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Creation of parallel algorithms for the solution of problems of gas dynamics on multi-core computers and GPU

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Problem formulation

We consider the problems of gas dynamics simulation on multi-processor computers and graphics processors. Such problems are typical in climate modeling, supernova explosions, engineering aerodynamics modeling, etc. Modeling of three-dimensional gas-dynamic flows refers to the number of complex dynamic processes that have specific requirements to the used difference schemes. For these tasks, the difference schemes used to be the most accurately reproduce the behavior of matter in the vicinity of large ruptures and reliably describe small perturbations away from the shock fronts. By the schemes of this kind belong Total Variation Diminishing (TVD) schemes and others.

Problem formulation

Carrying out detailed three-dimensional calculations on grids requires large computational resources. The interest in this regard is the use of new technologies - the graphics processor (GPU) based on CUDA technology. The use of graphics processors enables the development of more efficient parallel algorithms for intensive numerical calculations.

In the present report we focus on the developing of parallel algorithms for solving various problems of gas dynamics.

Problem formulation

The equations describing the hydrodynamic motion, are the laws of conservation of mass, momentum and energy

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0,$$

$$\frac{\partial (\rho v_i)}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i v_j + P\delta_{ij}) = -\rho \frac{\partial \phi}{\partial x_i},$$

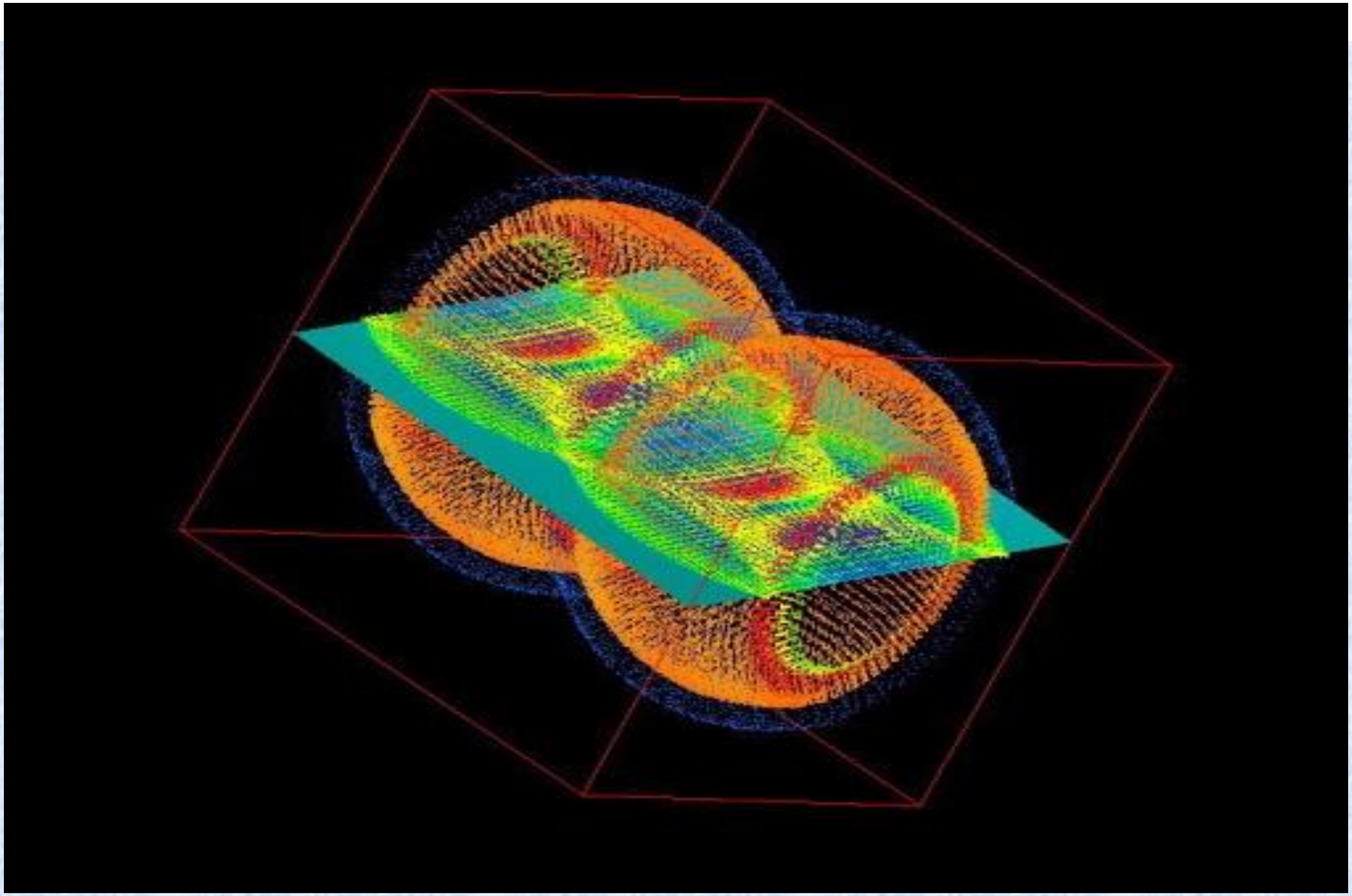
$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x_i}[(e+P)v_i] = -\rho v_i \frac{\partial \phi}{\partial x_i}.$$

Problem formulation

In these equations, the value of the gravitational potential is determined from the Poisson equation $\Delta\Phi = 4\pi G\rho$. The equation of state is used in the form: $e = 1/2\rho v2 + \varepsilon$. In the above equations ρ - density, v - velocity, P - pressure, ε - the specific internal energy, e - total energy.

Task 1. On the following slides presented results of testing culculation Sedov-Taylor tasks of interaction of two shock wave generated by the point explosions of equal power. The numerical results shown at the moment of the dimensionless time unit t = 1.2.

