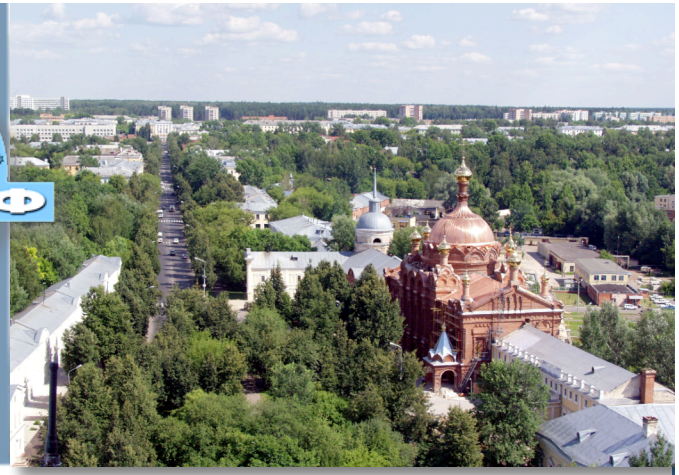
Institute of Theoretical and Mathematical Physics



Russian Federal Nuclear Center -

VNIIEF

Eulerian Numerical Techniques

EGAK and TREK for Simulation of Multidimensional Multi-material Flows

Yanilkin Yu.

RFNC-VNIIEF, 607190, Sarov, Nizhni Novgorod region

Joint Russian-American Five-Laboratory Conference on Computation Mathematics|Physics

19-23 June 2005, Crowne Plaza, Vienna Austria

Authors

Yanilkin Yu.V., Belyaev S.P., Bondarenko Yu.A., Gavrilova E.S., Goncharov E.A., Gorbenko A.D., Gorodnichev A.V., Gubkov E.V., Guzhova A.R., Degtyarenko L.I., Zharova G.V., Kolobyanin V.Yu., Sofronov V.N., Stadnik A.L., Khovrin N.A., Chernysheva O.N., Chistyakova I.N., Shemyakov V.N.

Main advantages of Eulerian methods

- crash-proof computations,
- easier preparation of initial data,
- less labor-intensity of calculations,
- less dependence of results on the computation executor skills.

Main problems of Eulerian methods

1. Lagrangian gas dynamics equation approximation for a multi-material medium because of occurrence of mixed cells.
2. A lower accuracy, as compared to Lagrangian methods.
3. Determination of interface positions and computation of their motion over the immovable computational grid.
4. Problems of simulation of various physical processes, namely: HE burning and detonation, heat transfer, elasticity-plasticity, etc.
5. Necessity of using of a heterogeneous grid.
6. The problem of efficient parallelization during implementation of codes on parallel computers.

Main features of the techniques EGAK (2D) and TREK (3D)

- ALE approach is used
- A single computational grid is used - cells are quadrangles in 2D case and hexahedrons, if it is 3D case
- The splitting method is used for modeling of various physical processes
- Use of explicit difference schemes in the main
- Use of the concentration method for mixed cells

Part 1.

Approximation of Lagrangian gas dynamics equations for multimaterial medium

The system of differential equations of multi-material gas dynamics

$$\frac{d\vec{u}}{dt} = -\frac{1}{\rho}\,\mathrm{grad}\left(P + q\right) \qquad (1)$$

$$\frac{d\rho_i}{dt} = -\rho_i \,\mathrm{div}\,\vec{u}_i \qquad (2)$$

$$\frac{d\beta_i}{dt} = \beta_i\left(\mathrm{div}\,\vec{u}_i - \mathrm{div}\,\vec{u}\right) \qquad (3)$$

$$\frac{de_i}{dt} = -\frac{P_i + q_i}{\rho_i}\,\mathrm{div}\,\vec{u}_i \qquad (4)$$

$$P_i = P_i\left(\rho_i, e_i\right) \qquad (5)$$

Main closure assumptions used in the techniques EGAK and TREK

- equal compressibility of materials (Bakhrakh et al., 1984) - **method 1;**

$$\mathrm{div}\vec{u}_1 = \mathrm{div}\vec{u}_2 = \mathrm{div}\vec{u}_3 = ...$$

- equal pressures of materials (Zharova and Yanilkin, 1992) - **method 2;**

$$P = P_1 = P_2 = P_3 = ...$$

- equal material pressure increments (Bondarenko and Yanilkin, 2000) - **method 3**;

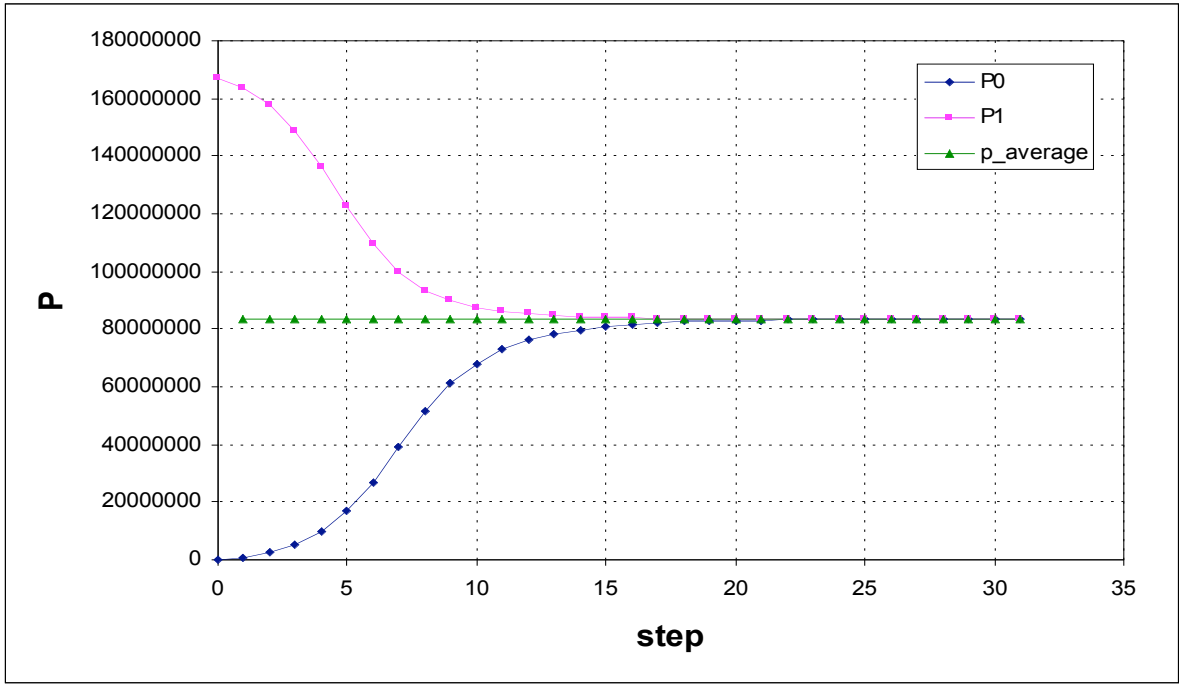
$$\Delta P_i = \Delta P_k = \Delta P$$

- equal material pressure increments + material pressure equalization algorithm (Goncharov and Yanilkin, 2004) - **method 3P**;

Problem 1. Thermodynamic equilibrium achievement with no gas dynamic motion

$\rho_1=1.25,\ e_1=2*10^5,\ \beta_1=0.5,\ \gamma = 5/3$

$\rho_2=50,\ e_2=5*10^6,\ \beta_2=0.5,\ \gamma = 5/3$



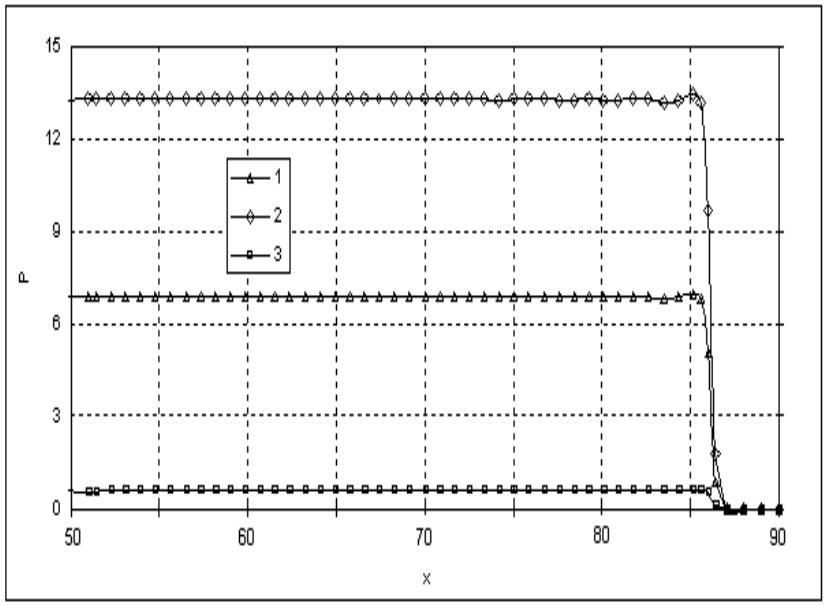
The material pressures and average pressure versus the number of computational steps

Problem 2. A shock wave propagation through a mixture of two gases

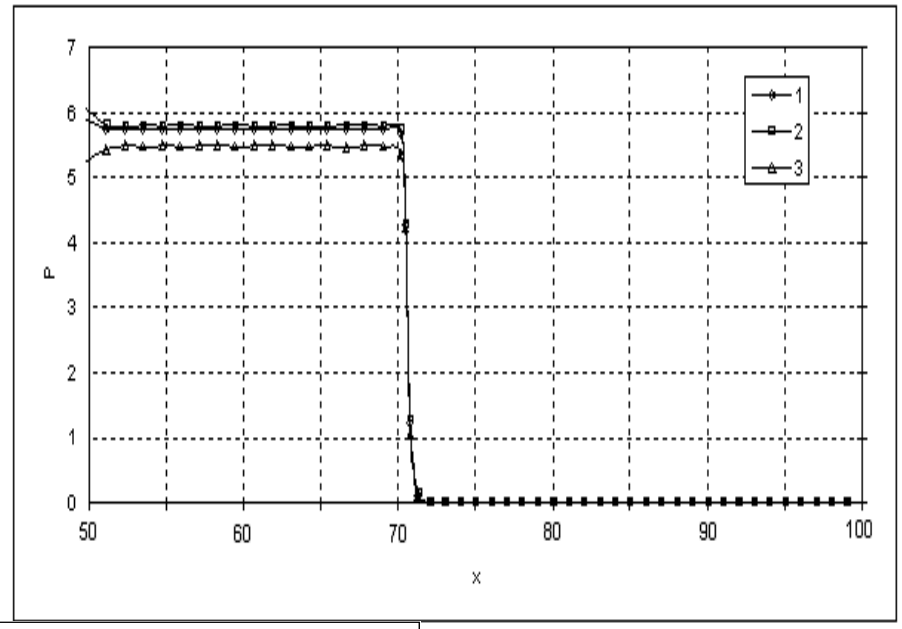
- There is a mixture of two gases within the region $0<x<100$, the gases are in completely mixed and equilibrium state ($P=0$, $u=0$).
- The first gas: $\rho=1$, $\gamma=3$.
- The second gas: $\rho=1$, $\gamma=1.2$.
- On the left boundary $ux=2$.

