

Institute of Theoretical and Mathematical Physics



Russian Federal Nuclear Center -

VNIIEF

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

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Abstract

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.



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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.



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Introduction

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.



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Introduction

- **The DMK and MEDUZA** techniques are based on the application of unstructured 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 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.



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Introduction

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 VNIIEF (**Bakhrakh et al.**) for computation of so-called “mixed” cells occurring in this case. Such approach is used in the **EGAK** and **TREK** Eulerian techniques, the **LEGAК-2D**, **LEGAК-3D**, **MIMOZA**, **RAMZES-KP** Eulerian-Lagrangian techniques. The algorithms, resident in the concentration method, are also used in the **MEDUZA** non-regular technique

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. Most techniques use **special donor-acceptor algorithm** of convective flow computation to avoid computation diffusion. Apart from this, the specified methods are characterized by the topology of used regular grids and finite-difference schemes.



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Introduction

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.



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Introduction

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, 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 (**VKL**), developed in the frames of the **LEGAK** technique. The method of contact line detachment (VKL) as the lines, which motion is calculated in a certain way, traces back to Nokh’s work (1964).

Another VNIIEF approach to the development of numerical algorithms is the realization of the discrete method of smoothed particles (the **SPH** technique).



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LEGAK-3D Method

The main part of the Report contains a more detailed description of the Regular Lagrangian-Eulerian technique LEGAK-3D, 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



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Principles of the LEGAK technique

The LEGAK technique is the finite-difference Lagrangian-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:

1. 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;
2. Continuous concordant representation of the flows of mass, energy, momentum and other values at the approximation of convective terms of the initial system of equations;
3. Donor-acceptor algorithm 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.



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Principles of the LEGAK technique

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 \mathbf{S} , is

used:

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

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

$$F(M, M\bar{u}, Me); G(\rho, \rho\bar{u}, \rho e);$$

$$H \left\{ \rho, \text{grad } p + \text{div } \hat{k}, p \text{ div } \bar{u} + sp(\hat{k} \hat{D}) \right\};$$

$M = \rho v$ 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.



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Principles of the LEGAK technique

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:

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

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:

$$\frac{dF}{dt} + \int_S G^{(1)} (u^{(1)} - u^*) dS = 0. \quad (3)$$

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



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Principles of the LEGAK technique

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. 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 (D-3, MIMOZA, TREK) was used.



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Principles of the LEGAK technique

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

$a_i = M_i / M$ is mass and $\beta_i = V_i / V$ is volume concentrations of components;

e_i is the specific (for the unit mass of the given substance) intrinsic energy

M_i, V_i are the mass and the volume of the substance number i ,
contained inside the computational cell

Each substance has its own equation of state $P_i = P_i(\rho_i, e_i)$

To determine the variation of densities of the components at the Lagrangian stage, it is supposed, that: $div \bar{u}_i = div \bar{u}$.

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:

$$\rho_i = \alpha_i \rho / \beta_i \quad P = \sum_{i=1}^N \beta_i P_i(\rho_i, e_i), \text{ where } N \text{ is the number of substances in a mixed cell,}$$

ρ_i is the density of the substance number i



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Principles of the LEGAK technique

The difference scheme (the two-layer explicit one) has the first order of accuracy 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, $k = 0.5$



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Program realization of the LEGAK-3D technique