The numerical results



The velocities field

The numerical results

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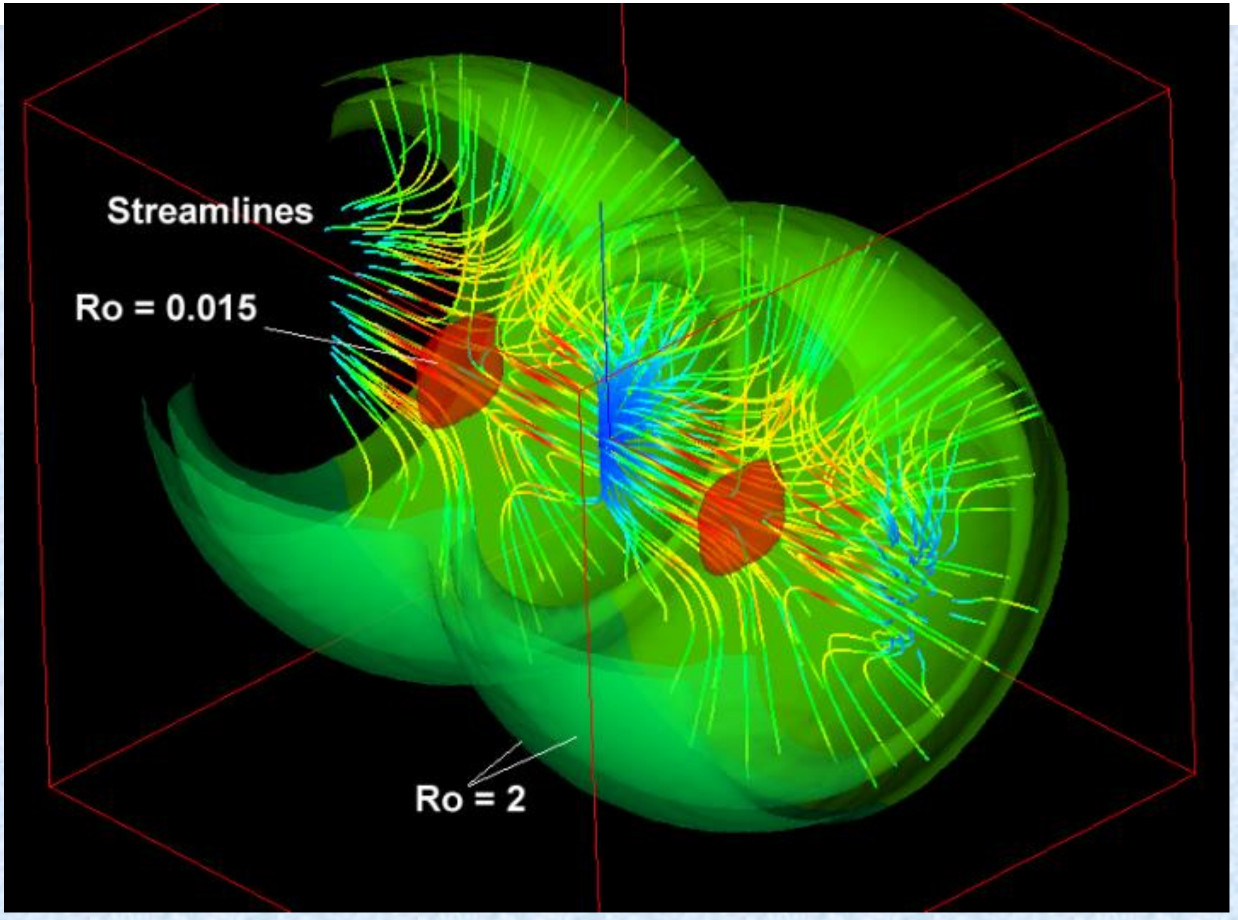


Density distribution

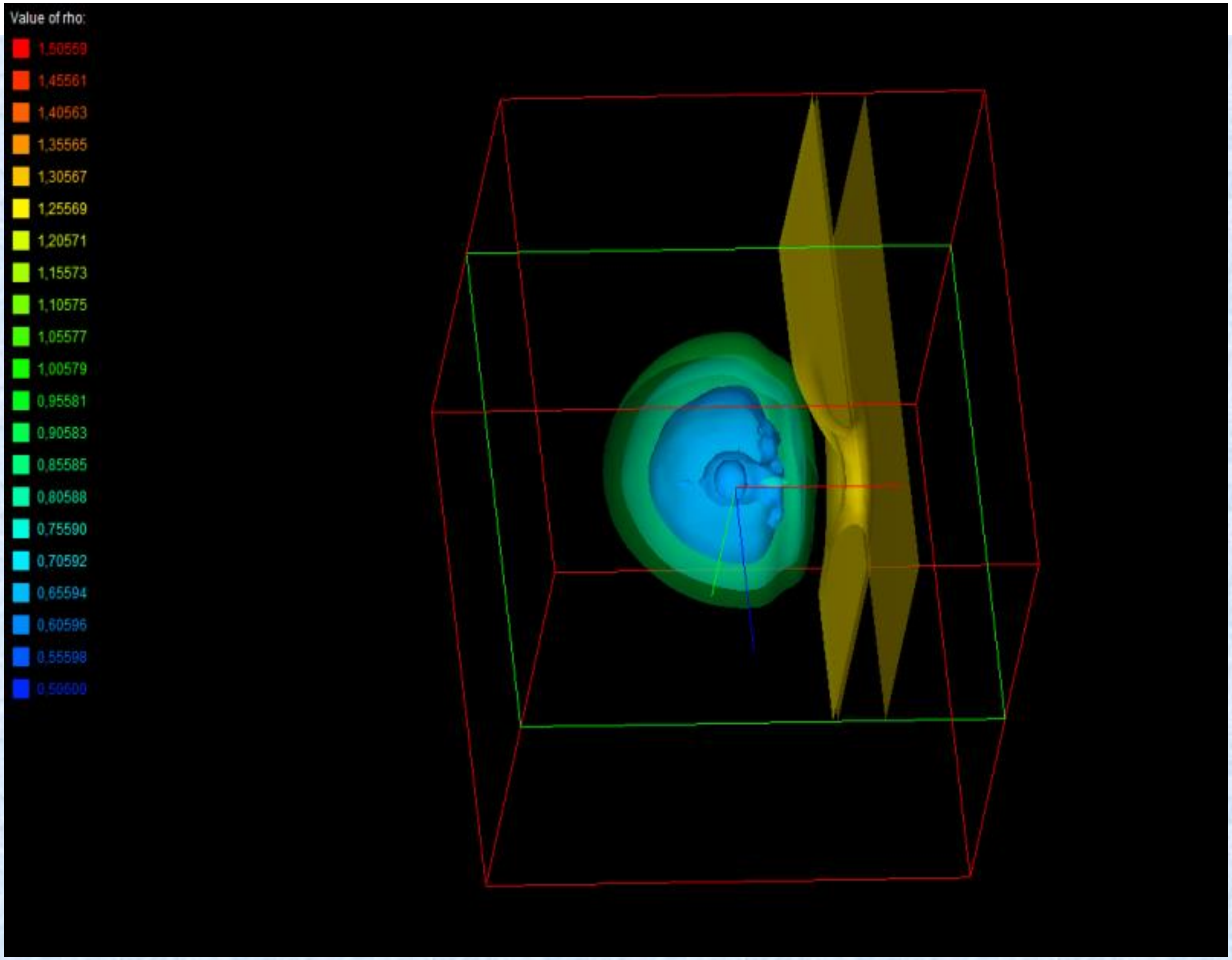
The numerical results - interaction of a plane shock wave with spherical cavities filled with gas

Task 2. Consider the problem of the interaction of a plane shock wave with spherical cavities filled with gas to other values of the thermodynamic parameters. These problems are typical for modeling of fuel combustion, evaporation vesicles, etc.

Suppose that R: $\{0 \le x \le 1, 0 \le y \le 1, 0 \le z \le 1\}$ is a parallelepiped filled with a stationary gas density $\rho 0 = 1.0$ and the pressure $p0 = 1.0$. Inside the box located a spherical region of radius $r = r0$, centered at the point $(x0, y0, z0)$. On the right, at coordinates $x = x^*$, is disposed plane shock wave that moves to the left. Initial conditions to the right from shock wave and outside the spherical bubble are defined as follows $(p, \rho, u, v, w)^T = (p_h, \rho_h, u_h, v_h, w_h)^T$. Inside a spherical cavity pressure and density equal to $p = p_b = 1.0$, $\rho = p_b = 0.1$. Behind the shock wave values are determined using the Rankine-Hugoniot relations.