Pressure profiles in problem 2

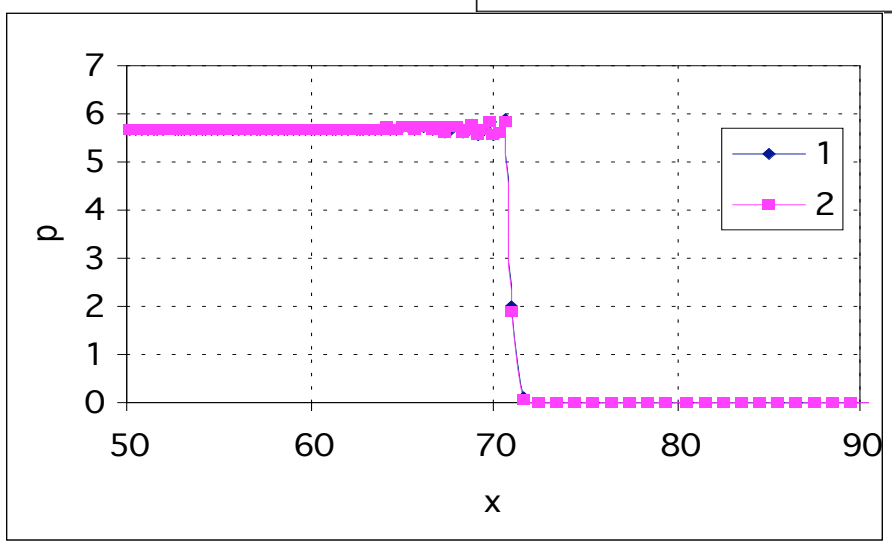
1 – average; 2 –material 1; 3 –material 2.



method 1



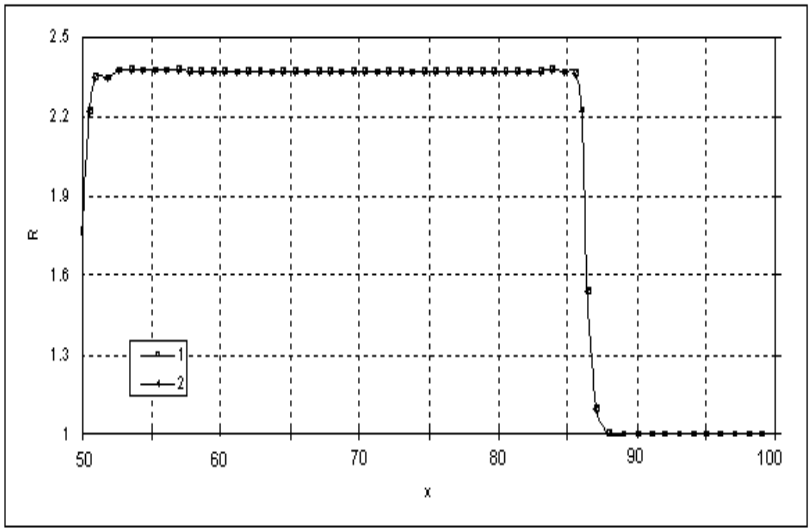
method 3



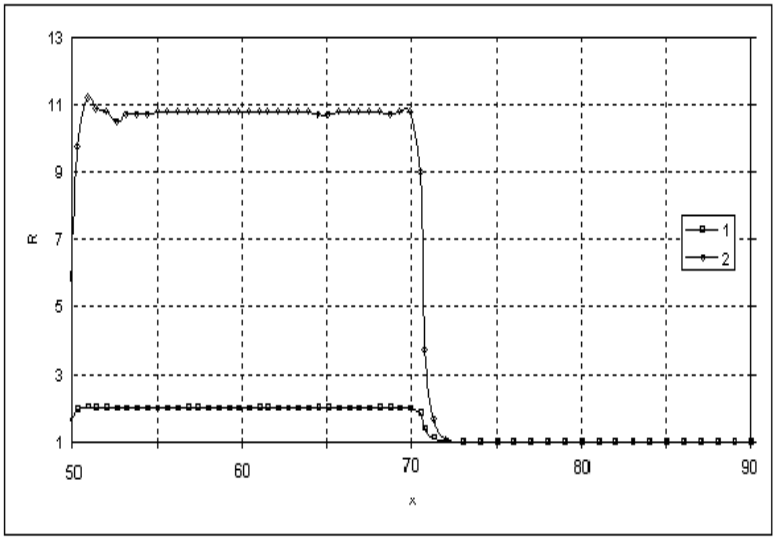
method 3P and method 2

Density profiles in problem 2

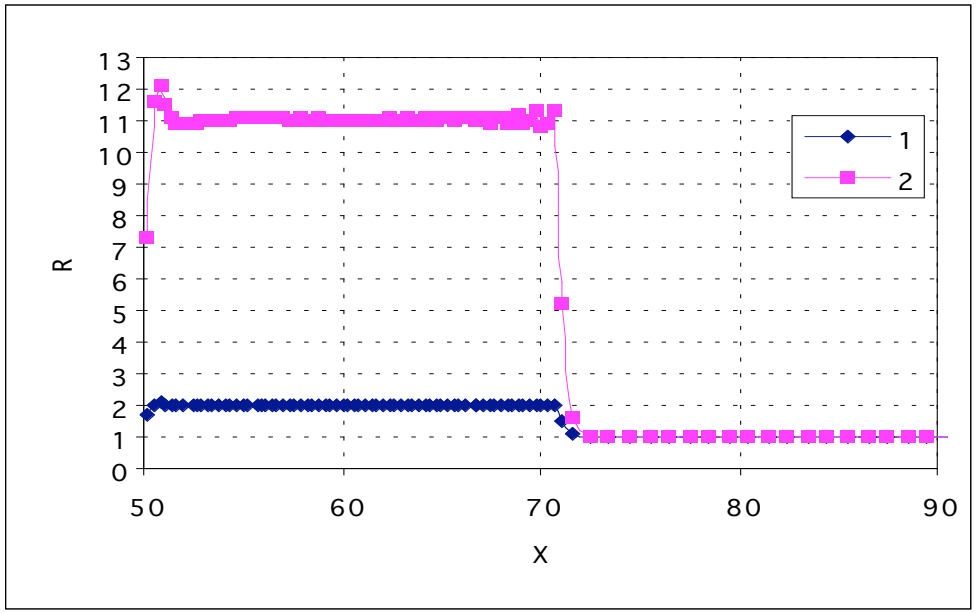
1–material 1; 2 –material 2.



method 1



method 3



method 3P

Part 2.

Specific features of using the donor method (DM), concentration method (CM), and PPM method

Determination of material flows across a cell side (face)

k-2	k-1	k	k+1	k+2
β^n_{k-2}	β^n_{k-1}	β^n_k	β^{n+1}_{k+1}	β^n_{k+2}

Volume flows:

$$\Delta V_i = \Delta V \cdot \beta^i_{\Delta V}$$

Mass and energy flows:

$$\Delta M_i = \Delta V_i \cdot \rho^i_{\Delta V};$$

$$\Delta E_i = \Delta M_i \cdot e^i_{\Delta V}$$

Use of various methods

- **Determination of volume flows:**

  it is possible to reconstruct an interface – method CM,

  otherwise – method PPM,

- **Determination of mass and energy flows:**

  method DM,

  method PPM.

- **Determination of momentum flows:**

  linear reconstruction of velocity + method DM,

  linear reconstruction of velocity + method PPM.

Some problems of using PPM

k-2	k-1	k		k+1	k+2
f_{k-2}^{n}	f_{k-1}^{n}	f_{k}^{n}	→	f_{k+1}^{n}	f_{k+2}^{n}

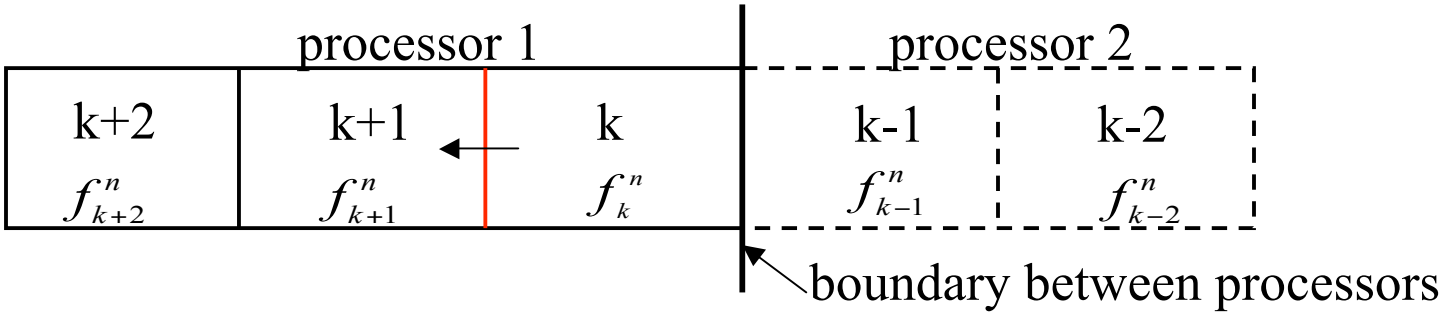
1) Not each of the 5 cells contains a given material

k-2	k-1	k		k+1	k+2
f_{k-2}^{n}	0	f_{k}^{n}	→	f_{k+1}^{n}	f_{k+2}^{n}

In cell (k-1) is not given material $\Rightarrow f_{k-1}^{n} = f_{k}^{n}$

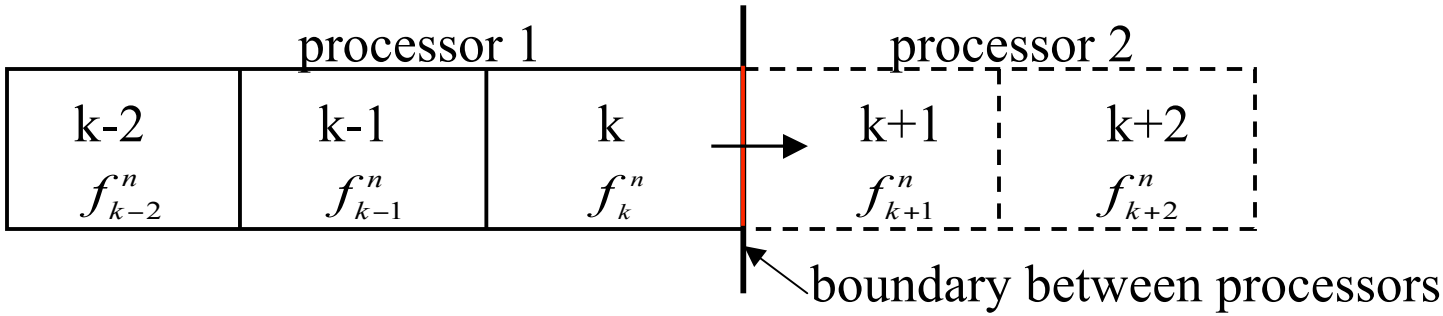
Some problems of using PPM

2) Some required cells are out of the current processor (only TREK)



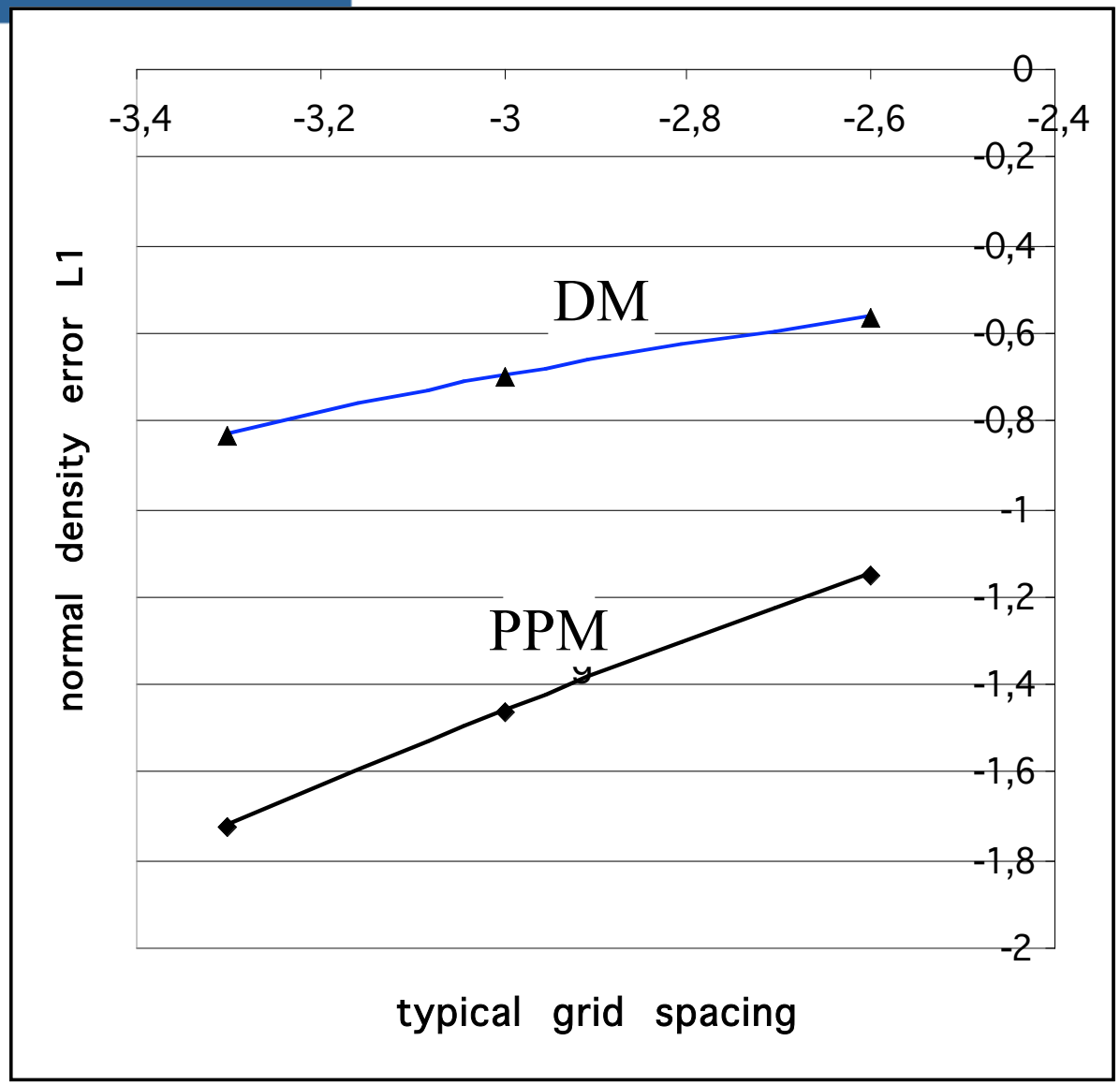
The state of cell (k-1) is available, the state of cell (k-2) is copied from cell (k-1)