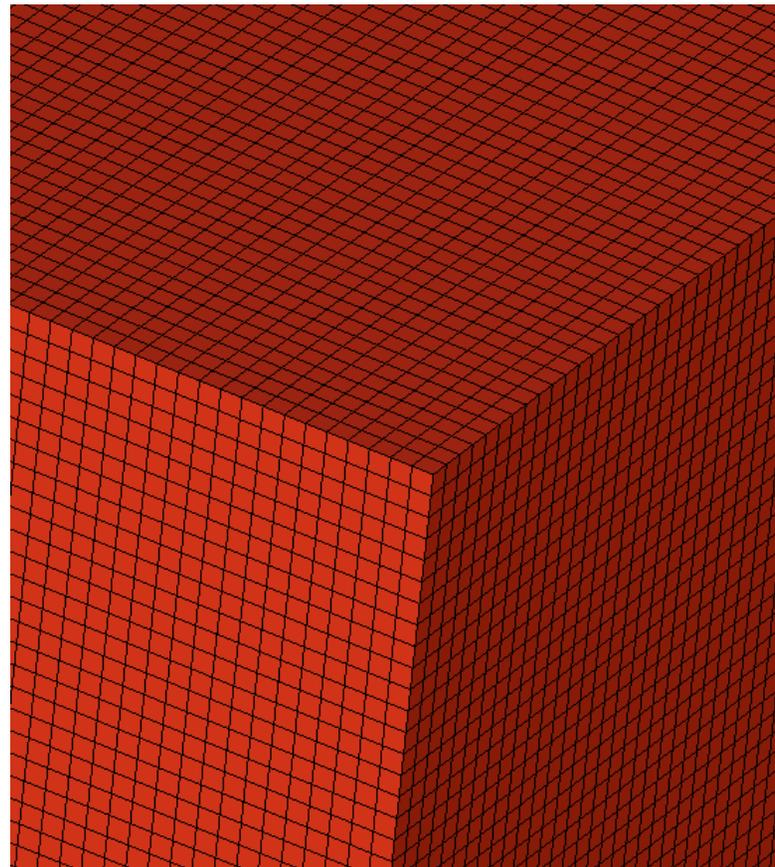
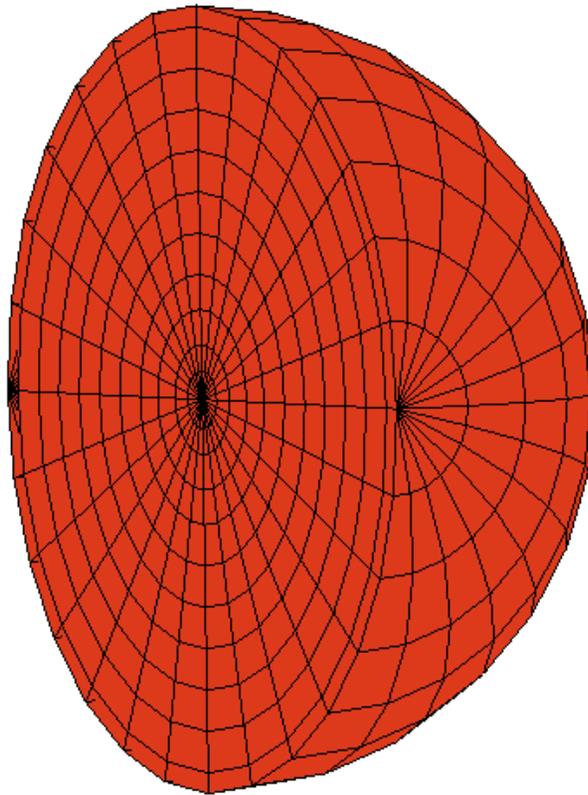
The basic principles of program realization of the LEGAK-3D technique coincide with the principles of realization of LEGAK-2D, made for the computation of axially symmetrical flows.

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-2D technique.



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Program realization of the LEGAK-3D technique





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Program realization of the LEGAK-3D technique

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 through “intrasheet” edges of hexahedrons).

The types of computational grids in the sheets are the same as in the LEGAK-2D technique.



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Program realization of the LEGAK-3D 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.



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Program realization of the LEGAK-3D technique

The software realization of the LEGAK-3D technique, as well as the LEGAK-2D 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.



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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-2D parallelization was used. At that the main principles of parallelization remained unchanged:

- No software limitations of the number of used processors (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.

Parallelization of the LEGAK-3D technique

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).

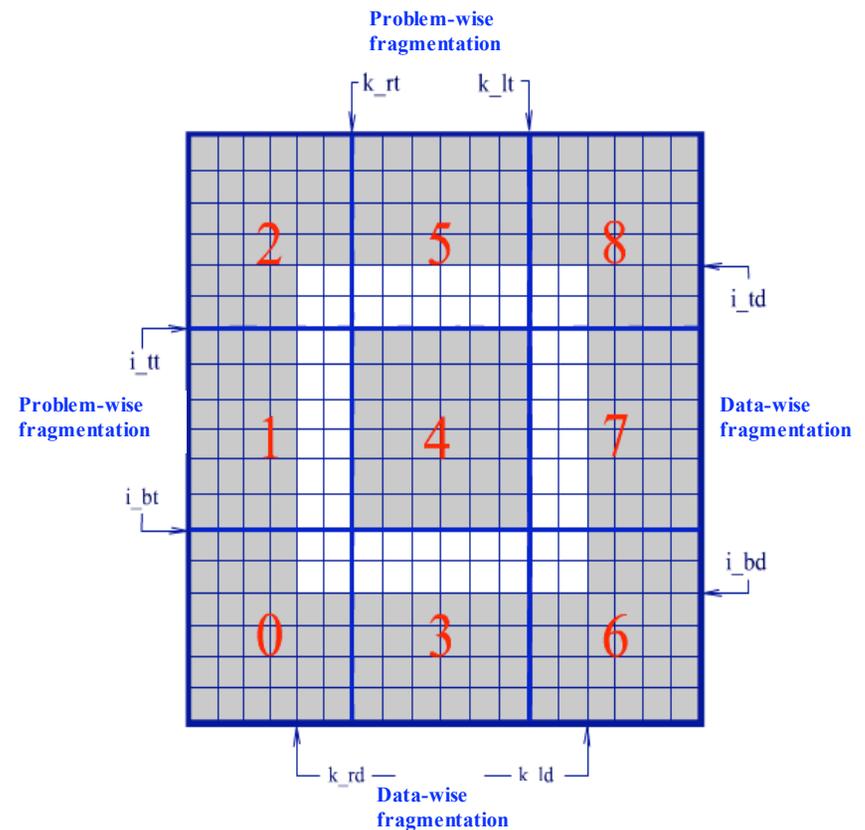
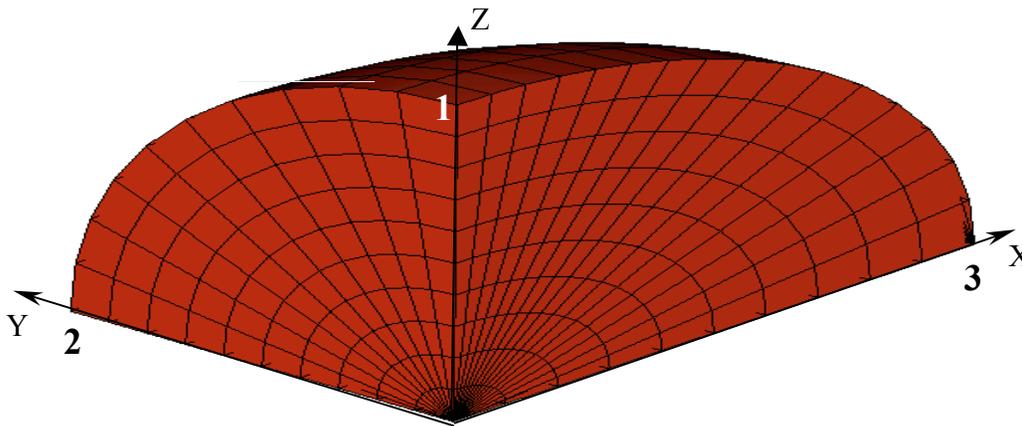