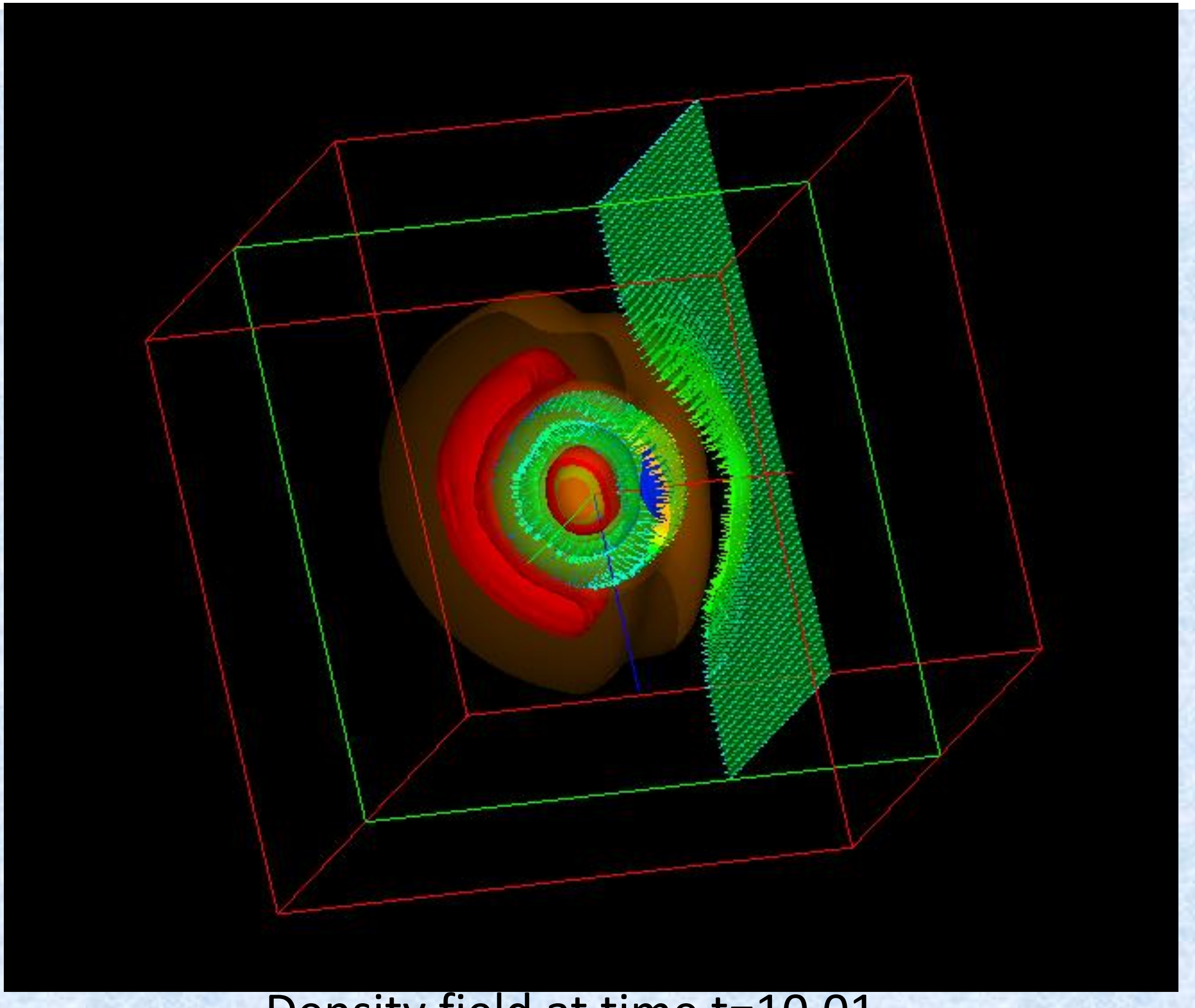
On following slides are shown graphs of density at the time moments $t = 5.021$ and $t = 10.01$ respectively.