3) Calculation of the flow across a boundary between processors (only TREK)



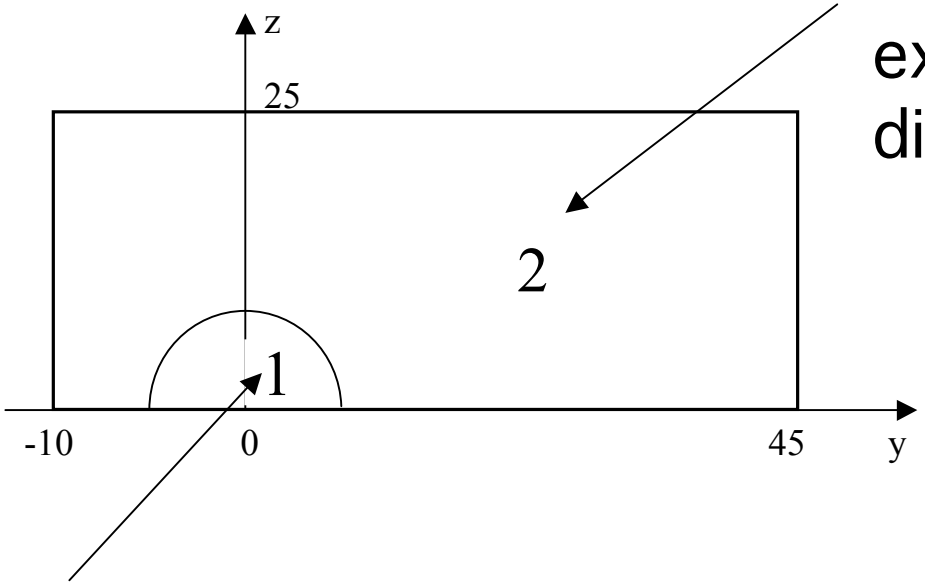
The method DM is used

Problem 3 (Blast Waves)



Convergence curves

Problem 4. Explosion in exponential atmosphere



Region 2: atmosphere with exponential density distribution along Y-axis,

$$\rho = \rho_0 \exp(-y), \ \ \rho_0 = 1$$

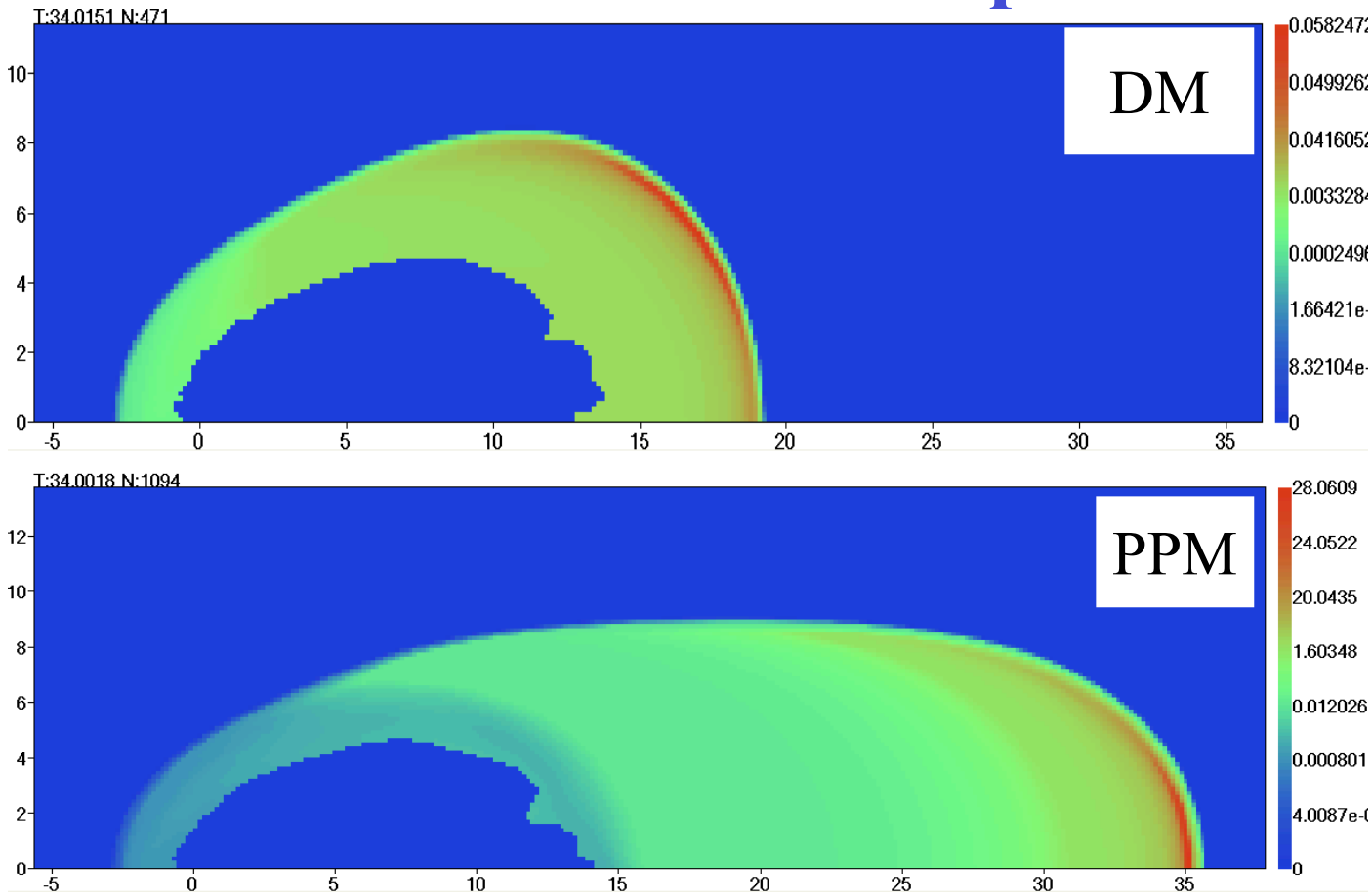
Region 1: EP with radius $R_0 = 0.75$

$$\rho = 1, \ \ e = \frac{E}{4/3 \ \pi R_0^3 \rho} \quad (E = 1)$$

Explosion in exponential atmosphere

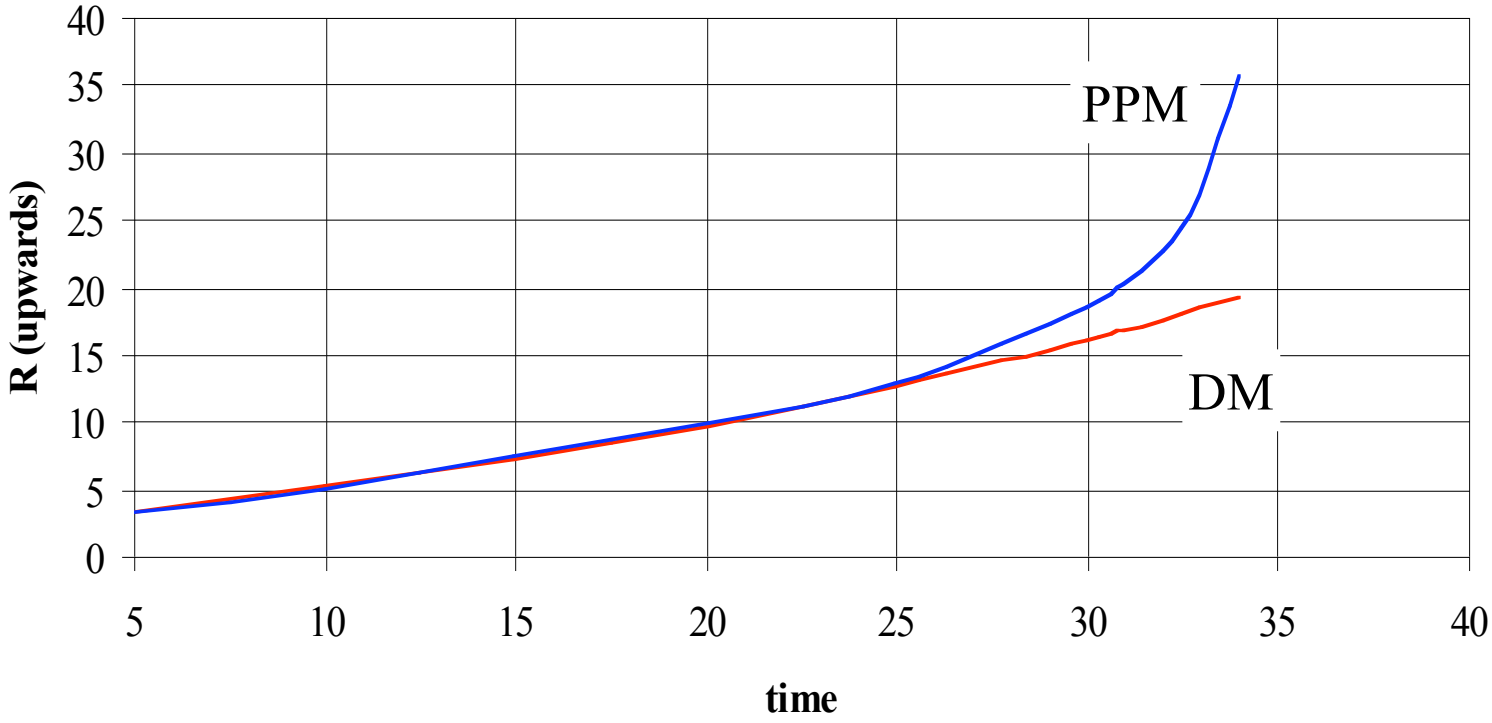
a)

b)



Internal energy of the atmosphere at time t=34

Explosion in exponential atmosphere



Зависимость радиуса ударной волны от времени

Part 3.

Heat conductivity equation approximation for multimaterial case

Division into two phases

1. Solution of an arbitrary heat conductivity equation for the mean energy

2. Heat exchange between materials in mixed cells

Phase 1.

LI scheme (Lokutsiyevsky, 1984; Zhukov, 1986)

$$\rho \frac{\partial e}{\partial t} = \mathrm{div}\left(\kappa \cdot \mathrm{grad}T\right)$$

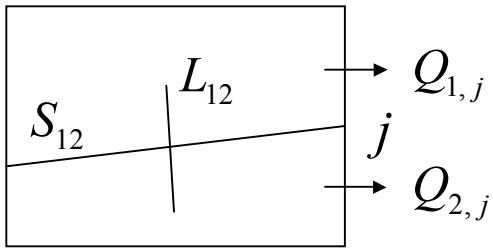
$$\frac{1}{\kappa} = \sum_l \frac{\alpha_l}{\kappa_l\left(T, \rho_l\right)}. \qquad \alpha_l = \frac{\rho_l \cdot \beta_l}{\rho}$$

$$\frac{e_{cell}^{n+1} - e_{cell}^{n}}{\tau^n} = \left(\frac{\mathrm{div}\left(\kappa \cdot \mathrm{grad}T\right)}{\rho}\right)_{cell}^{n+1}$$

Phase 2.