Fig.1. Example of problem fragmentation into 9 fragments (3×3 per sheet)

Examples of computations with the LEGAK-3D technique

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



$x \geq 0, y \geq 0, z \geq 0$
 $a_x=3, a_y=2, a_z=1$
 An ideal gas ($\gamma=7/5$)

Table 1. Problem 1 computation results.

Grid	U_x	U_y	U_z	$S_1 = \frac{a_y}{a_x}$	$S_2 = \frac{a_z}{a_y}$	$S_3 = \frac{a_z}{a_x}$
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

$$P_0 = (1 - \eta^2)^{\frac{\gamma}{\gamma-1}},$$

$$\rho_0 = (1 - \eta^2)^{\frac{1}{\gamma-1}}.$$

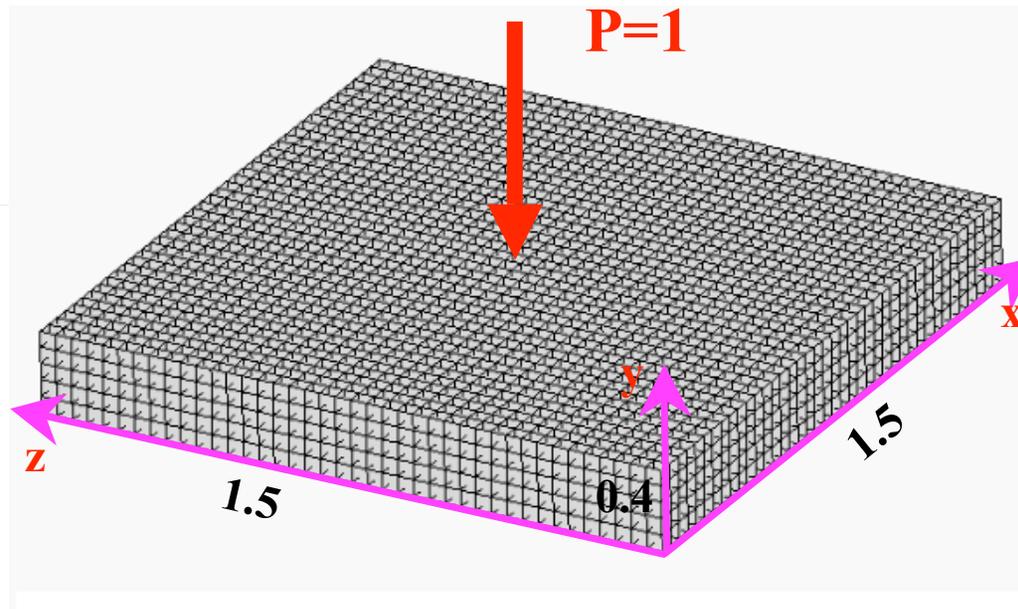
$$\eta^2 = \frac{x^2}{a_x^2} + \frac{y^2}{a_y^2} + \frac{z^2}{a_z^2}$$



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Examples of computations with the LEGAK-3D technique

Problem 2. Development of Richtmyer-Mechkov's 3D instability



$$p = c_{\zeta\hat{a}}^2 (\rho - \rho_0) \quad y = y_0 - A_0 \left(\cos \frac{\pi x}{l_1} + \cos \frac{\pi z}{l_2} \right)$$