The numerical results



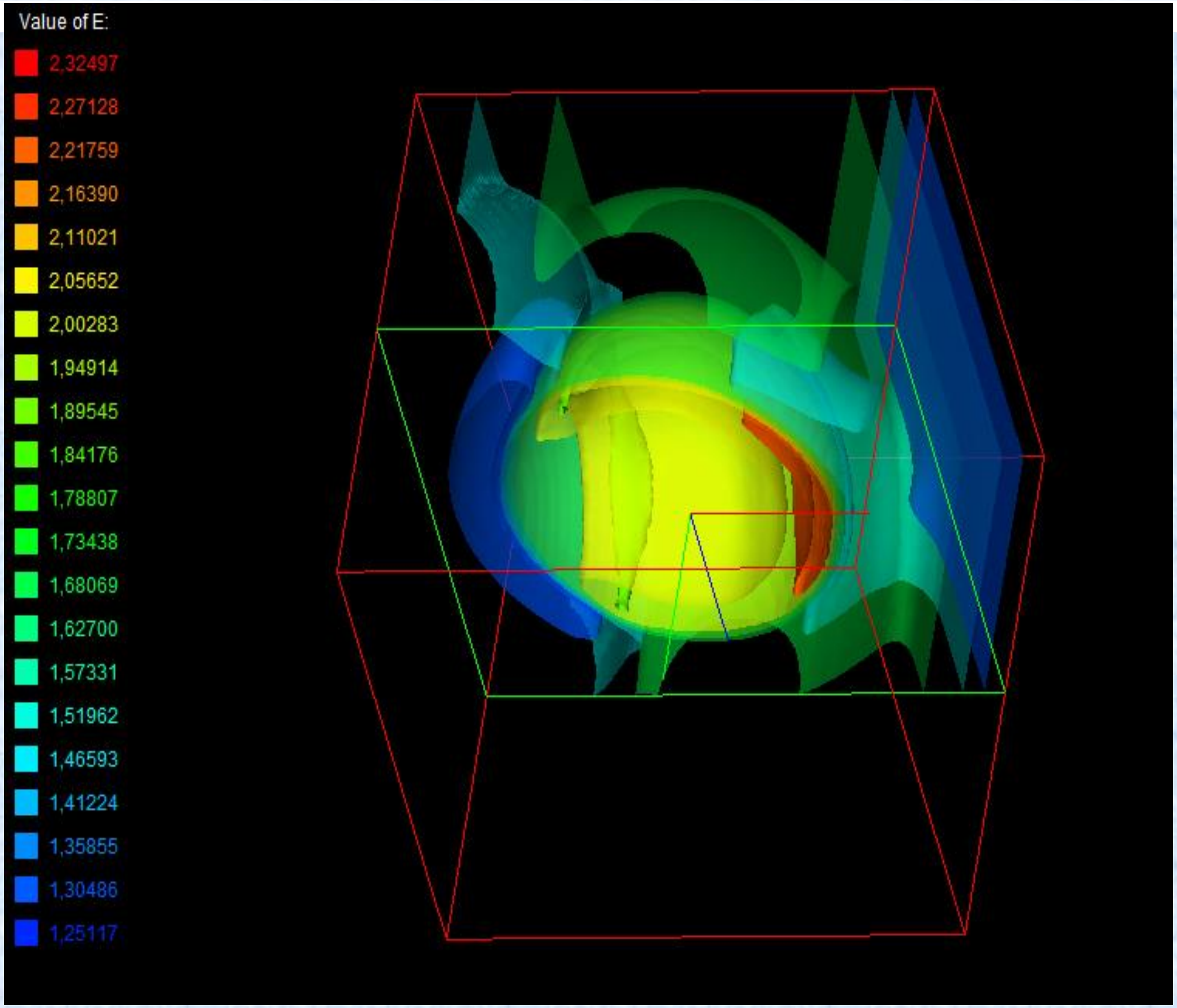
Density profile at time t = 5.021

The numerical results



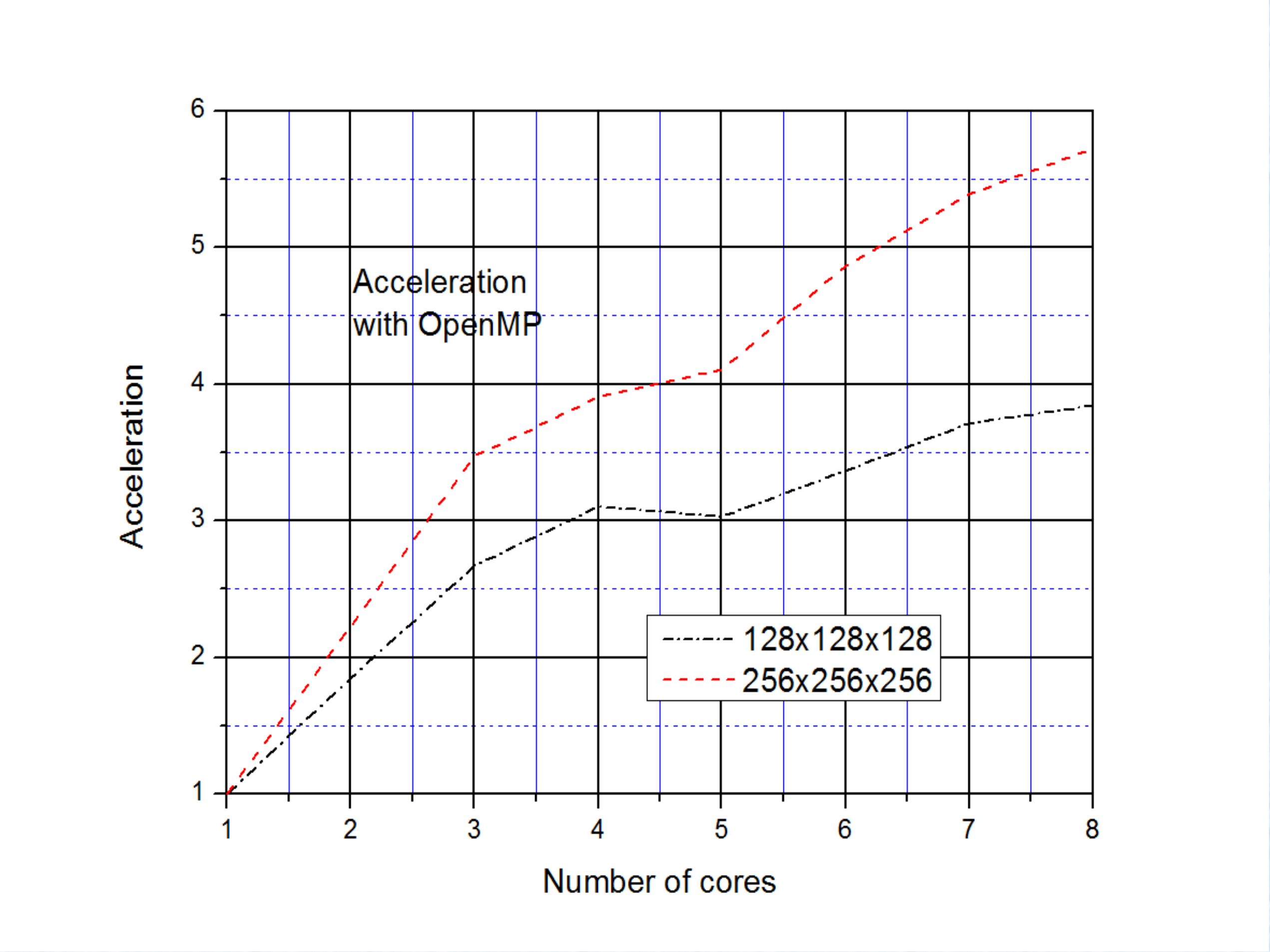
Density field at time t=10.01

The numerical results



Profile of power distribution at time t = 20.057

The numerical results



Calculations carried out on GPU GeForce 570 GTX, which give the acceleration compared to the single-core processor on the grid 256x256x256 to 15.2 times

Graph acceleration of computations for different grids

Conclusions.

In the presented work described the use of finite difference schemes and program for the solution of multi-dimensial problems of gas dynamics on graphics accelerators.

For this purpose we used Total Variation Diminishing (TVD) scheme, that has a high resolution in the shock waves and in high gradient areas. The calculations were carried out on grids sizes from 64x64x64 to 512x512x512 nodes using OpenMP and CUDA technologies.

Curried out test calculations have shown that the proposed schemes and programs allow accurately and efficiently to solve complex problems related to the gas-dynamic flows.

Mathematical modeling of impulsive loading of explosive charge

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Problem formulation

We studied the impact of the shock wave from the detonation booster on cylindrical charge with detonator. The main charge is modeled as a shell, filled with explosive, the exploder is located in the end of the shell and has a higher sensitivity than the main charge. To describe materials, composing the shell and the explosive substance we use elastoplastic model. We propose here a second order accurate finite-difference numerical scheme that is an extension of Wilkins scheme.

The system of governing equations can be written as

(1.1) continuity equation

$$\frac{\partial\rho}{\partial t}+v\frac{\partial\rho}{\partial r}+u\frac{\partial\rho}{\partial z}+\rho(\frac{\partial v}{\partial r}+\frac{\partial u}{\partial z})+\frac{\rho v}{r}=0,$$

(1.2) equation of motion

$$\frac{\partial v}{\partial t}+v\frac{\partial v}{\partial r}+u\frac{\partial u}{\partial z}-\frac{1}{\rho}(\frac{\partial\sigma_r}{\partial r}+\frac{\partial\sigma_{rz}}{\partial z}+\frac{\sigma_r-\sigma_\varphi}{r})=0,$$

$$\frac{\partial u}{\partial t}+v\frac{\partial u}{\partial r}+u\frac{\partial u}{\partial z}-\frac{1}{\rho}(\frac{\partial\sigma_r}{\partial z}+\frac{\partial\sigma_{rz}}{\partial r}+\frac{\sigma_{rz}}{r})=0,$$

(2) The defining equation of Prandtle-Reis plasticity theory

$$\frac{\partial s_r}{\partial t}+v\frac{\partial s_r}{\partial r}+u\frac{\partial s_r}{\partial z}+\lambda s_r=2G(\frac{\partial v}{\partial r}-\frac{1}{3\rho}\frac{\partial \rho}{\partial t}),$$

$$\frac{\partial s_\varphi}{\partial t}+v\frac{\partial s_\varphi}{\partial r}+u\frac{\partial s_r}{\partial z}+\lambda s_\varphi=2G(\frac{v}{r}-\frac{1}{3\rho}\frac{\partial \rho}{\partial t}),$$

$$\frac{\partial s_z}{\partial t}+v\frac{\partial s_z}{\partial r}+u\frac{\partial s_z}{\partial z}+\lambda s_z=2G(\frac{\partial u}{\partial z}-\frac{1}{3\rho}\frac{\partial \rho}{\partial t}),$$

$$\frac{\partial s_{rz}}{\partial t}+v\frac{\partial s_{rz}}{\partial r}+u\frac{\partial s_{rz}}{\partial z}+\lambda s_{rz}=G(\frac{\partial v}{\partial z}+\frac{\partial u}{\partial r}),$$

plastic condition of Mises

$$s_r^2+s_z^2+s_\varphi^2+2s_{rz}^2=\frac{2}{3}Y_e^2.$$

Shteinberg-Guinan model

$$Y = Y_0(1+\beta\varepsilon_u^p)^n(1-b\sigma(\frac{\rho_0}{\rho})^{1/3} - h(T-T_0)),$$