The system of equations describing heat transfer between materials inside a mixed cell

$$\begin{cases} M_1 \dfrac{e_1^{n+1} - e_1^n}{\tau} = S_{12}\chi_{12} \dfrac{T_2^{n+1} - T_1^{n+1}}{L_{12}} + \sum_{j=1}^{6} Q_{1,j} \\ M_2 \dfrac{e_2^{n+1} - e_2^n}{\tau} = -S_{12}\chi_{12} \dfrac{T_2^{n+1} - T_1^{n+1}}{L_{12}} + \sum_{j=1}^{6} Q_{2,j} \end{cases}$$



2D cross-section of a mixed cell

M_i - mass of materials

e_i^n - specific internal energy of the i-th component at time t^n

$e_i^{n+1} = e_i(T_i^{n+1})$ - specific internal energy of the i-th component at time t^{n+1}

χ_{12} - mean value of heat conductivity coefficient at an interface

S_{12} - contact area between components (cross-section area)

L_{12} - distance between the centers of volumes occupied by components

$Q_{i,j}$ - the i-th component heat flow across the j-th face

Phase 2. Distribution of heat flows across faces of cells between materials

$$Q_{i,j} = S_j q_j \frac{S_{i,j}\chi_{i,j}}{\sum_{k=1}^{2} S_{k,j}\chi_{k,j}}, \quad j = 1,\ldots,6, \quad i = 1,2$$

q_j - the mean heat flow unit area entering a cell across the j-th face and calculated in Phase 1

S_j - area of the j-th face of cell

$S_{i,j}$ - the part of the j-th xell face area occupied by the i-th component

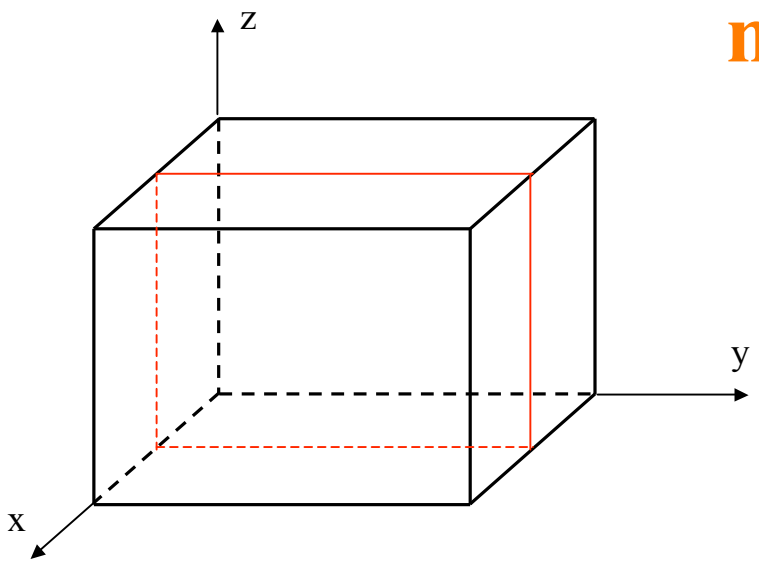
$\chi_{i,j}$ - heat conductivity coefficient of the i-th component, related to the j-th face of cell

Test computations

There were three options of settings for computations:

- The interface coincides with the computational grid lines (Lagrangian computation)
- The interface doesn't coincides with the computational grid lines, assumption of equal material temperatures in mixed cells is used (**method 1**)
- The interface doesn't coincides with the computational grid lines, heat exchange between materials in mixed cells takes place (**method 2**)

Problem 5. Heat exchange in a two-component medium



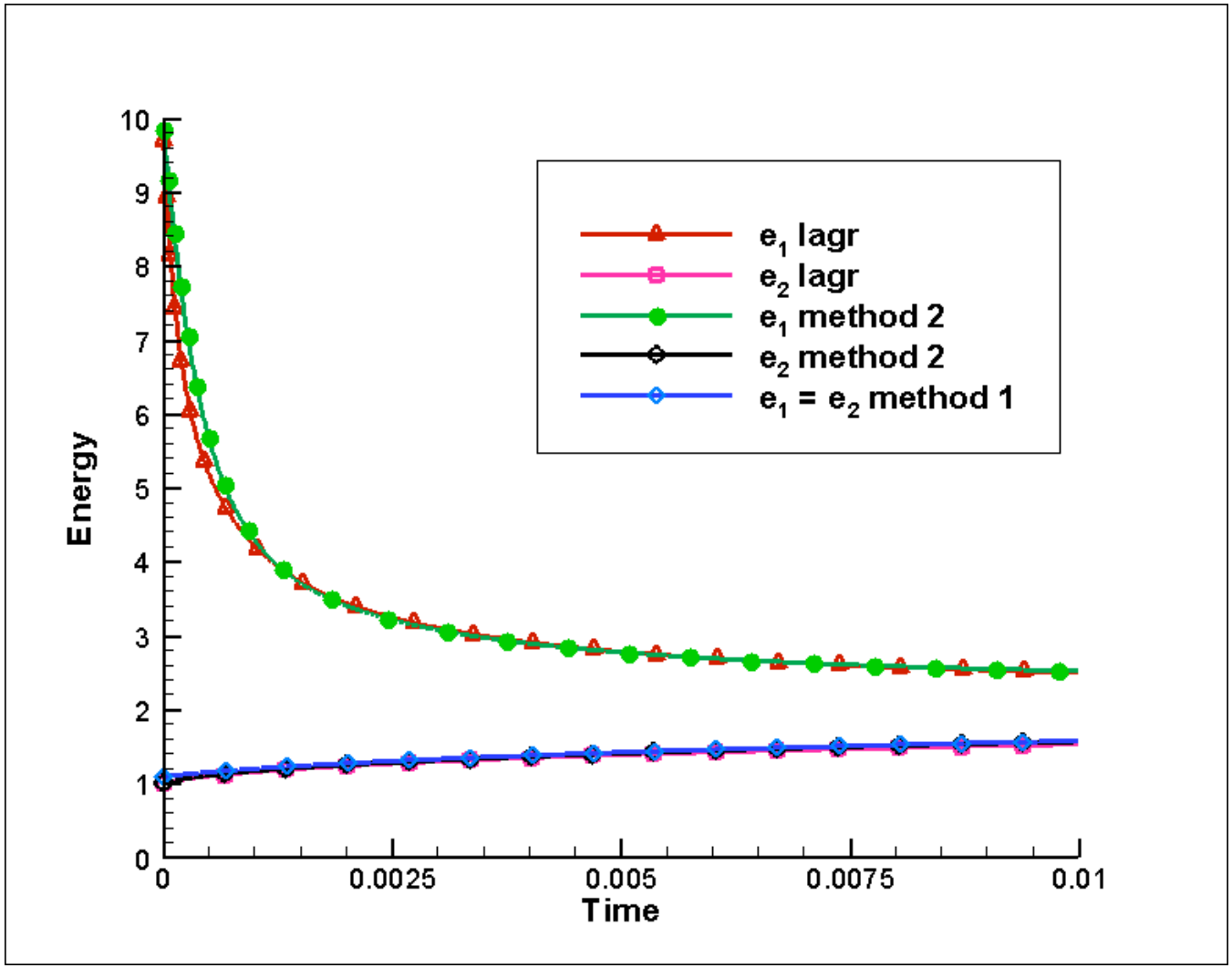
Rectangular parallelepiped

$(-2 \le x \le 2, \quad 0 \le y \le 3, \quad 0 \le z \le 0.2)$

is cut by plane $x = 0$ into two parts

Region 1: $e_1 = 10 \quad \rho_1 = 0.1 \quad \chi_1 = 1 \quad C_V = 1$

Region 2: $e_2 = 1 \quad \rho_2 = 10 \quad \chi_2 = 0.5 \quad C_V = 1$



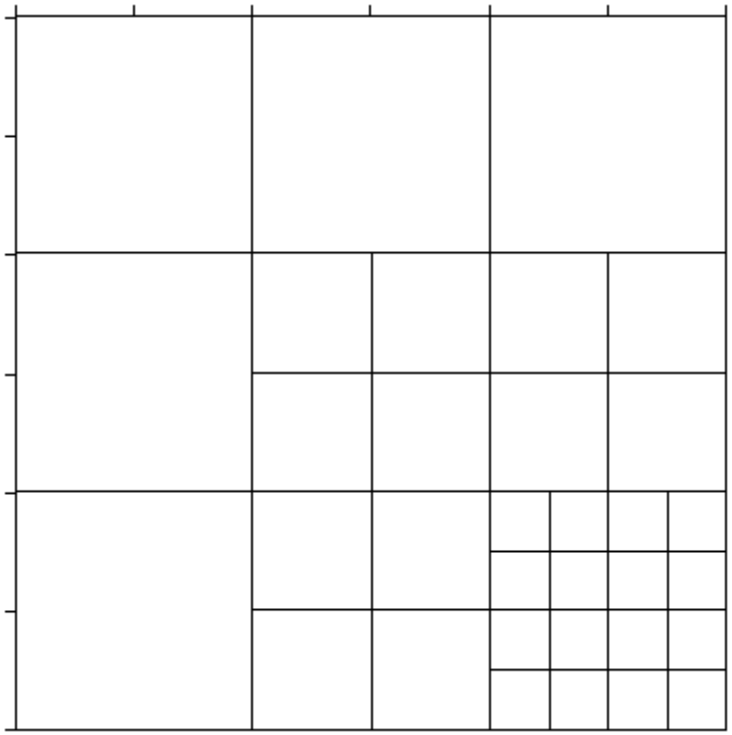
Specific internal energy vs-time inside a mixed cell

Part 4.