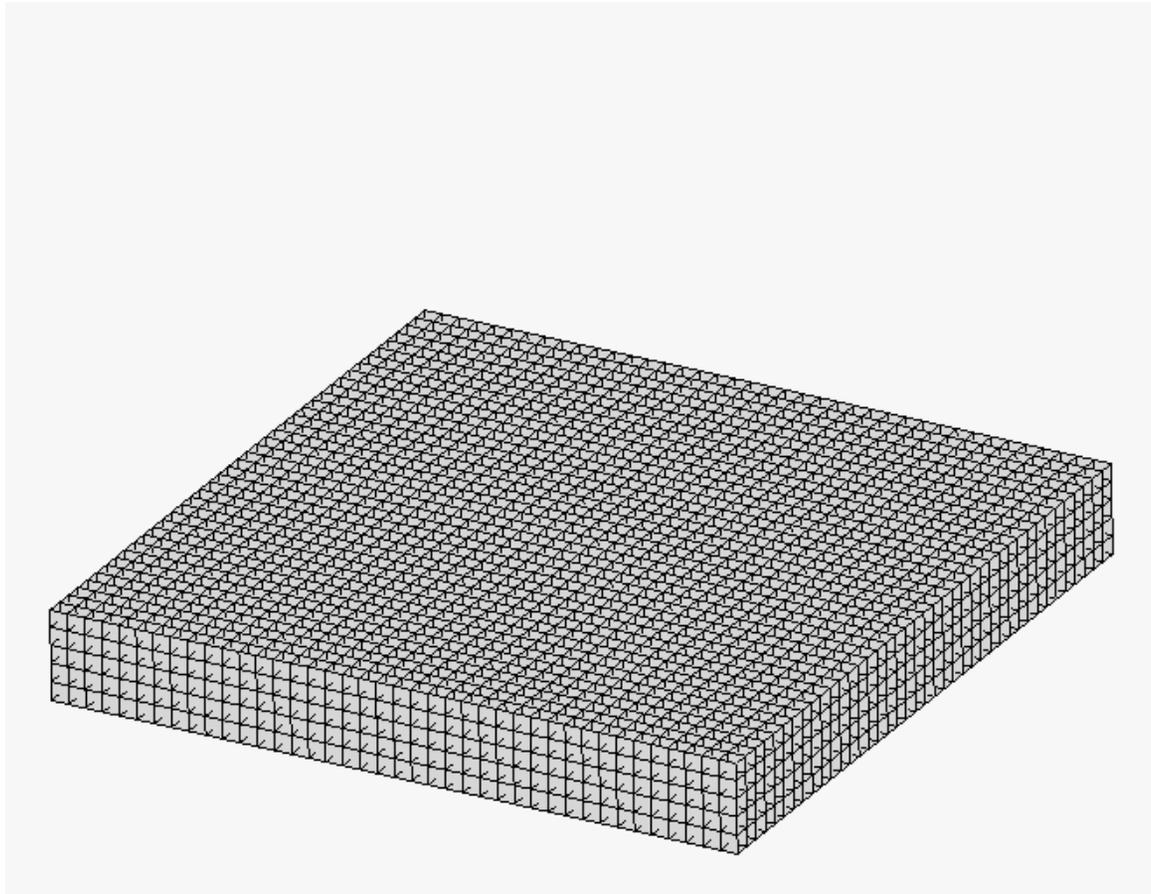
$$\tilde{n}_{\zeta\hat{a}} = 1 \quad l_1 = l_2 = 1.5 \quad \rho_0 = 20 \quad A_0 = 0.004$$



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Examples of computations with the LEGAK-3D technique