(3)

$$Y_0 = 0,$$

$$Y_0(1+\beta\varepsilon_u^p)^n \le Y_{\max},$$

$$T > T_m$$

$$T_m = T_{m0}(\frac{\rho_0}{\rho})^{2/3}\exp(2\gamma_0(1-\frac{\rho_0}{\rho}))$$

$\varepsilon_u^p = \sqrt{2\varepsilon_{ij}^p\varepsilon_{ij}^p/3}$ - the plastic deformation tensor intensity

T_m - is the materials melting temperature

$Y_0, Y_{\max}, \mu_{00}, T_{m0}, \beta, b, \gamma_0$ - materials constants

ES state equation before the detonation is written in the form of Teta law:

$$p = \frac{C_k}{n}\left[\left(\frac{\rho}{\rho_0}\right)^n - 1\right] (5)$$

$$\rho_0 = 1720 kg / m^3, C_k = 0.123, n = 3$$

The polytrope state equation for the detonation products was written in the form :

$$P = A\rho^\gamma (6)$$

$$A = 0.0764, \gamma = 3.0$$

Lyahov soil model

$$\rho = \rho_0 \left\{ \alpha_1 \left(\frac{p}{p_0}\right)^{-\frac{1}{k_1}} + \alpha_2 \left[\frac{k_2(p-p_0)}{\rho_2 c_2^2} + 1 \right]^{-\frac{1}{k_2}} + \alpha_3 \left[\frac{k_3(p-p_0)}{\rho_3 c_3^2} + 1 \right]^{-\frac{1}{k_3}} \right\}^{-1} \quad (9)$$

$$\alpha_1 + \alpha_2 + \alpha_3 = 1$$

$\alpha_1, \alpha_2, \alpha_3$ respectively gaseous, liquid and solid components

ρ_1, ρ_2, ρ_3 are the values of density

c_1, c_2, c_3 sound velocity corresponding to the gaseous, liquid and solid components

Soil model

$$\rho_0 = \alpha_1\rho_1 + \alpha_2\rho_2 + \alpha_3\rho_3 (10)$$

k_1, k_2, k_3 are isentrope indicators for the corresponding components

In order to reduce the equation (9) to a form, convenient for numerical

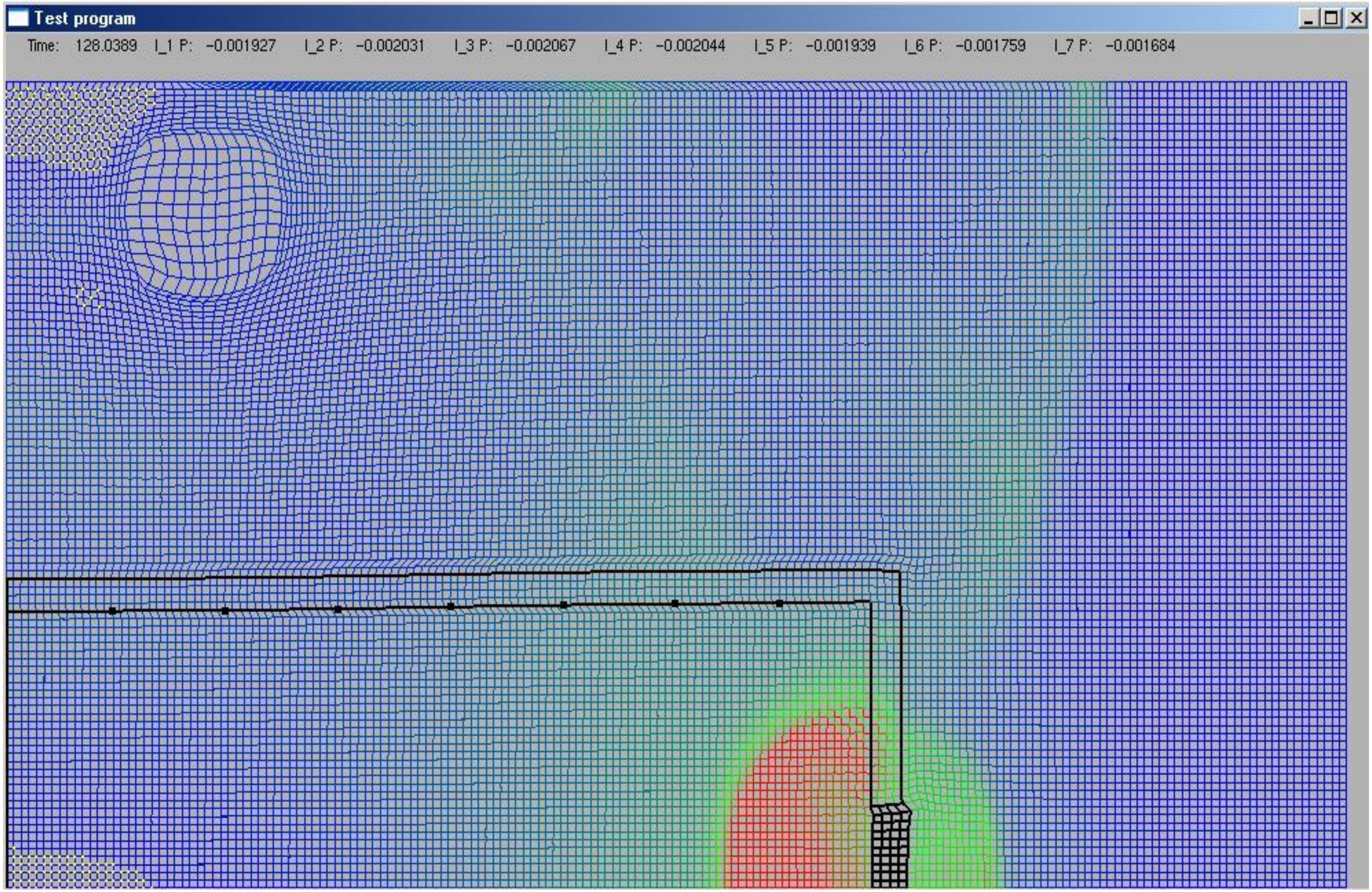
calculations, we approximate it with a polynomial of third degree in a