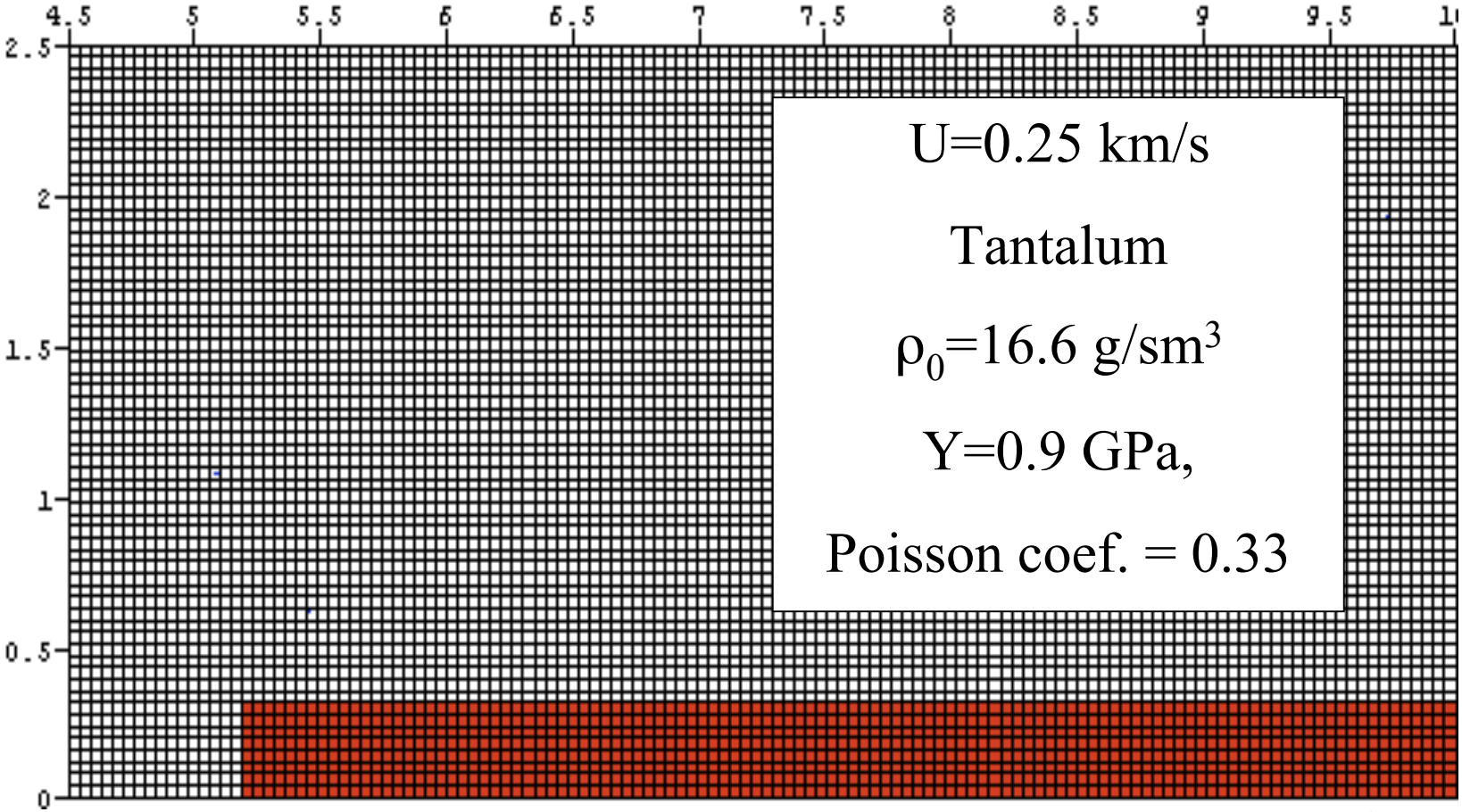
Use of a refined mesh

Refined mesh

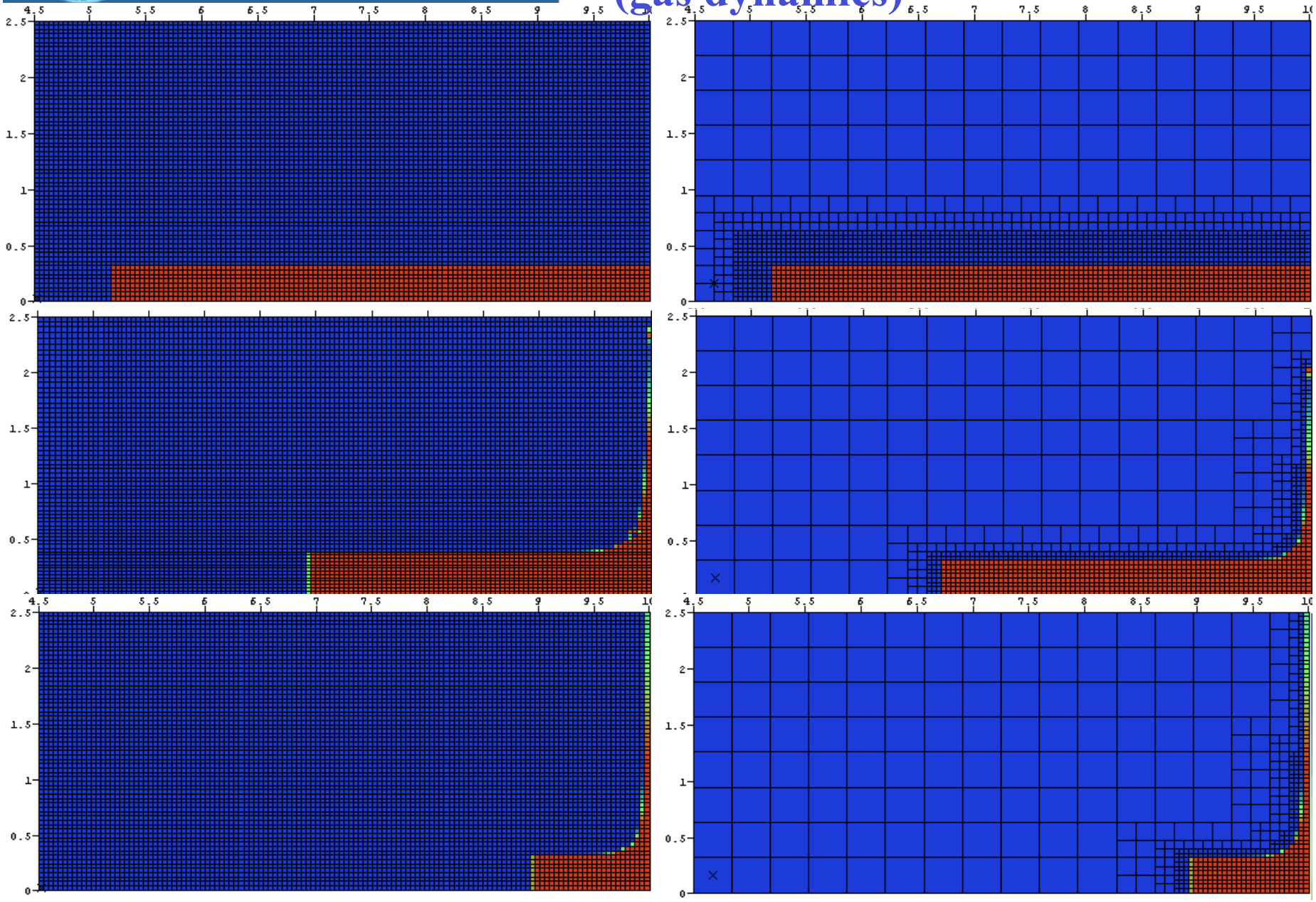
- Both addition of new cells and elimination of old ones are performed automatically by the program;
- The refinement method is the same at all levels (number of levels <= 5);
- New cells are obtained by drawing lines to connect center points of larger cell sides;
- The difference between adjacent cells cannot exceed one level;
- All mother cells are retained.



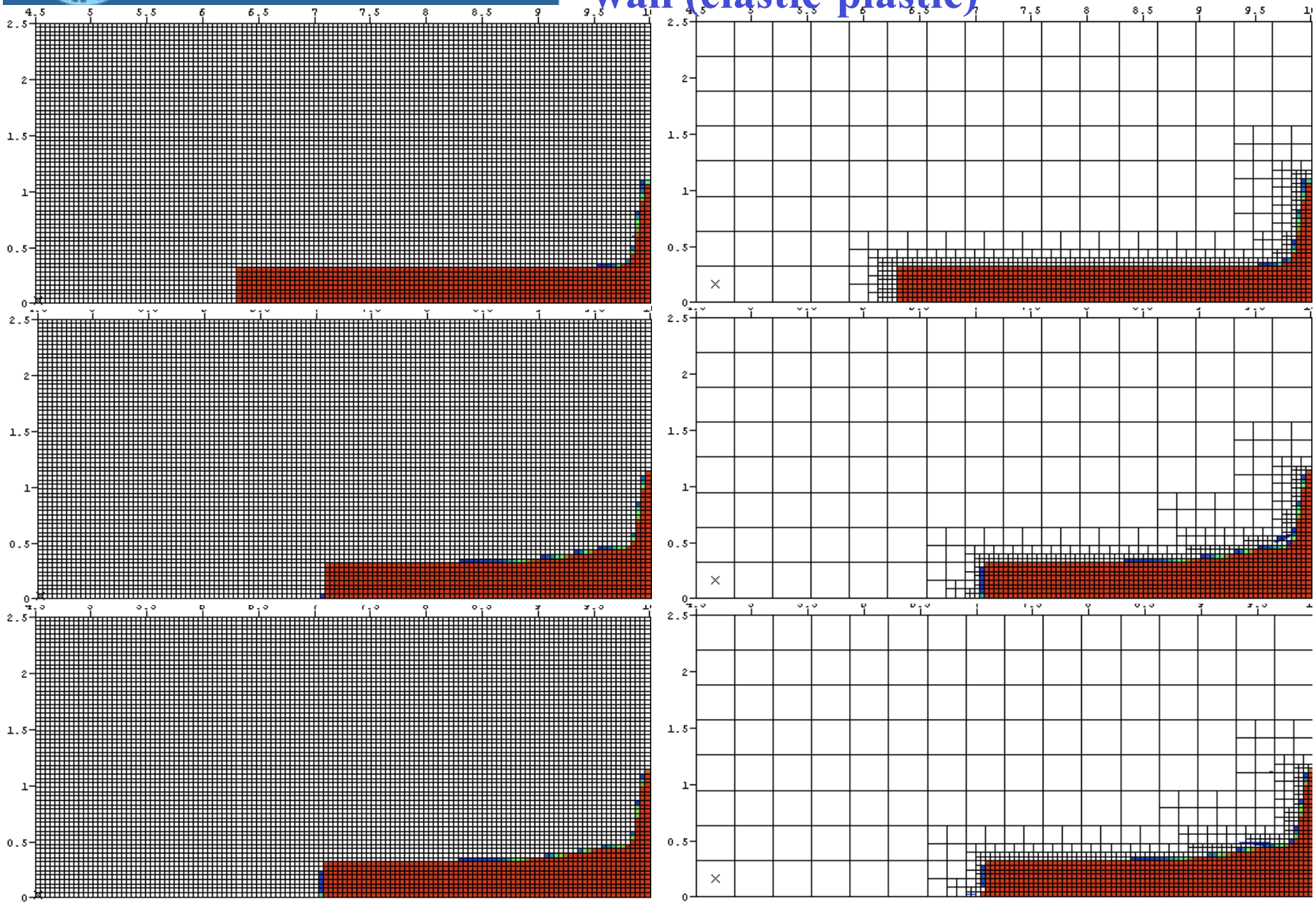
Problem 6. A cylinder impact on a rigid wall



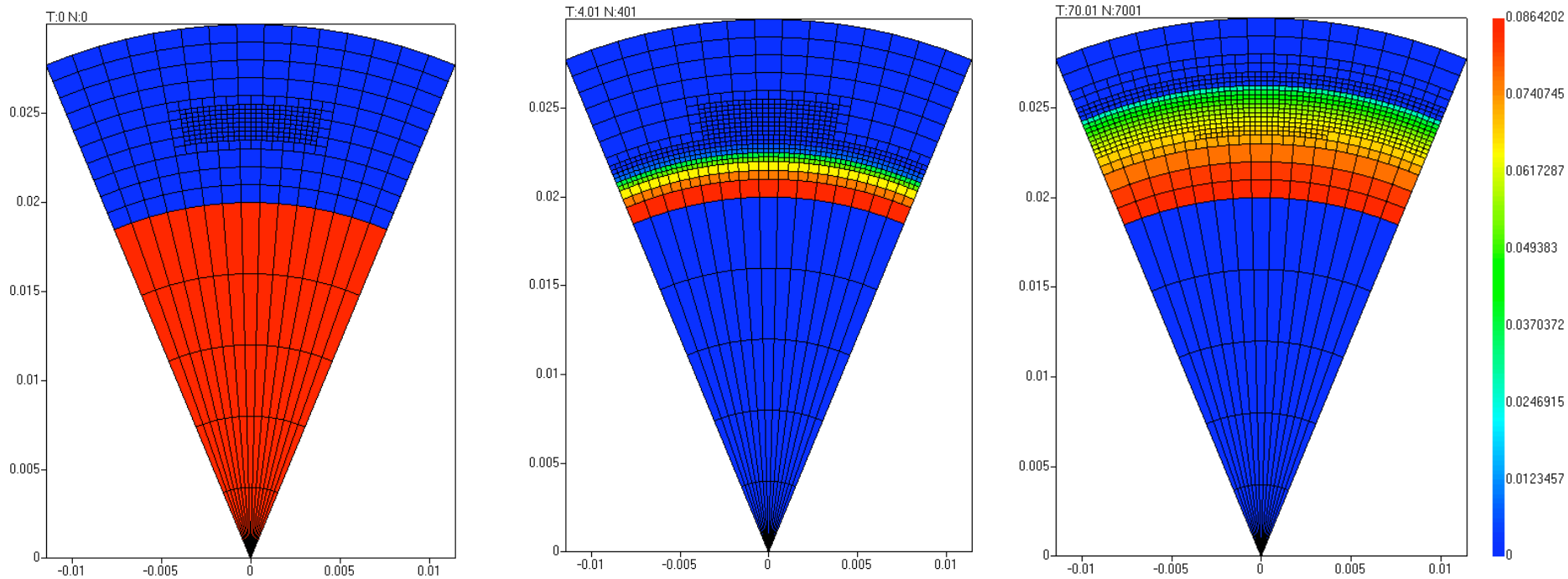
A cylinder impact on a rigid wall (gas dynamics)

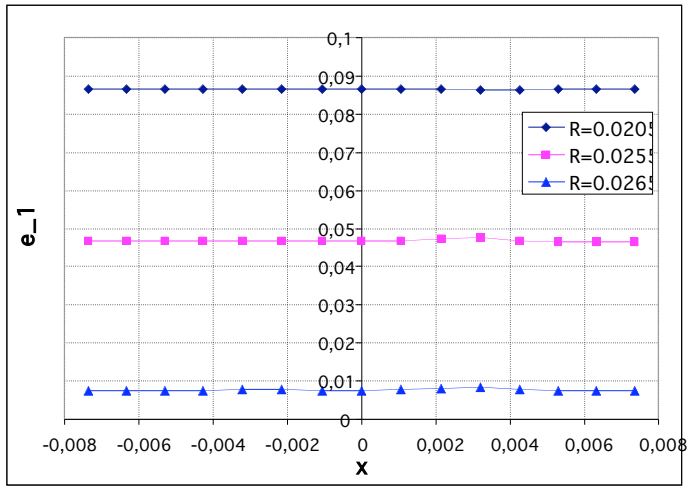


A cylinder impact on a rigid wall (elastic-plastic)



Problem 7. Heat wave propagation

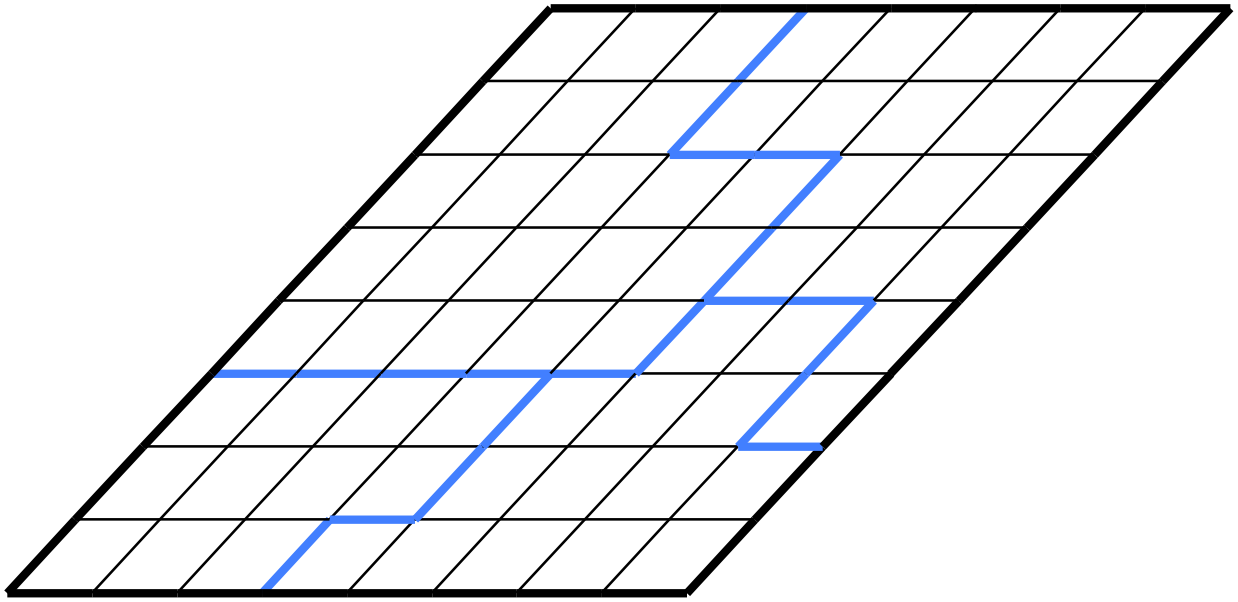




Part 5.