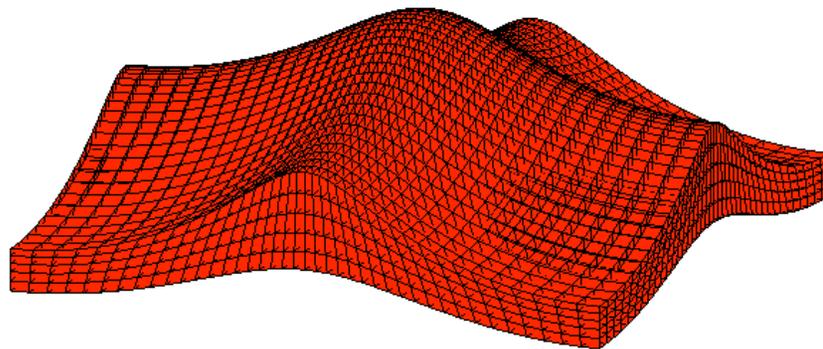
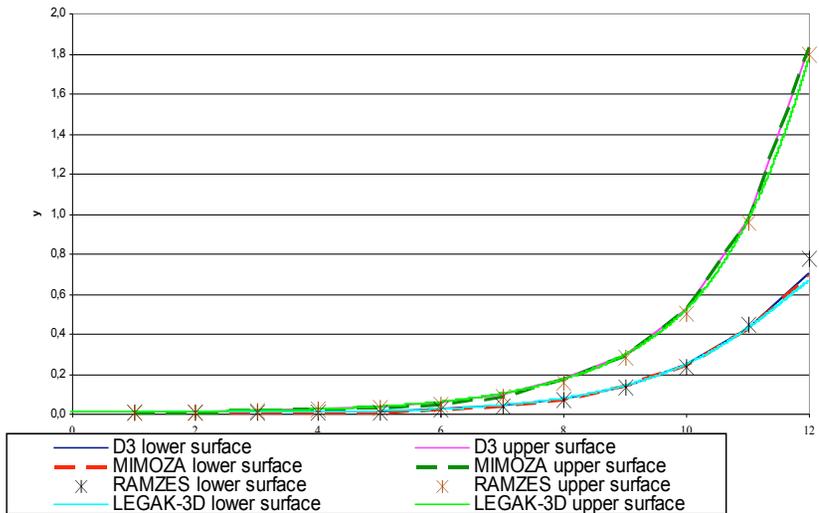
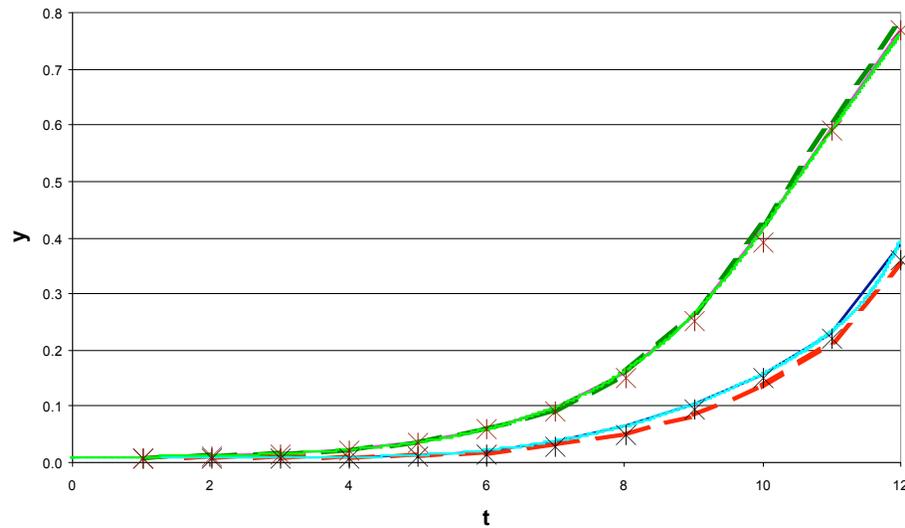
Problem 2. Development of Richtmyer-Mechkov's 3D instability



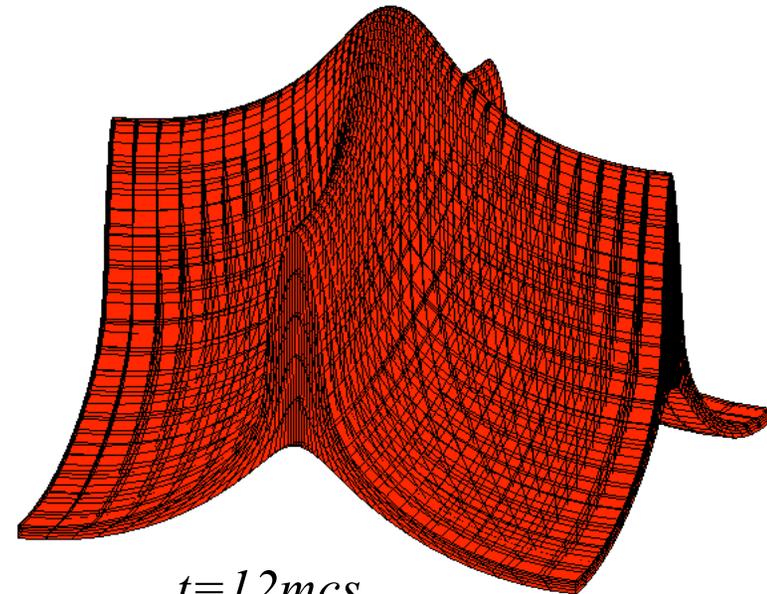


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Examples of computations with the LEGAK-3D technique