degree of compression

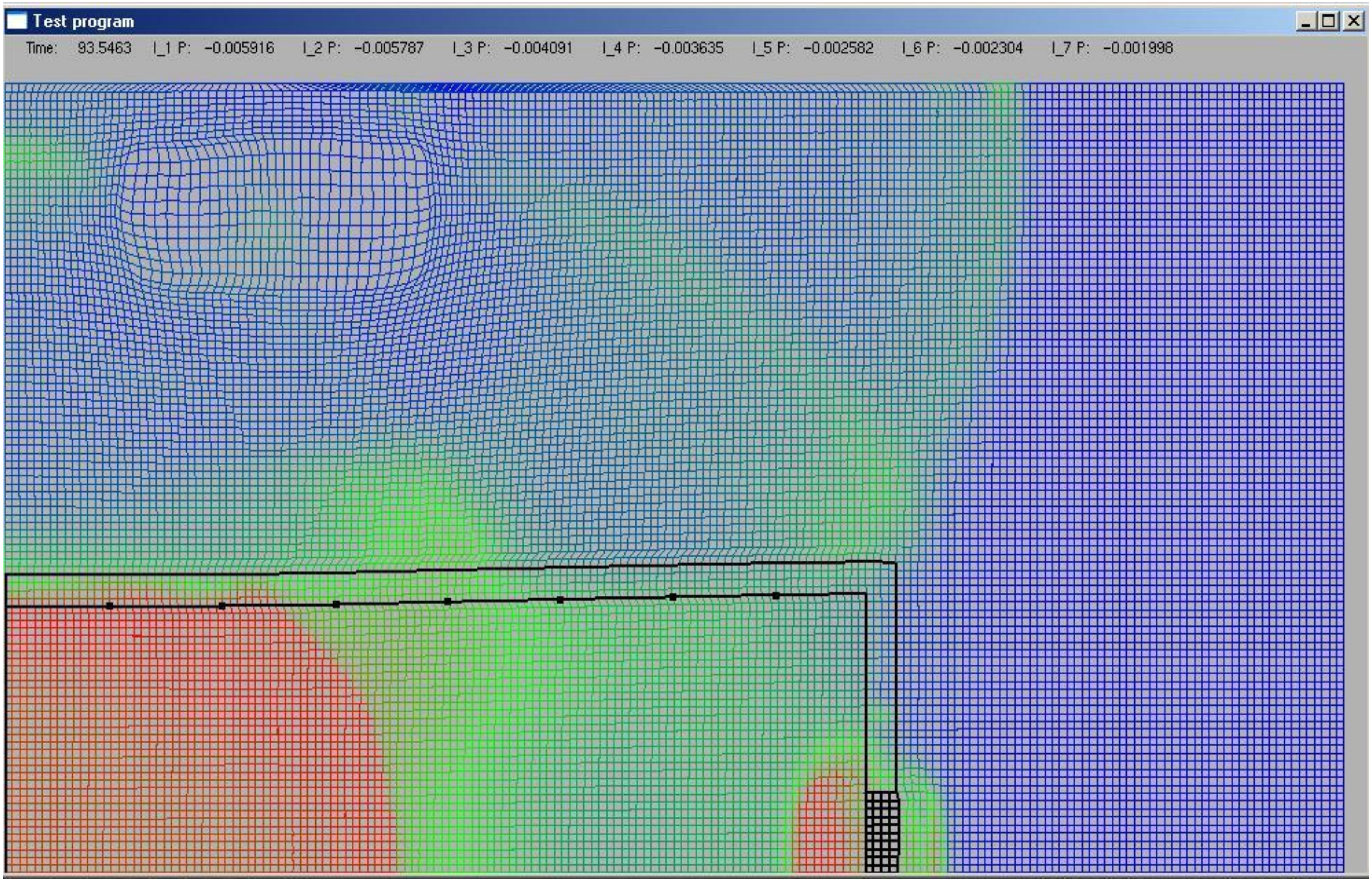
$$\mu = \frac{\rho}{\rho_0} - 1$$

$$p = a_0 + a_1\mu + a_2\mu^2 + a_3\mu^3 (11)$$

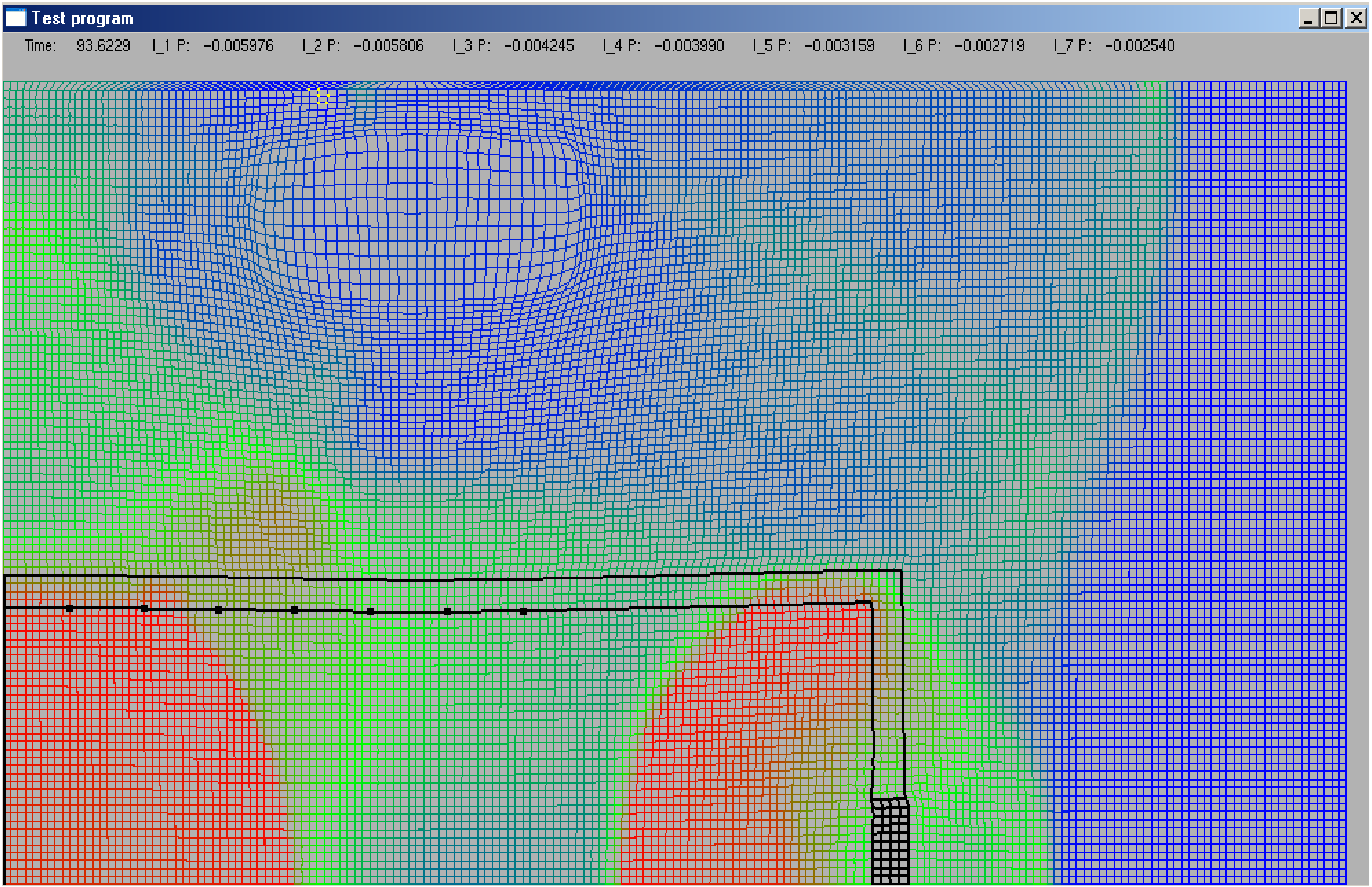
Variant 1. The calculation area, t=128 мks.