Specific features of parallelization

Geometric decomposition



Specific features of the parallel code

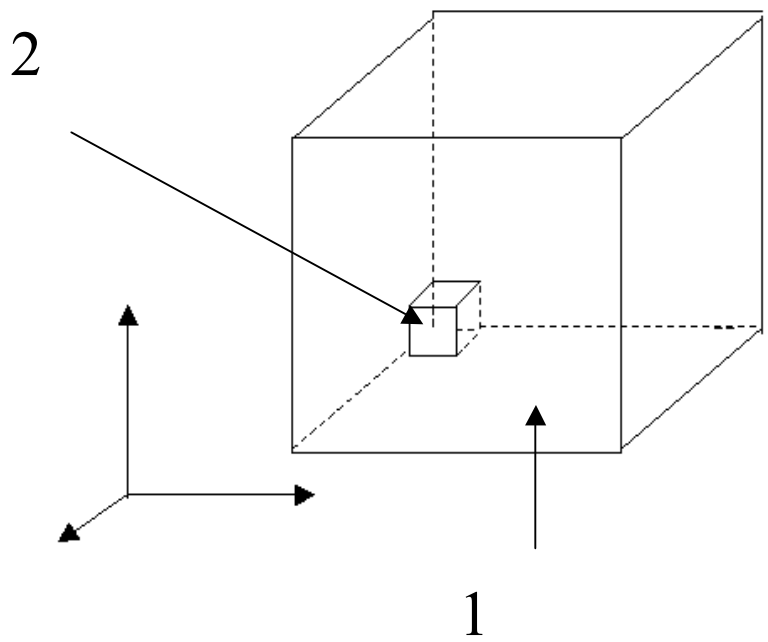
- First, calculations at boundary processor points are performed. The calculated values are immediately transmitted to the neighboring processors.

- Then calculations at inside-processor points are performed against the background of these calculations, data transmissions from the neighboring processors are received in the order of priorities

Irregular pointwise parallelization

- Irregular pointwise parallelization is a key point of this approach. Calculation of quantities, determined at one computational point is a unit work for allocation to processors.
-
- The code is arranged as a loop in an arbitrary list of the numbers of points.

Problem 8. Gas dynamics test



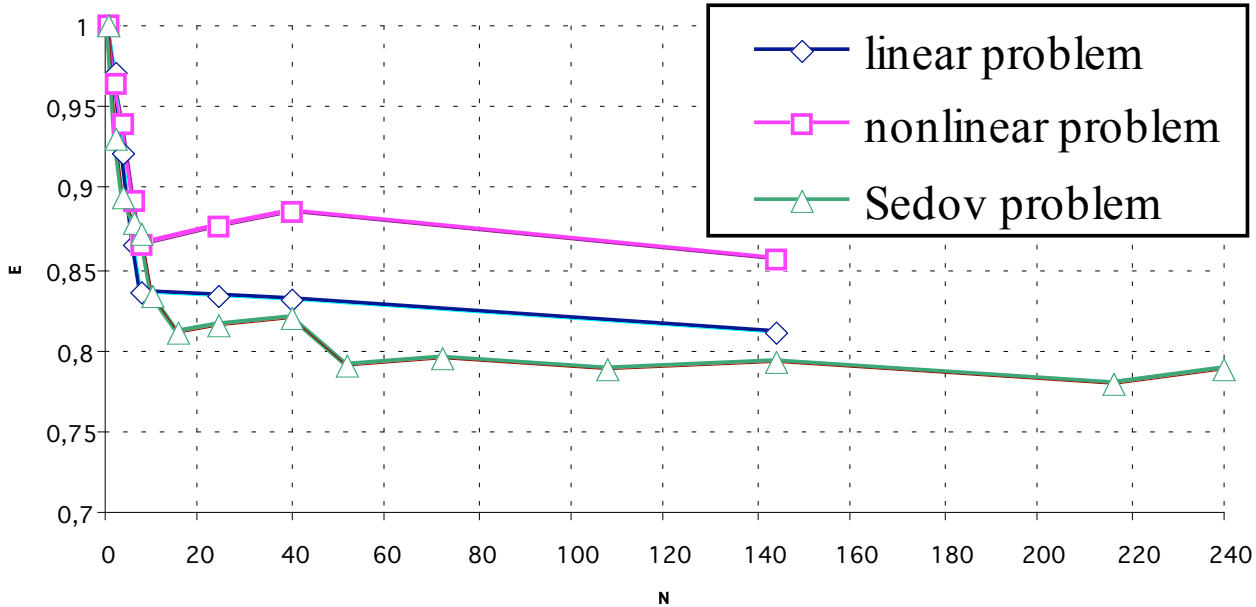
$h_x=h_y=h_z=0.1.$
Region 1 - $\rho_0= 1$, $e= 0$, $u_0= 0$, $\gamma=1.4$
Region 2 (cube with side =1) - $\rho_0= 1$, $e= 1.0$, $u_0= 0$, $\gamma=1.4$.

Problems 9 and 10.
Thermal conductivity test problems

- **linear problem of a cooling down cube;**

- **nonlinear problem - heat wave propagation.**

Efficiency in the problem multiplication mode. (105*105*105 cells per processor)



Conclusion

- The report describes same innovations allowing a significant improvement of accuracy of 2D and 3D numerical simulations using EGAK and TREK codes.

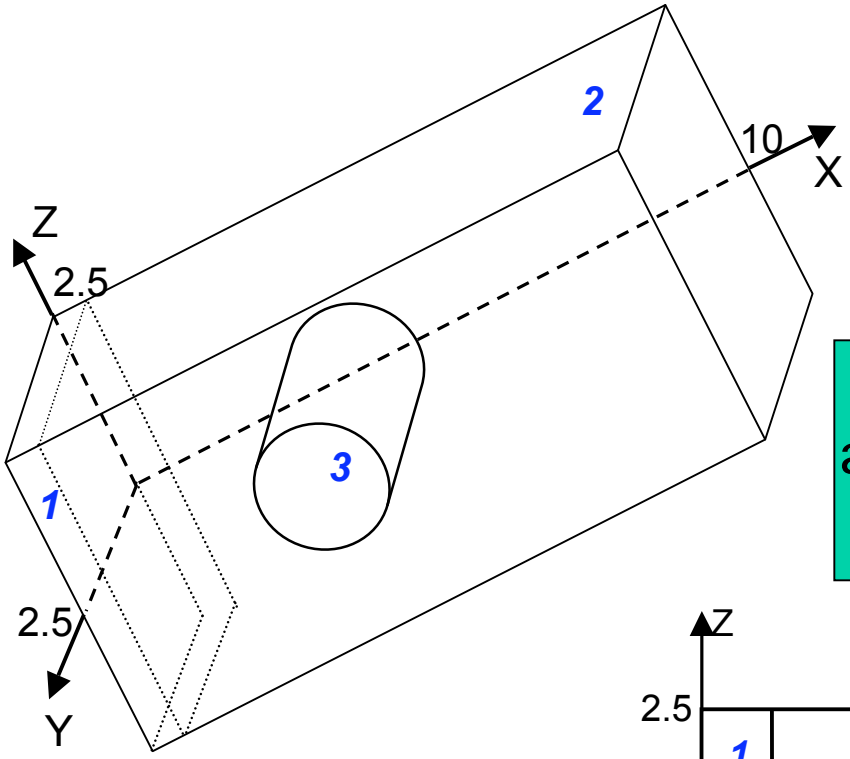
- As a result, the accuracy of Eulerian methods is almost the same as the accuracy of Lagrangian methods, this makes them attractive for numerical studies of complex problems.

- These techniques are currently used for numerical studies of a wide range of problems with multidimensional flows, in particular, those related to turbulent mixing.

Part 8.