$t=10mcs$



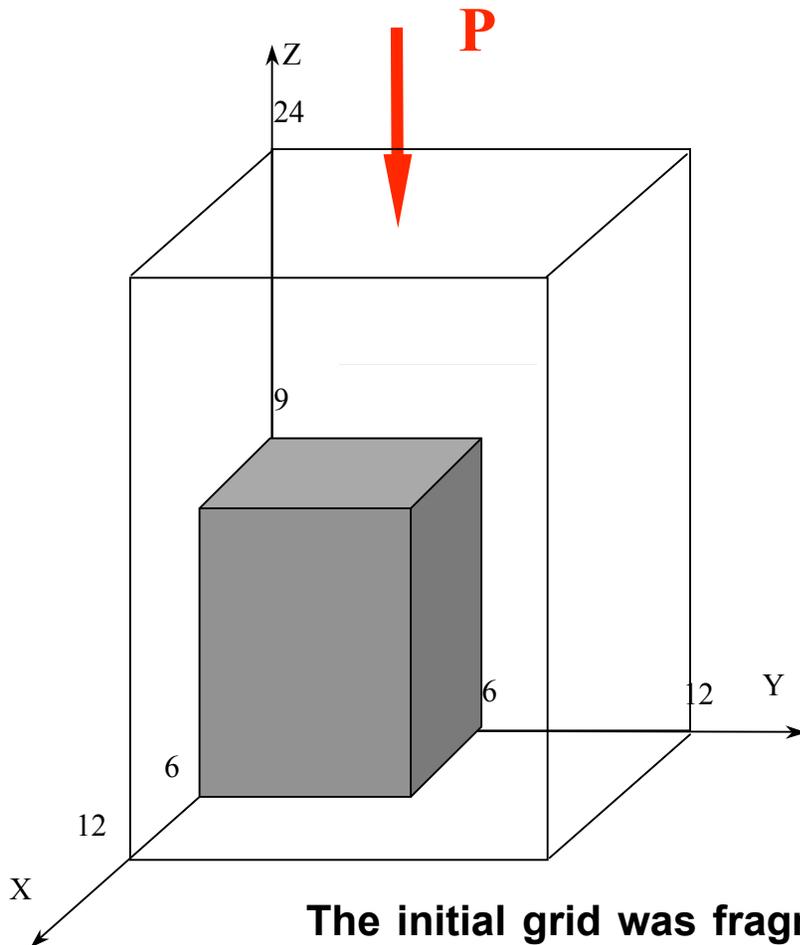
$t=12mcs$



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Examples of computations with the LEGAK-3D technique

Problem 3. Computation of Richtmyer-Mechkov's instability



$$0 \leq X \leq 12\tilde{n}i \quad 0 \leq Y \leq 12\tilde{n}i \quad 0 \leq Z \leq 24\tilde{n}i$$

$$\text{air: } \begin{aligned} \rho &= 0.001205 \text{ g} / \tilde{n}i^3 \\ e &= 0.2033195 \text{ kJ} / \text{g} \end{aligned} \quad \gamma = 1.4$$

$$\text{freon: } \begin{aligned} \rho &= 0.00513 \text{ g} / \tilde{n}i^3 \\ e &= 0.1374339 \text{ kJ} / \text{g} \end{aligned} \quad \gamma = 1.139$$

$$0 \leq X \leq 6\tilde{n}i \quad 0 \leq Y \leq 6\tilde{n}i \quad 0 \leq Z \leq 9\tilde{n}i$$

$$P = 2.2148 \cdot 10^{-4} \text{ GPa}$$

The initial grid was fragmented into 101 rows, 101 columns and 101 sheets in the directions Z, X, Y respectively



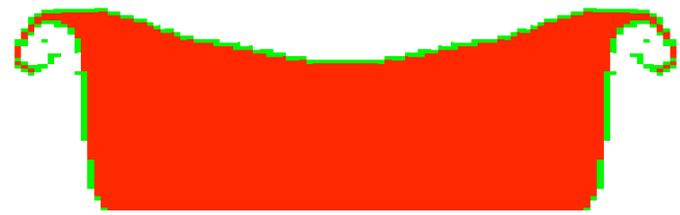
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Examples of computations with the LEGAK-3D technique

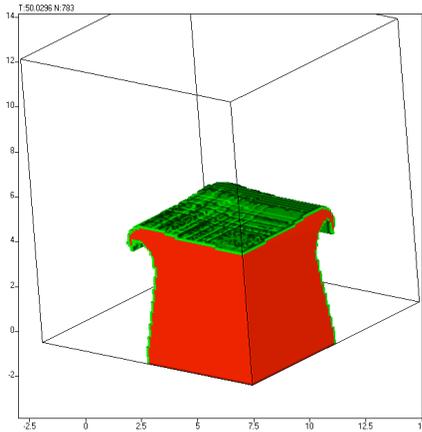
Problem 3. Computation of Richtmyer-Mechkov's instability



