 rows, in the interval $9 \le Z \le 24$ cm it contained 10 rows. The grid was uniform considering spacings between columns and sheets.

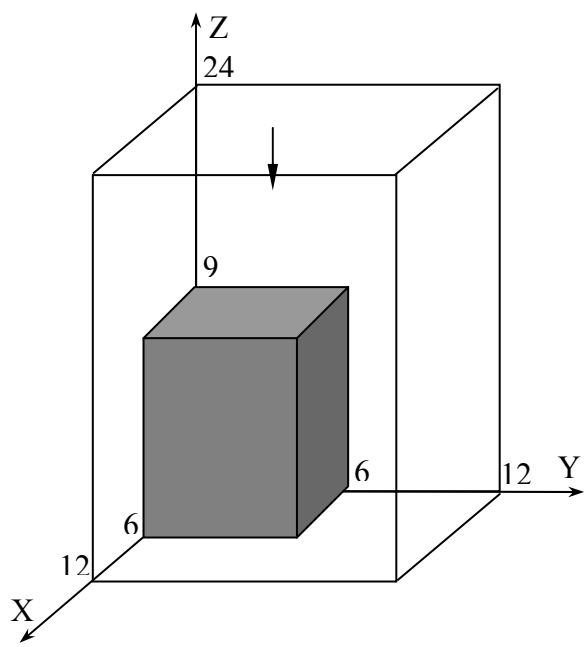


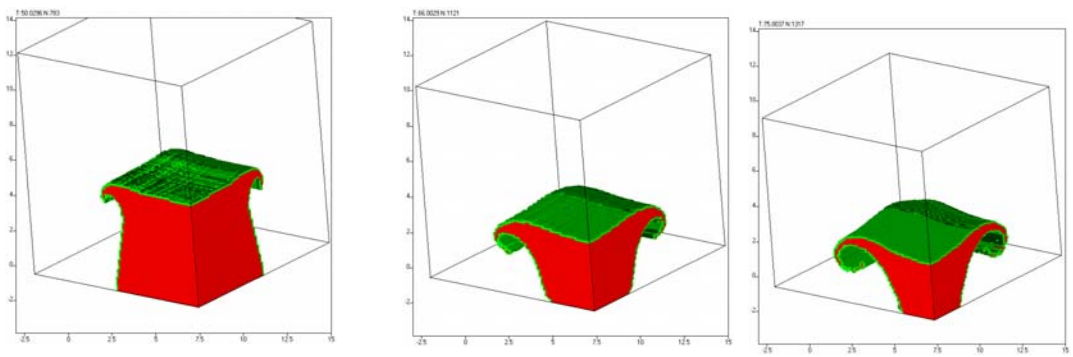
Fig. 5. Initial geometry of problem 3.

The domain $0 \le Z \le 9$ cm was stationary up to the moment of time *t*=650 mcs. After that moment the grid was kept uniform in the spacings. In Fig.6 domain cross-sections with planes X=0, Y=0 and X=Y (diagonal cross-section) at the moment of time *t*=750 mcs are presented (the cross-section was plotted on the ground of solution symmetry). In Fig. 7 the instability development is presented for different moments of time.

a ***b*** ***c***

Fig. 6. Problem 3. Domain cross-sections for the moment of time t=750 mcs:

a is the cross-section with plane X=0; *b* is the cross-section with plane Y=0; *c* is the cross-section with plane X=Y.



a ***b*** ***c***

Fig 7. Problem 3. Instability development at different moments of time: *a* – t=500 mcs; *b* – t=660 mcs; *c* – t=750 mcs.

Computation results of this problem obtained with the LEGAK-3D complex agree well with the results, obtained with the MEDUZA-3D complex (Bakhrakh et al., 2004).

Problem 4. Expansion and compaction of the spherical shell. The initial problem geometry with the concentration field is presented in Fig.8.

The domain 0<r<814 cm is filled with vacuum. The domain 8.14 cm<r<8.8 cm is the shell with the equation of state of the Mee-Gruneisen type with the parameters $\rho_{00} = 7.82 g/cm^3, \quad \gamma = 3.5474, \quad c_0 = 4.9 km/s, \quad n = 3$. In the domain 8.8 cm<r<15 cm explosive is disposed. The equation of state for the explosive and the explosion product are $P = (\gamma - 1)\rho e, \quad \gamma = 3$. The domain 15 cm<r<30 cm is filled with vacuum.

Initial conditions:

$$\rho_{\text{shell}} = 7.82 g/cm^3,\ \rho_{\text{explosive}} = 1.67 g/cm^3.$$
$$E_{\text{shell}} = E_{\text{explosive}} = U_{\text{shell}} = U_{\text{explosive}} = 0$$

Parameters of the explosive: caloricity Q=3.61 kJ/g, detonation rate D = 7.6 km/s.

Initiation of detonation takes place in the point with coordinates *x=0.0, y=15.0 cm, z=0.0* (Fig. 10, point C).