Some calculations

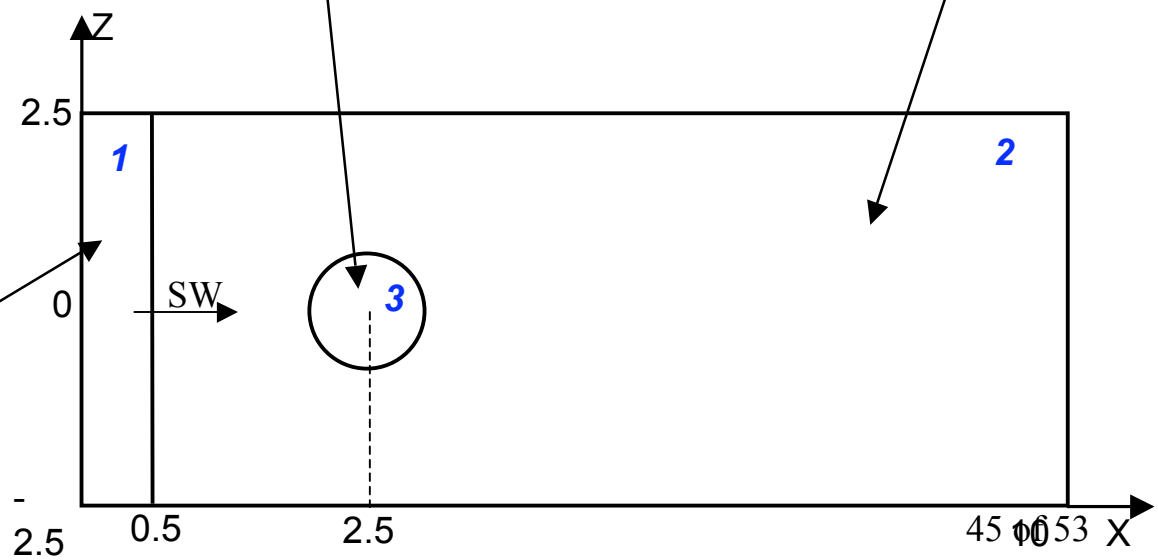
Problem 11. Benjamin experiment



Region 3:
air / SF6 mixture,
radius R=0.5

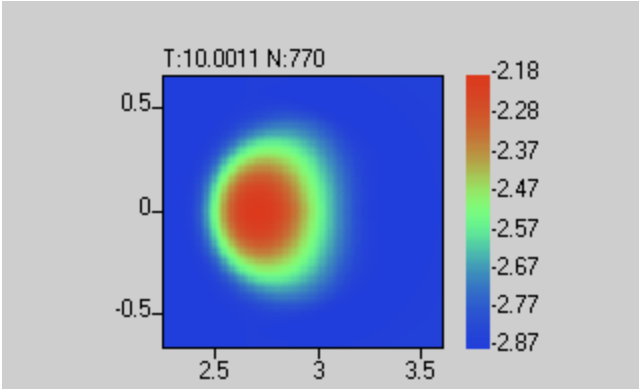
Region 2:
undisturbed air

Region 1:
disturbed air

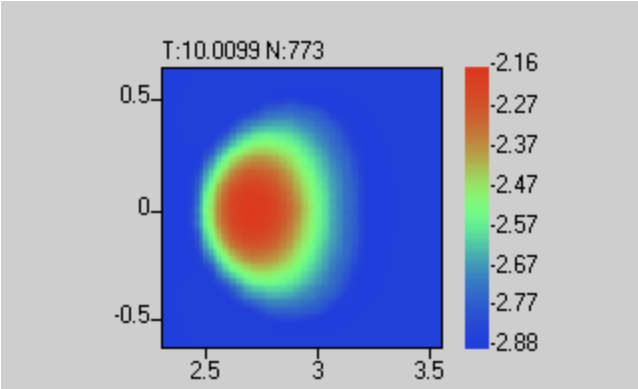


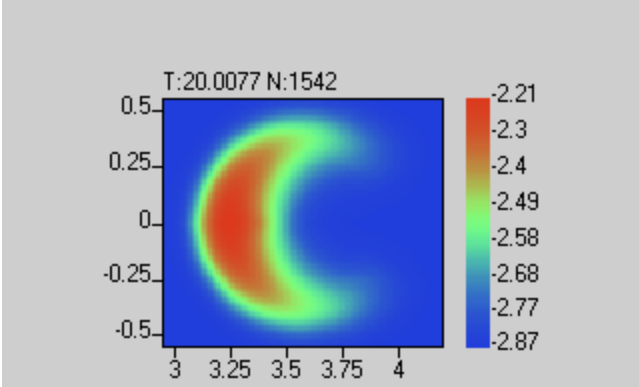
Density raster pictures

method DM | method PPM

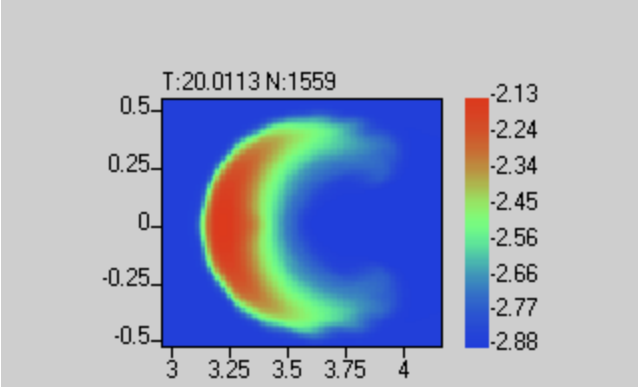


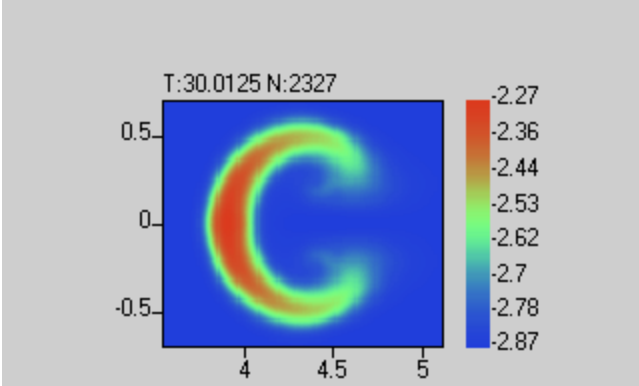
t=100mks



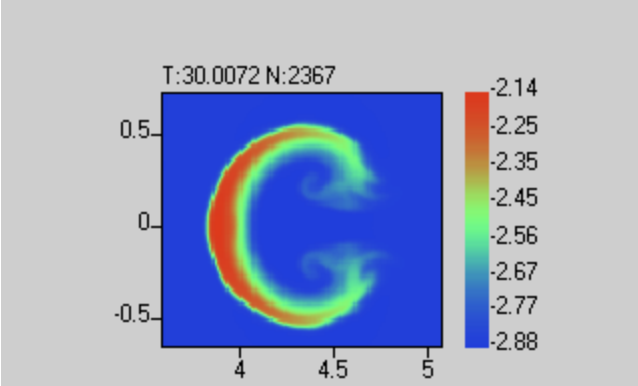


t=200mks



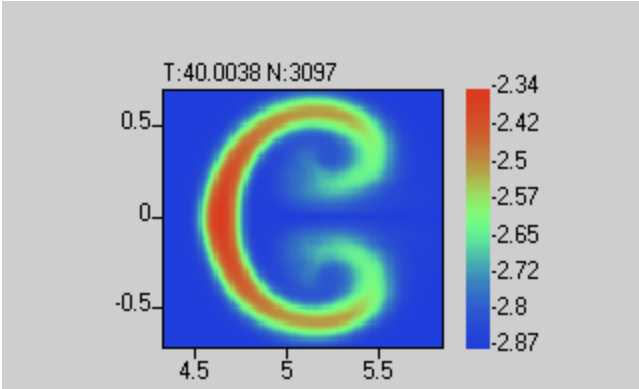


t=300mks

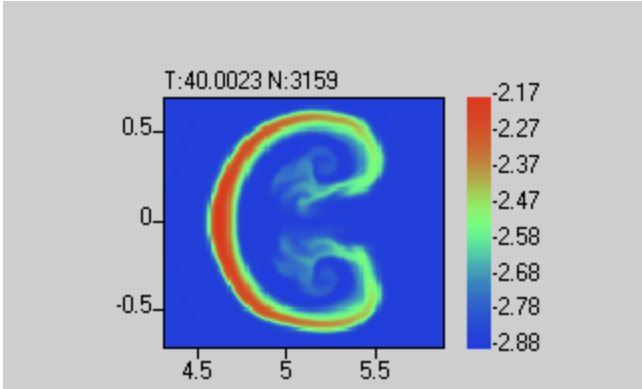


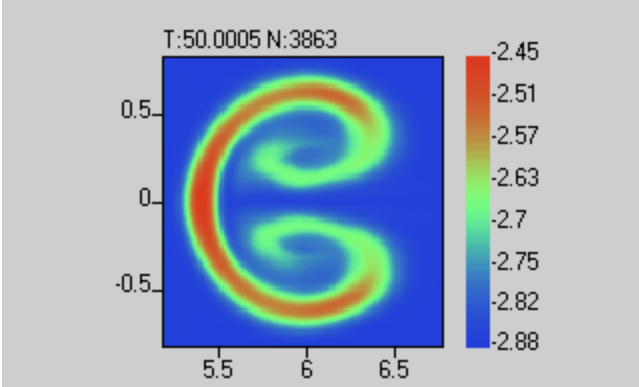
Density raster pictures

method DM | method PPM

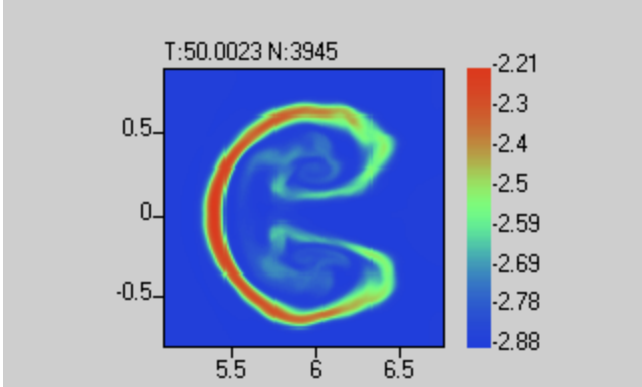


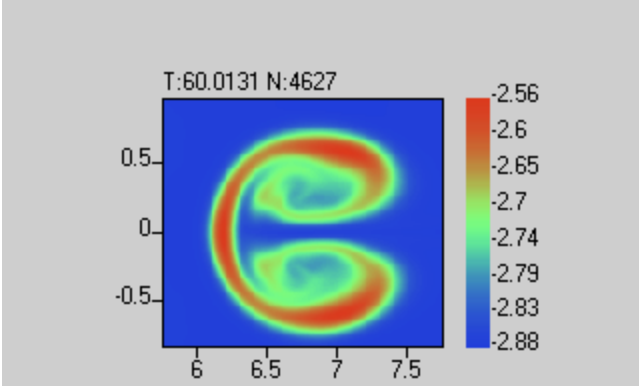
t=400mks



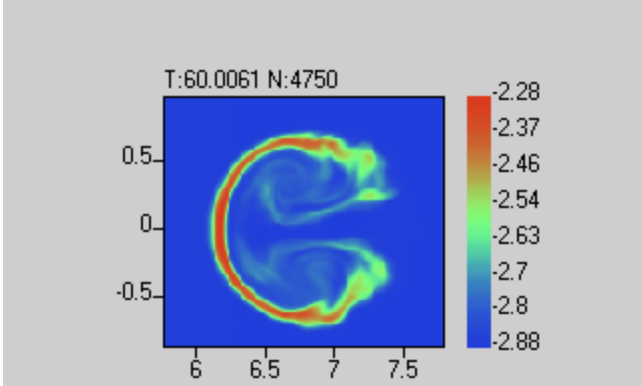


t=500mks





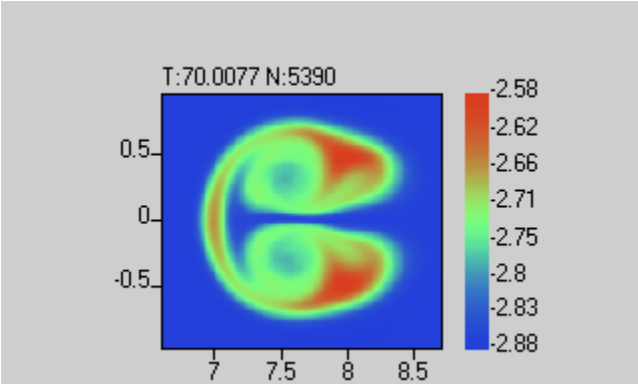
t=600mks



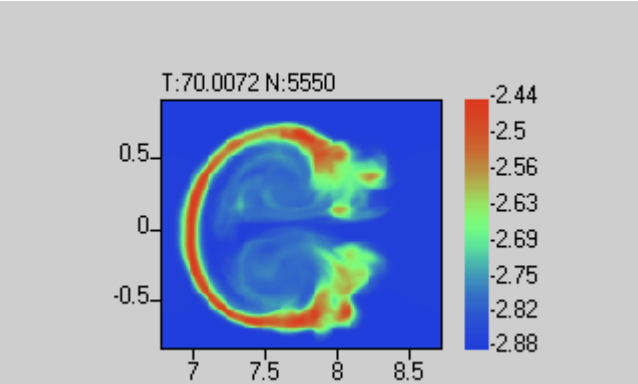
Density raster pictures

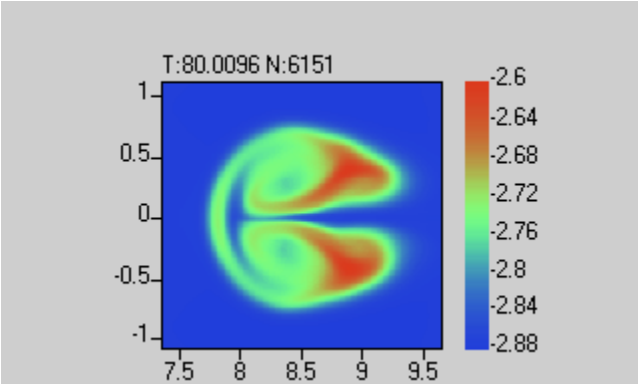