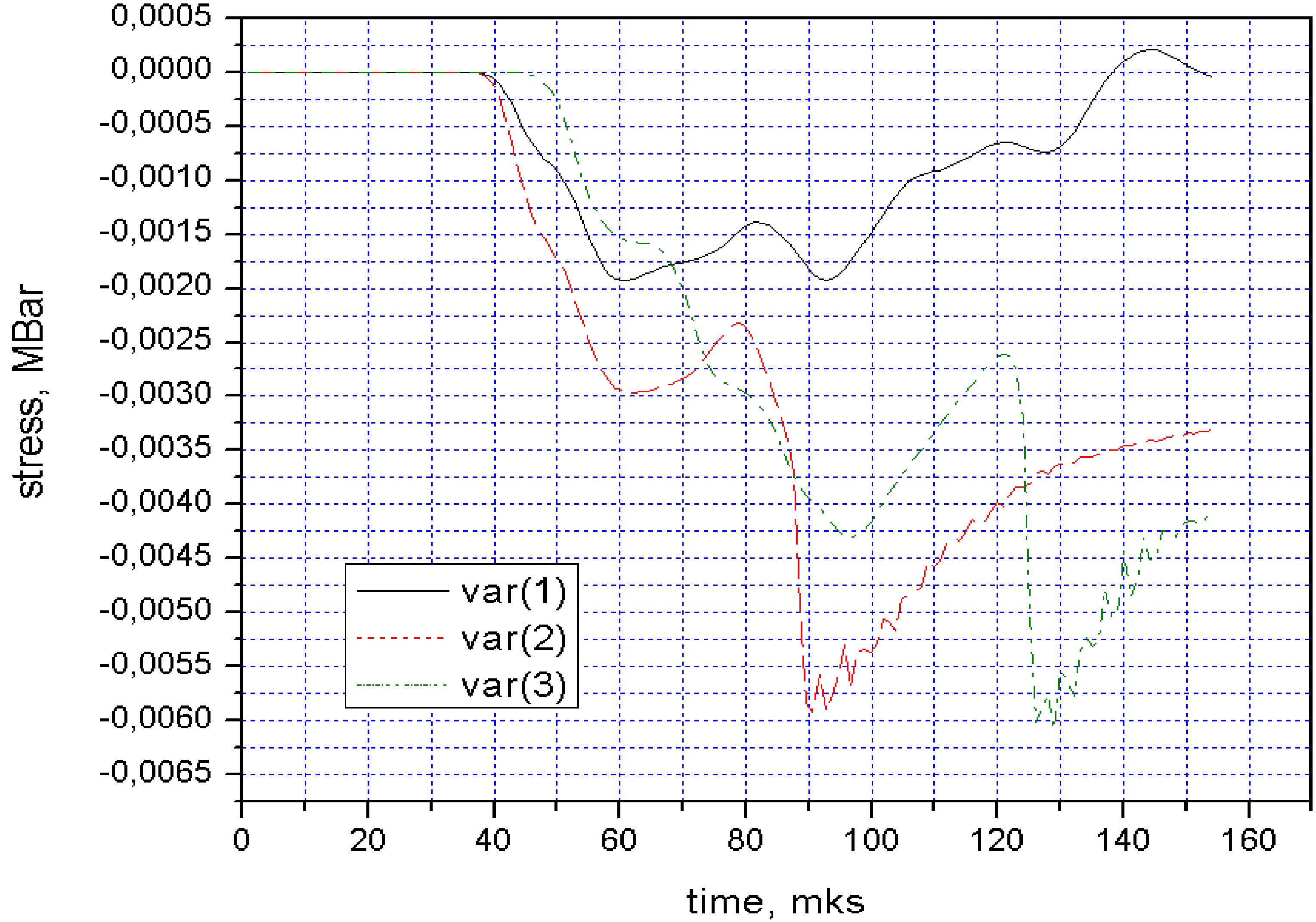
Variant 2. The calculation area, t= 93.5 мks.



Variant 3. The calculation area, t= 93.6 мks.

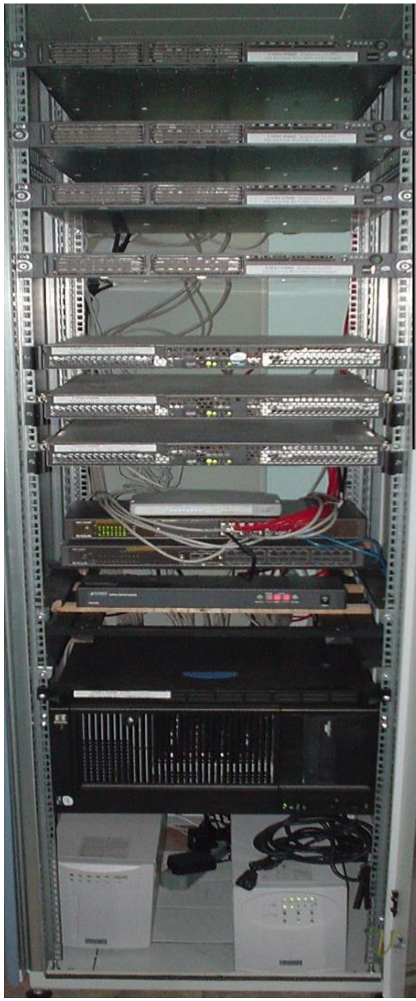


Stress at the steel/TNT



Local HPC resources for training, applications testing and debugging

48-core IMI-RENAM cluster



MS Windows Compute Cluster 2003

Cluster Status Last Refreshed: 24.05.2011 13:02:02

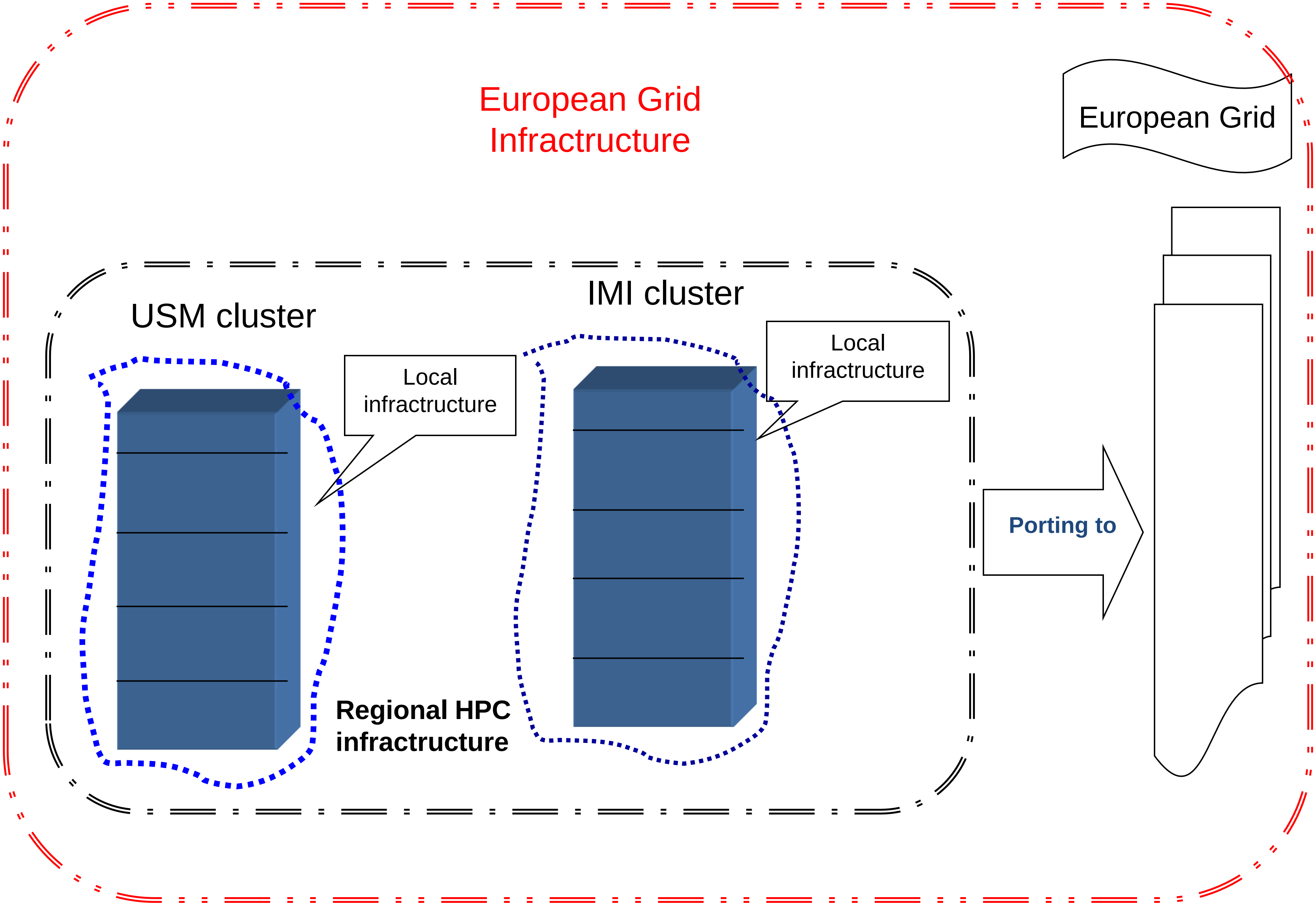
Compute Nodes:

Ready nodes:	8
Paused nodes:	0
Unreachable nodes:	0
Pending for approval nodes:	0
Total nodes:	8

Processors:

Processors in use:	14
Idle processors:	8
Total processors:	22

Name	Status	Jobs Run...	CPUs	CPUs in Use	OS Vers...	Total Memory
VMWCIMI01	Ready	0	4	0	5.2.3790	2043
VMWCIMI02	Ready	1	4	4	5.2.3790	4091
VMWCIMI03	Ready	1	4	4	5.2.3790	2043
VMWCIMI04	Ready	1	4	4	5.2.3790	2043
VMWCIMI05	Ready	0	2	0	5.2.3790	507
VMWCIMI06	Ready	1	2	2	5.2.3790	507
VMWCIMI07	Ready	0	1	0	5.2.3790	507
VMWCIMI08	Ready	0	1	0	5.2.3790	507


European Grid
Infractructure
European Grid
USM cluster
IMI cluster
Local infractructure
Local infractructure
Porting to
Regional HPC infractructure

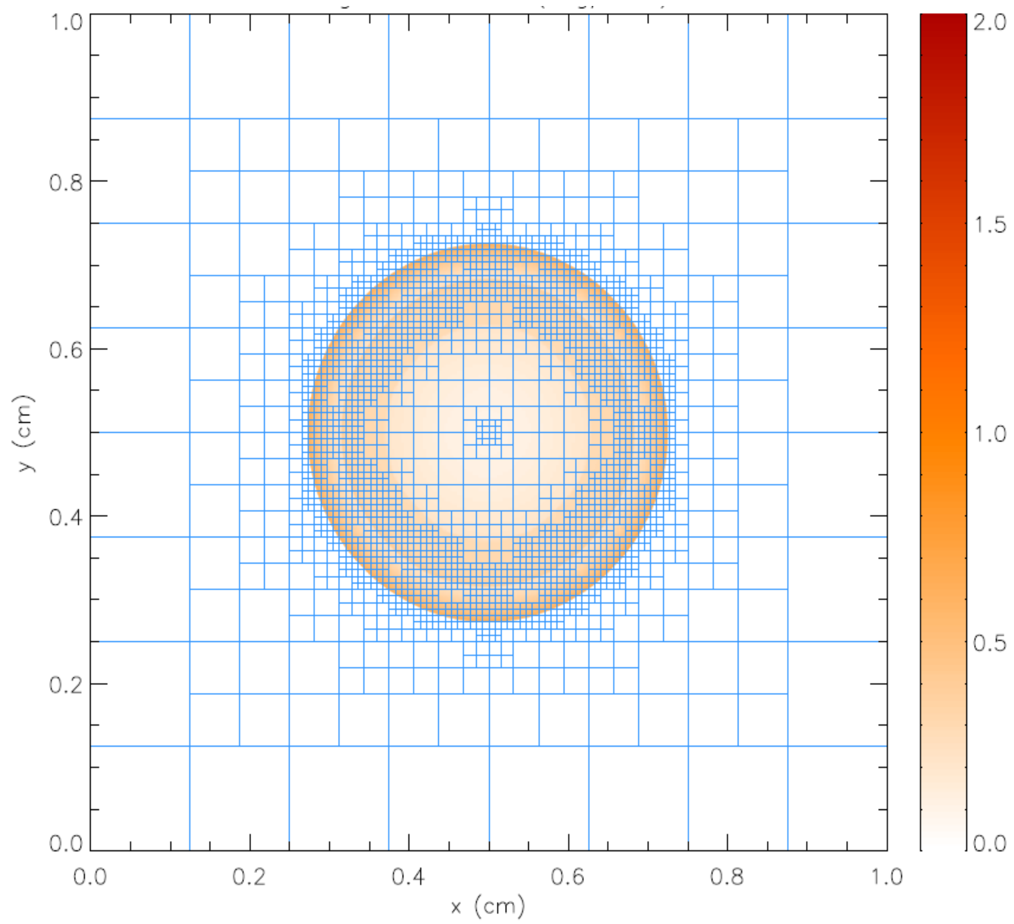
AMR_PAR application for the solving of continuum mechanics equations using Adaptive Mesh Refinement

The AMR_PAR application is considering a continuum mechanics problem, and namely the problem of modeling the explosion of a supernova type II and, for this example, created the algorithm and parallel program using the AMR method

Adaptive Mesh Refinement method can be applied to any other nowadays problem of continuum mechanics - to calculate the aerodynamics of aircraft, the calculations of the air flow of cars, a large number of other problems of mathematical modeling – the calculation of the flow of blood through the vessels, the calculations of the heart valves, etc. In all these cases, at the beginning of the problem we define a way to highlight areas in which we need to construct the grid, then the program builds a sequence of grids and makes a decision on them. The social impact depends on the problem to be solved, the use of AMR_PAR being of interest for heavy industry (e.g. car body design and development, aircraft aerodynamics), or for healthcare industry.

AMR Method

If necessary, in the areas with large gradients of pressure, temperature, etc., using the AMR method we can build sophisticated grid:



STCU Project. Objective

The project #5807 aims at analysis, adaptation, development, and porting to the regional high-performance computing (HPC) infrastructure of scalable applications for solving of tasks that need large volume of computational resources.

Within the project two new applications are preparing to run on HPC resources – for computer added design of semiconductor devices and decision-making processes modeling for economical systems. These applications are developing by research teams from the State University of Moldova with support of specialists from IMI ASM and RENAM Association.

Thank you for your attention!