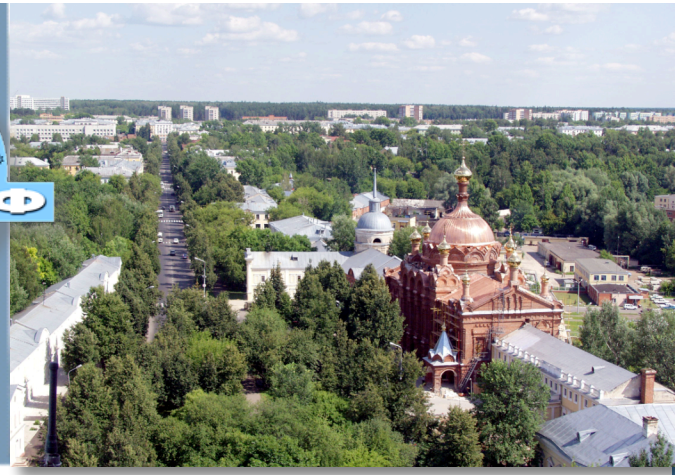
Institute of Theoretical and Mathematical Physics



Russian Federal Nuclear Center - VNIIEF

Solving Multidimensional Continuum Mechanics Problems on Unstructured Lagrange Meshes

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19-23 June 2005, Crowne Plaza, Vienna Austria

Problem Definition

$$\begin{cases} \dfrac{d\rho}{dt} = -\rho \operatorname{div} \vec{u}; \\ \rho \dfrac{d\vec{u}}{dt} = -\operatorname{grad} P + \operatorname{div} S + \dfrac{1}{4\pi}\left[\operatorname{rot} \vec{H} \times \vec{H}\right]; \\ \dfrac{d}{dt}\left(\dfrac{\vec{H}}{\rho}\right) = \left(\dfrac{\vec{H}}{\rho} \cdot \vec{\nabla}\right)\vec{u} \\ \dfrac{dE}{dt} = -P\dfrac{d}{dt}\left(\dfrac{1}{\rho}\right) + \dfrac{1}{\rho} S_p(SD) + \dfrac{1}{\rho}\operatorname{div}(\kappa \operatorname{grad} T); \\ \dfrac{d\vec{r}}{dt} = \vec{u}, \end{cases}$$

$$P = P^{\tilde{A}}(\rho, E)$$

ρ - matter density
E - specific internal energy
T - temperature
κ - heat conductivity factor
$\vec{u} = (u, v, w)$ – velocity vector
P - pressure
$\vec{r} = (x, y, z)$ – radius vector
S - strain tensor deviator
D - strain rate tensor
$S_p(SD)$ - first invariant of tensor SD
$\vec{H}$ - magnetic field strength vector

$S = 0$ - gas dynamics model

$S = S^{Yn}$, $P = P^{\Gamma}$ - elastoplastic model

$S = S^{Yn} + S^{B}$, $P = P^{\Gamma} + P^{B}$ - elastoviscoplastic model

Elastoplastic model

- Hooke law in the differential form:

$$\frac{\delta S^{\text{óï}}}{\delta t} = 2G\left(D - \frac{1}{3}S_p D\right)$$

where G - shear modulus;

- Mises flow rule: $\frac{3}{2}S_{ij}^{\text{óï}} S_{ij}^{\text{óï}} = Y^2$.

Elastoviscoplastic model

$$P = P^{\text{ã}} + P^{\text{â}} \quad S = S^{\text{óï}} + S^{\text{â}} \quad P^{\text{â}} = \frac{1}{3}\mu_1 S_P D \quad S^{\text{â}} = \mu_2\left(D - \frac{1}{3}S_P D\right)$$

P^B – the viscous pressure, S^B – the strain tensor deviator

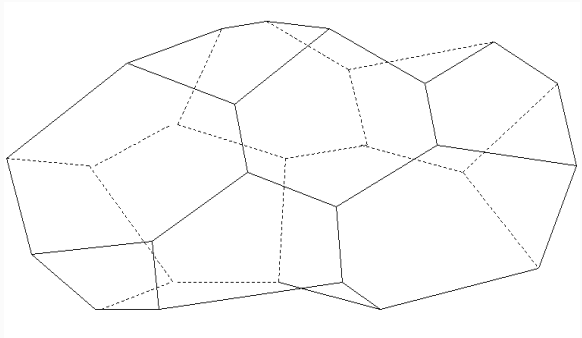
μ_1, μ_2 – the values of dynamic viscosity