The problem was computed up to the moment of maximum shell compaction..

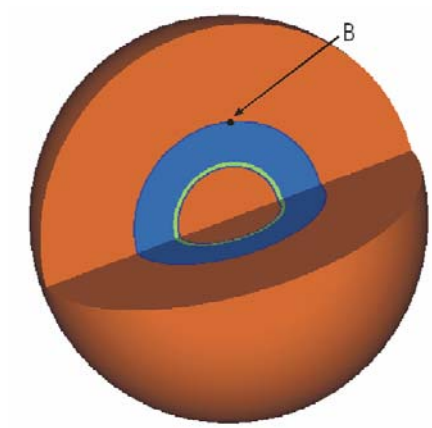
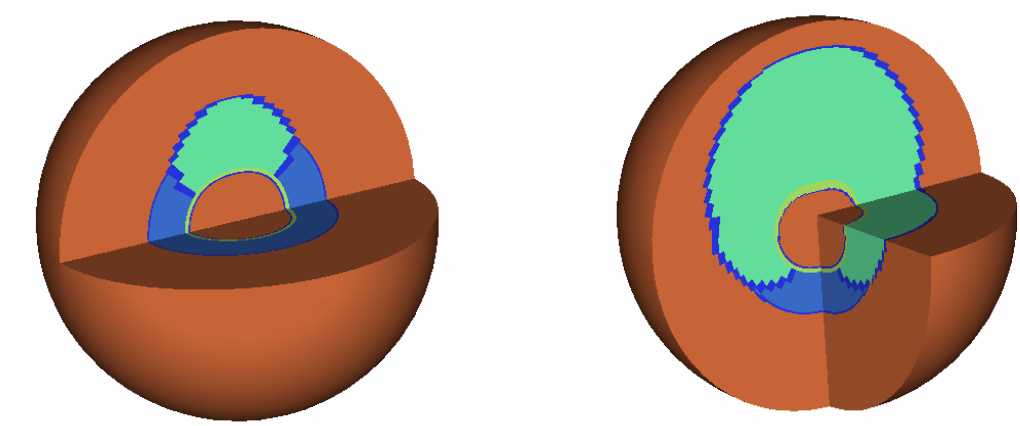


Fig. 8. Initial geometry of problem 4.

The computational domain is fragmented into 100 points in rows, 30 points in columns and 60 points in sheets (complete spread): 30 points at the radius are for vacuum and the shell, 70 points at the radius uniformly by spacing for the explosive and vacuum. The type of interpolation along the rows is angular-uniform, the type of interpolation along the columns is as follows: the explosive is separated from the shell with the Lagrangian line; for rest points the type of interpolation was: uniform splitting without interpolation. In Fig.9 the picture of detonation wave distribution is presented. In Fig.10 a fragment of the computational grid is presented for the moment of time t=50 mcs.

During the process the implosion of the shell takes place, at some moment of time its maximum density is achieved. During the computations the moment and the maximum value of the shell density was registered.



a ***b***

Fig. 9. Problem 4. 3D cross-section of the concentration field for the system: *a* - t=15 mcs; *b* – t= 35 mcs.

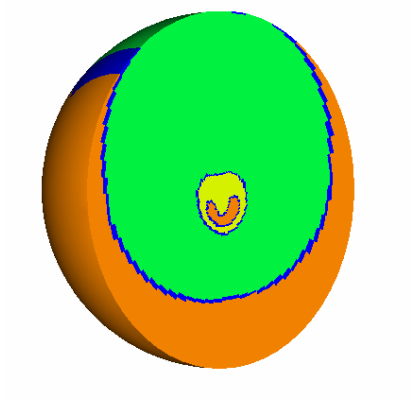


Fig. 10. Problem 4. Fragment of the computational domain for the moment of time t=50 mcs.

Also the problem was computed under the LEGAK-3D technique with initiation on the system axis.

Computation results are presented in Table 2.

Table 2. Problem computation results

Technique	Time of maximum shell compression, (mcs)	Maximum average shell density, (g/cm^3)
LEGAK-2D	60.8	8.93
LEGAK-3D	60.3	8.82

Conclusion

A short review of approaches to the development of 2D and 3D gas dynamic flow mathematical simulation, used by VNIIEF, is made.

As an example the LEGAK-3D regular Lagrangian-Eulerian technique is presented in more detail.

The LEGAK-3D technique for computation of 3D non-stationary flows of multi-component continuum operates on multi-processor computation systems with distributed memory.

The computations made with the LEGAK-3D technique proved its abilities.

The computations, made in the multi-processor mode, showed the acceptable efficiency of parallelization of the complex. In case of matrix decomposition into 10 rows, 10 columns and 100 sheets the efficiency was 60% for 100 processors.

Deeper parallelization (decomposition in the third dimension) is supposed to be carried out at the following stage of the development of LEGAK-3D program realization.

Acknowledgements

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