method DM

method PPM

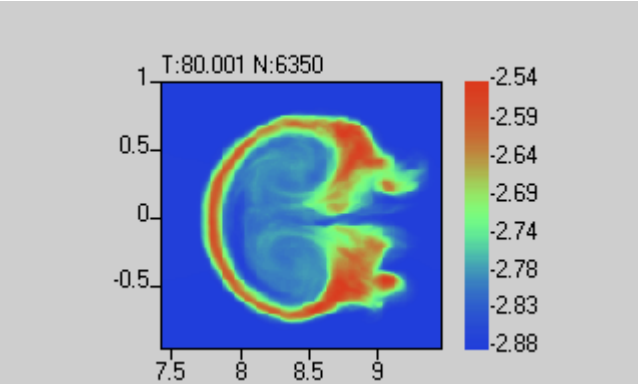


t=700mks



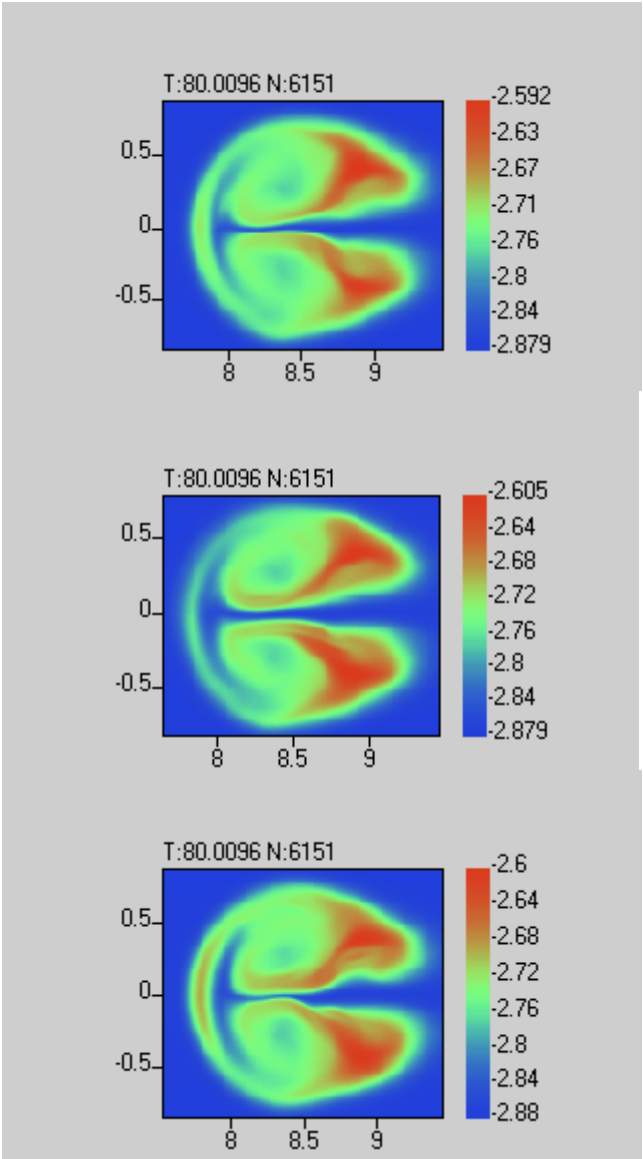


t=800mks

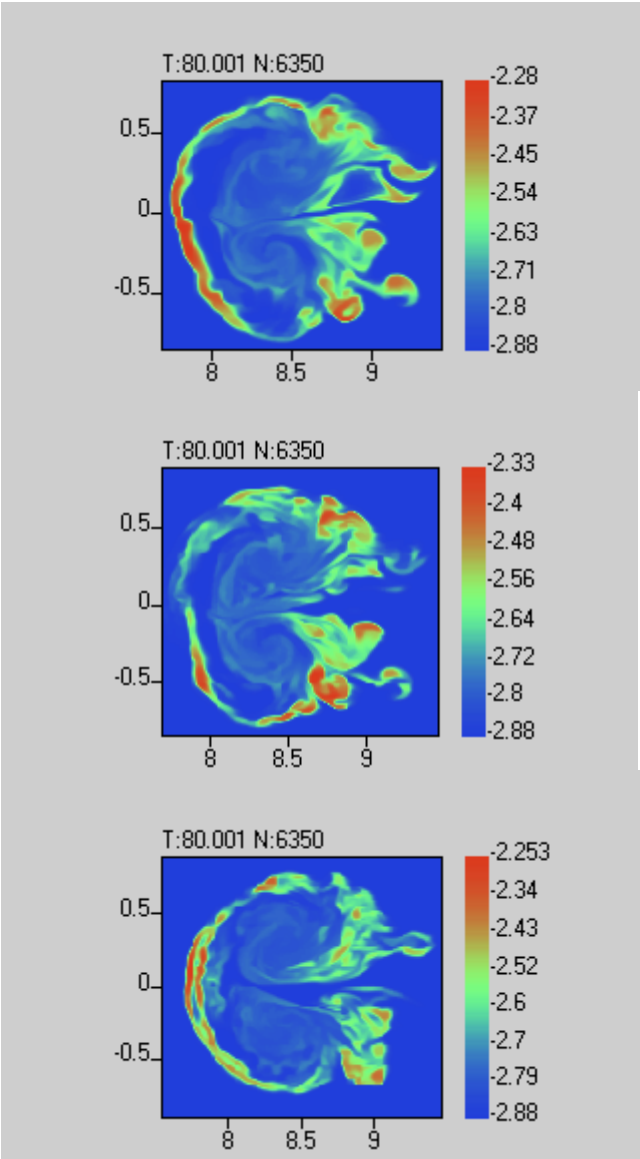


Density raster pictures (various sections)

method DM

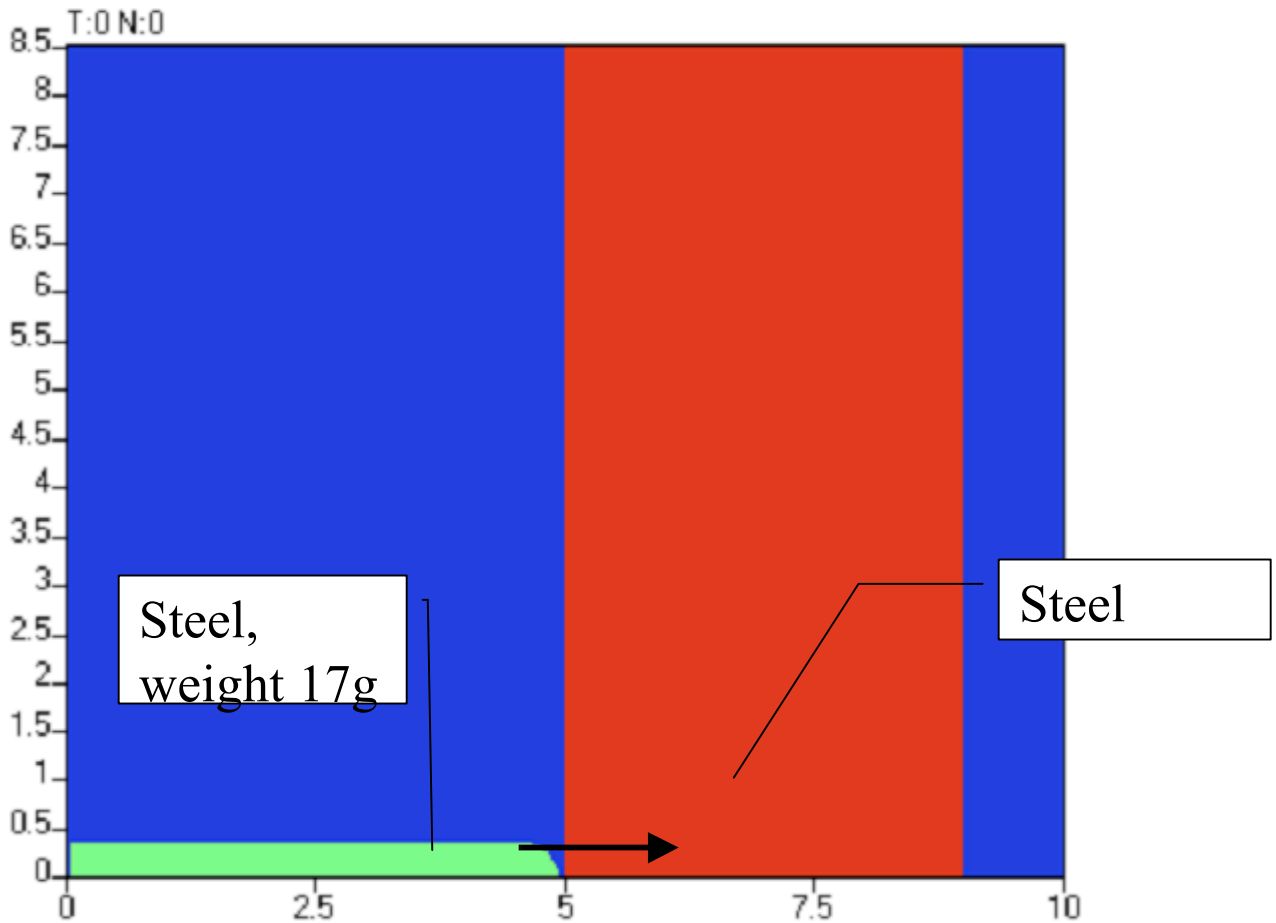


method PPM

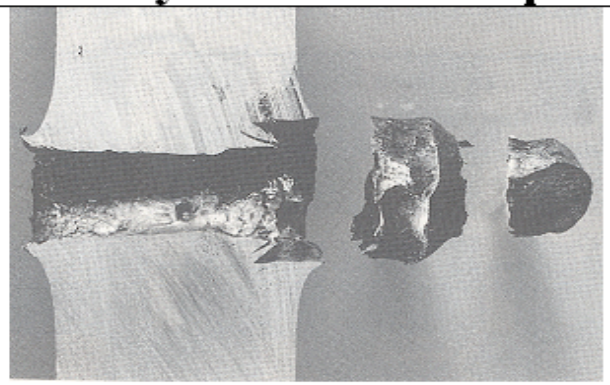
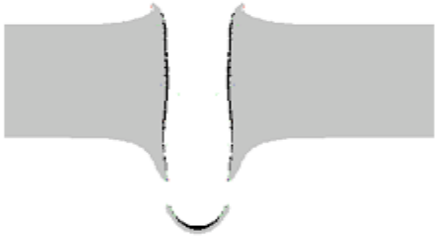
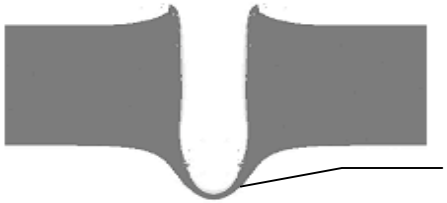
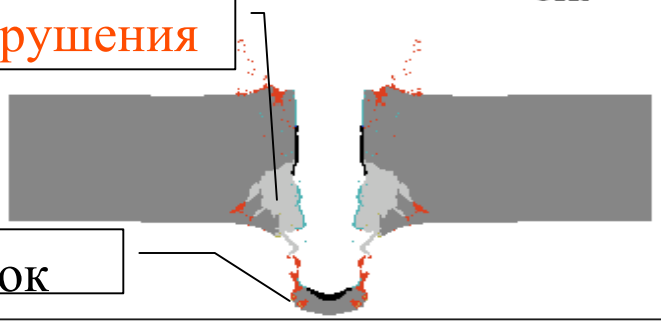
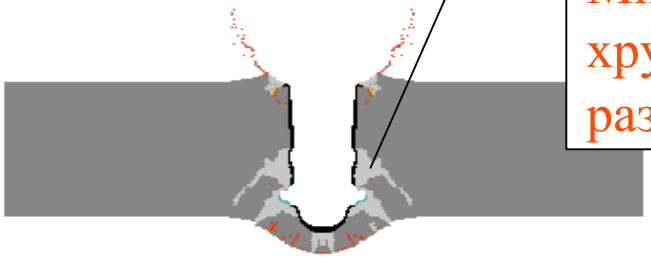


Problem 12. Target penetration

(Kanel destruction model)



Результаты расчетов

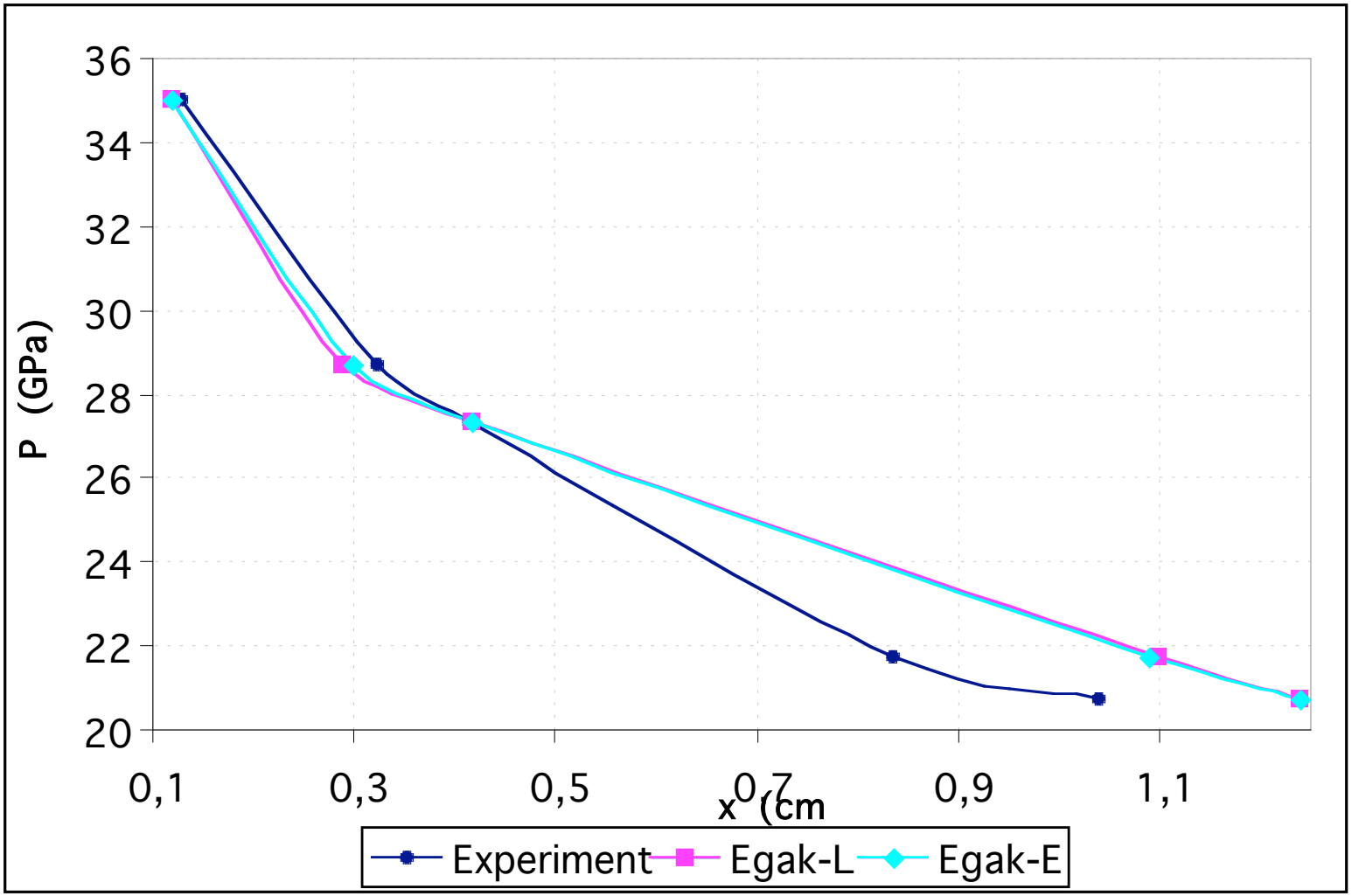
мишень 40мм	мишень 42мм
Результаты экспериментов, $V_{ударника}$=2100м/с	
	
ЭГАК, $\sigma_{тек}$ =0.9ГПа и $\sigma_{отк}$ =-0.9ГПа	
	
ЭГАК, модель разрушения Канеля, $\sigma_{тек}$ =1.1ГПа и $\sigma_{отк}$ =-1.1ГПа	
	

Мишень растягивается

Зона разрушения

Мишень хрупко разрушается

Осколок

Initiation of detonation in explosive material

Initiation of detonation in explosive material (results)