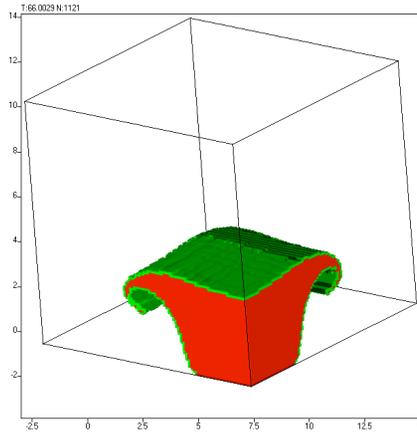
$t = 750\text{mcs}, X = 0$



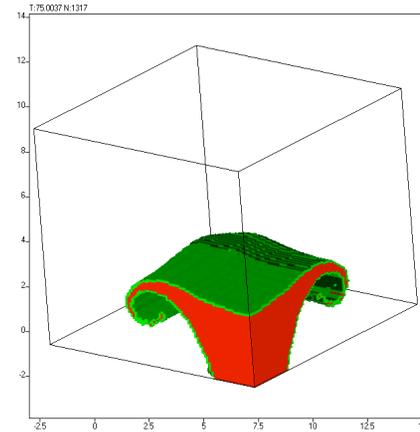
$t = 750\text{mks}, X = Y$



$t = 550\text{mcs}$



$t = 660\text{mks}$



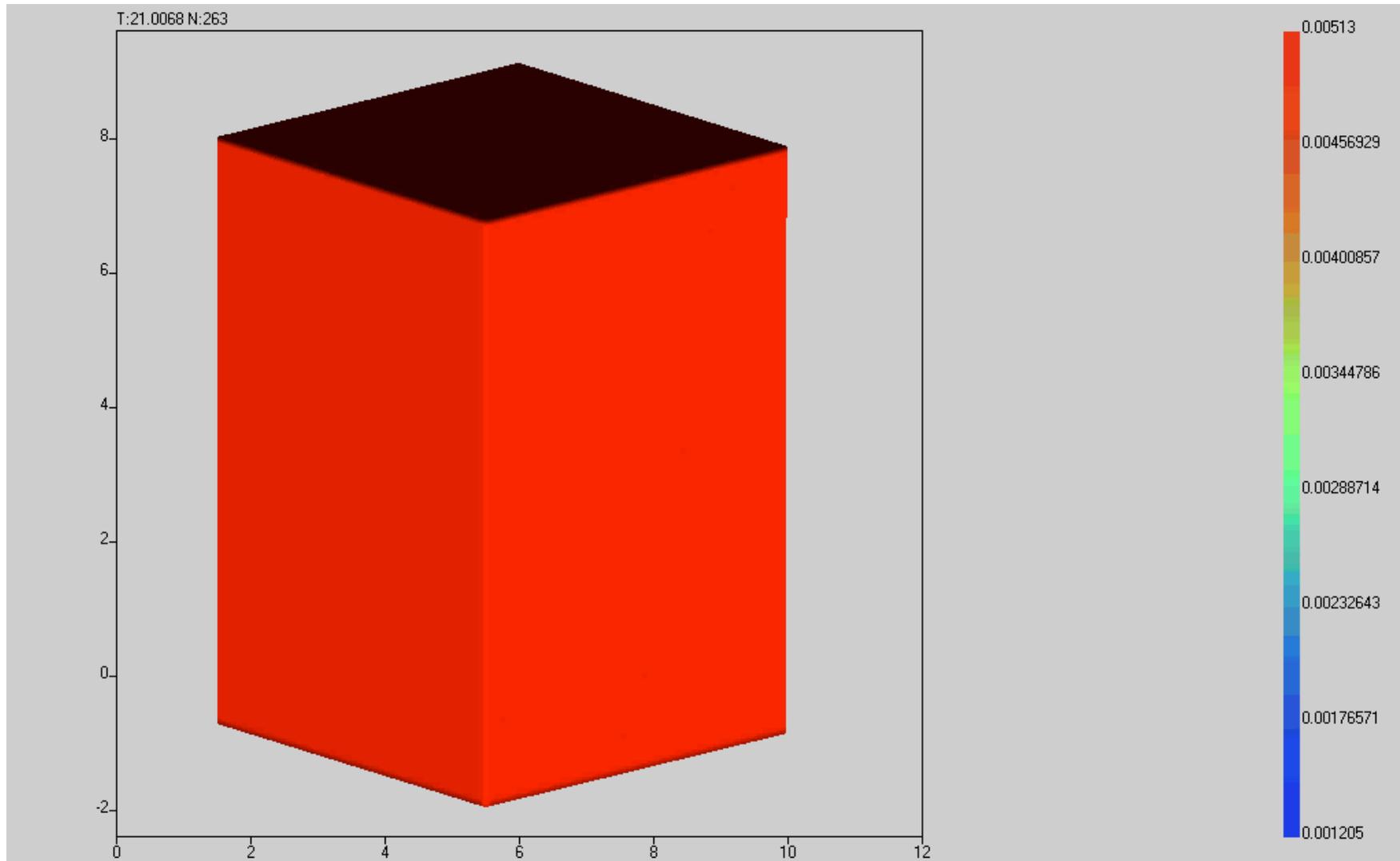
$t = 750\text{mcs}$



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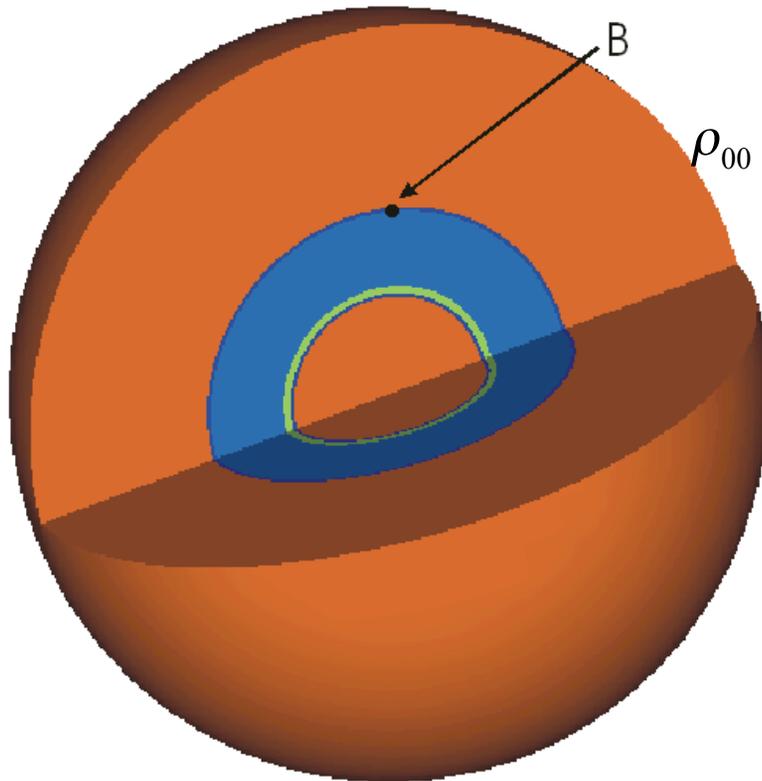
Examples of computations with the LEGAK-3D technique