3D Techniques developed in VNIIEF

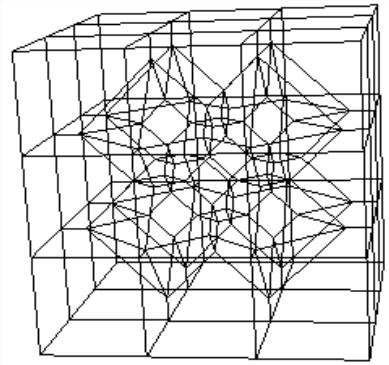
- TMK - technique to solve 3D gas dynamics and elastoplastic problems on unstructured polyhedral Lagrange meshes
- MEDUZA-3D - free-Lagrange technique centering of all gas dynamics values on the node, variable difference template for the numerical integration of differential equations.
- TIM - serves for 3D continuum mechanics computations on polyhedral unstructured Lagrange meshes. It allows computations to be performed on meshes with an arbitrary number of node connections.

TMK Technique

- Explicit difference scheme
- Velocities specified at mesh nodes
- Density, energy, pressure and strain specified in cells
- Four cells converging in any mesh node
- In order to maintain the mesh in good condition used the method of elastic impact
- Local polyhedral cell reconstruction technique



3D mesh cell

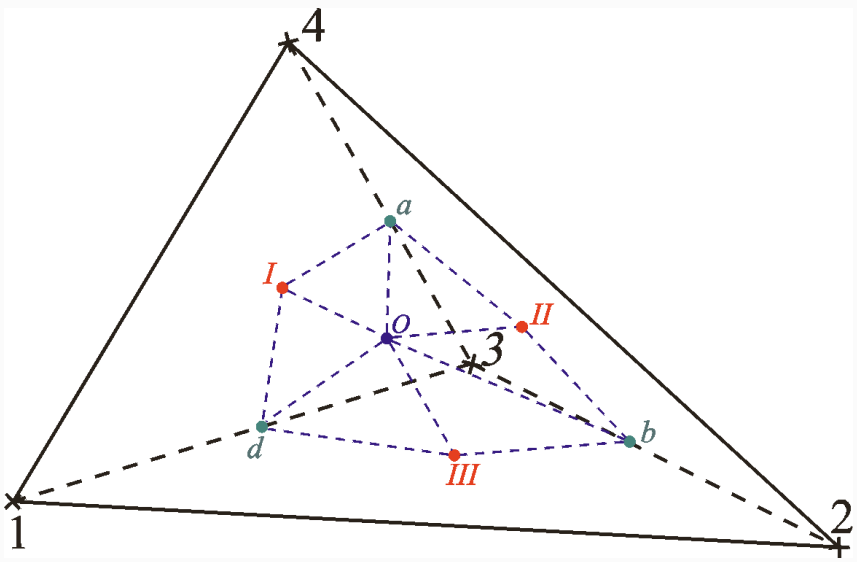


Dirichlet mesh contained in a cube

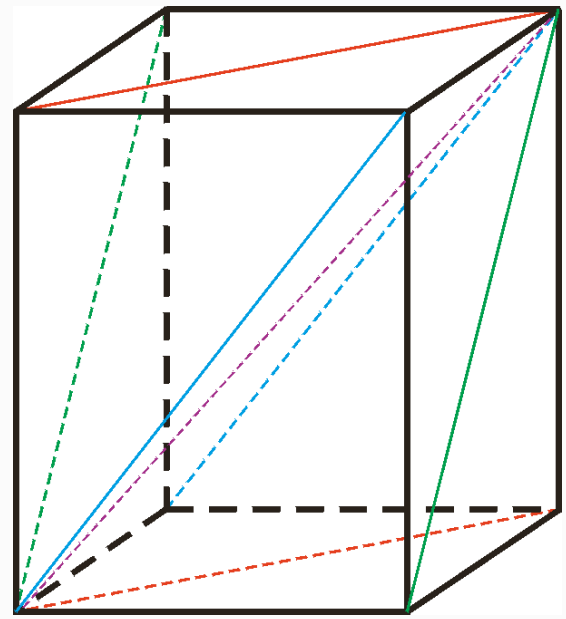
MEDUZA-3D Technique

- Generalization of the MEDUZA-2D technique for 2D problems
- Tetrahedron mesh
- Centering of all gas dynamics values on the node
- Variable difference template
- Possibility to change the mesh topology in running a problem
- Boundaries are described by mixed cells calculated by the lumping method