Problem 3. Computation of Richtmyer-Mechkov's instability



Examples of computations with the LEGAK-3D technique

Problem 4. Expansion and compaction of the spherical shell



vacuum: $0\text{cm} < r < 8.14\text{cm}$

shell: $8.14\text{cm} < r < 8.8\text{cm}$

$$\rho_{00} = 7.82\text{g} / \tilde{\text{m}}^3, \quad \gamma = 3.5474, \quad c_0 = 4.9\text{km/s}, \quad n = 3$$

Expl.: $8.8\text{cm} < r < 15\text{cm}$

$$P = (\gamma - 1)\rho e, \quad \gamma = 3$$

vacuum: $15\text{cm} < r < 30\text{cm}$

caloricity : $Q = 3.61\text{kJ/g}$

detonation rate : $D = 7.6\text{km/s}$

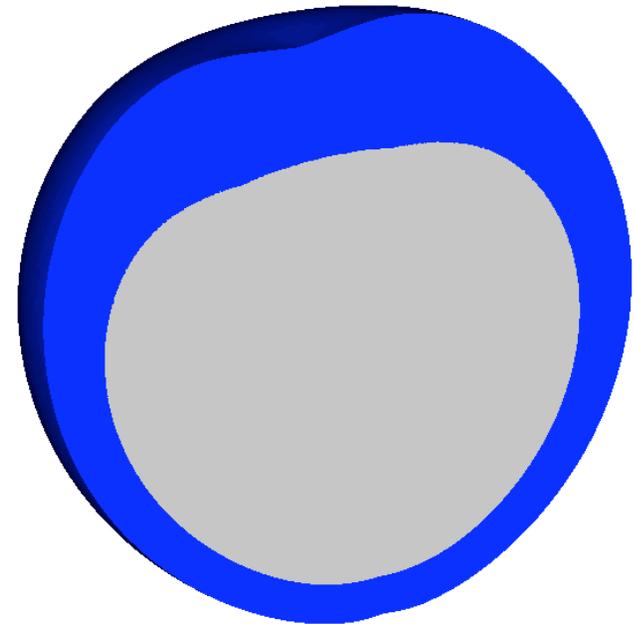
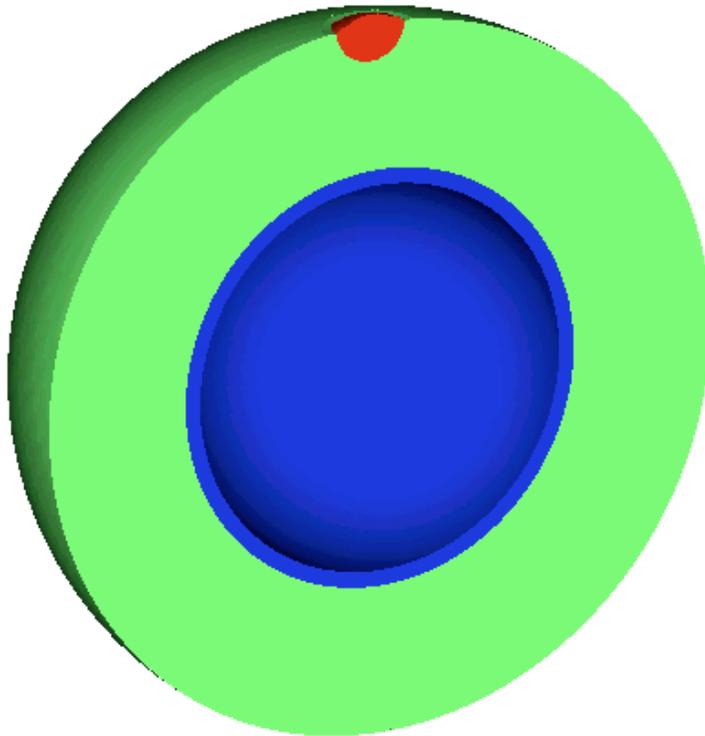
$$\rho_{shell} = 7.82\text{g} / \tilde{\text{m}}^3, \quad \rho_{expl} = 1.67\text{g} / \tilde{\text{m}}^3.$$



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Examples of Computations with the LEGAK-3D technique

Problem 4. Expansion and compaction of the spherical shell





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Conclusion

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

2. 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 technique. 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.



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THANK YOU for attention