MEDUZA-3D Technique



Six triangles of the integration surface related to node 3



Tetrahedration of a hexahedron

TIM Technique

- Meshes with an arbitrary number of node connections
- Valid both on the Dirichlet-Voronoi unstructured polyhedral meshes, and on hexahedral meshes and unstructured polyhedral meshes having an arbitrary number of neighborhoods in a node
- Uses the same computational algorithm for all the meshes
- Intended for solving gas dynamics, time-dependent elastoplasticity, magnetohydrodynamics and heat conductivity

TIM Technique

In generating a finite-difference scheme for solving system of differential equations, one uses the integro-interpolation process assuming that

- P, ρ, E, q, S_{ij}, ε, H, T – assigned to the cells centers and are constant within them;
- x,y,z,u,v,w are assigned to the nodes;
- faces are described by their piecewise linear representation

TIM Technique – Gas dynamics and Elastoplasticity

- Fully conservative explicit difference scheme with second order of accuracy in space and time
- Artificial viscosity uses a combination of the quadratic and linear viscosity.
- The velocities of mesh nodes are defined using the law of conservation of momentum in the integral form.

TIM Technique – Ideal Magnetohydrodynamics

- Magnetic field strength vector is defined in the centers of mesh cells
- Current density and electromagnetic force vectors are assigned to mesh nodes
- Explicit difference scheme

$$\frac{d\left(\vec{H}V\right)}{dt} \approx H_x \int_{\partial\Omega} \vec{u}\,dydz + H_y \int_{\partial\Omega} \vec{u}\,dzdx + H_z \int_{\partial\Omega} \vec{u}\,dxdy$$

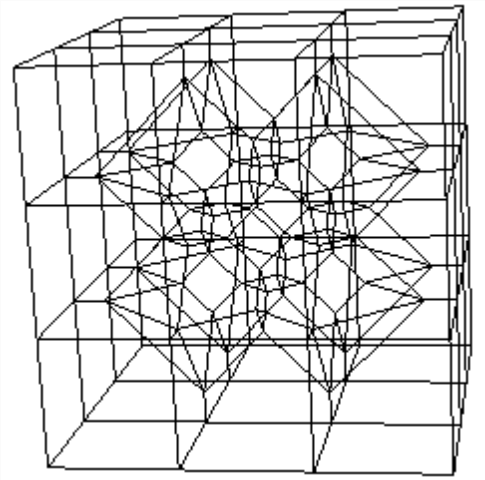
computational cell Ω, cell volume *V*

The integrals in the right-hand member of this equation are substituted by finite sums.

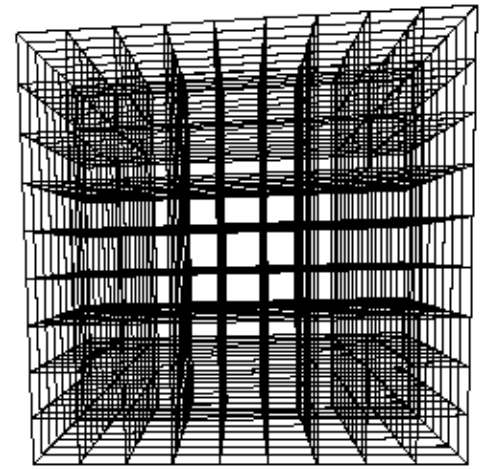
TIM Technique – Heat conductivity

- Value of temperature is defined in cell centers
- Heat flow vector is defined at the nodes
- The difference scheme is constructed using the process of generalized derivation of discontinuous functions and is implicit and conservative
- The approximation of the differential operator in the heat conductivity equation has the second order of accuracy in space
- The resulting difference system of linear equations has a symmetric and positively definite matrix
- The system of equations is solved by the iteration method of conjugate gradients using different types of preconditioners

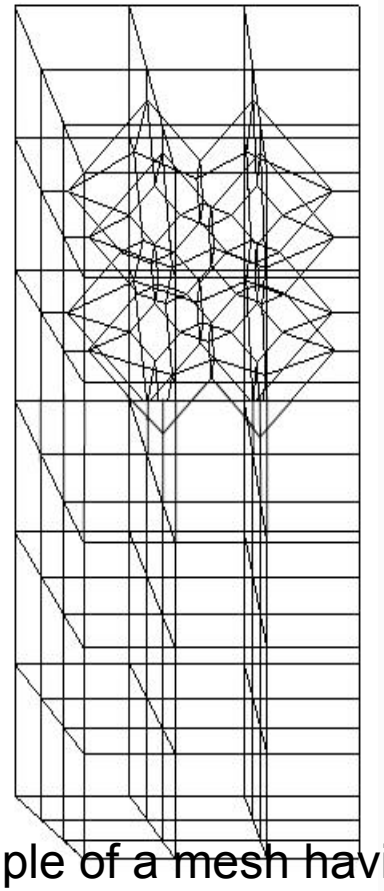
TIM Technique - Types of initial meshes



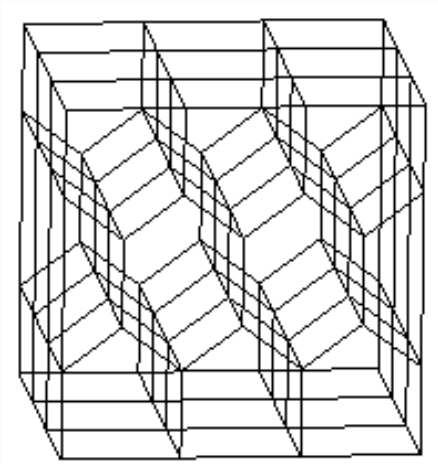
The Dirichlet-Voronoi mesh

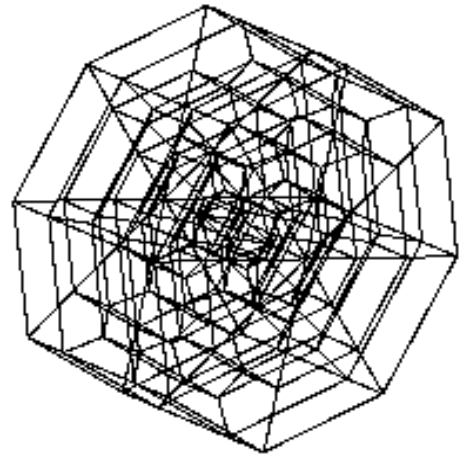


A hexahedral mesh



Example of a mesh having hexahedral and Dirichlet-Voronoi cells in one domain



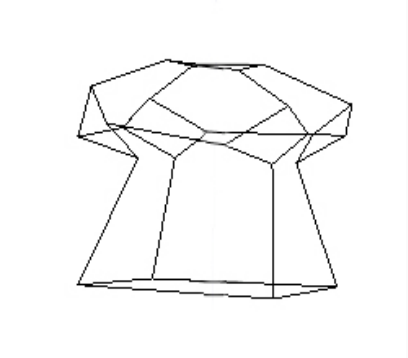


Unstructured meshes derived from a 2D mesh

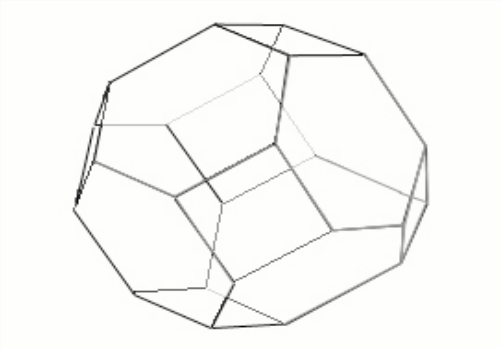
TIM Technique - Mesh maintenance

Method 1. Mesh maintenance is performed by imposition of differentiable connections:

- meshes containing “stellar” cells



- meshes with convex dihedral cell angles



- meshes with convex polyhedral cell angles

TIM Technique - Mesh maintenance

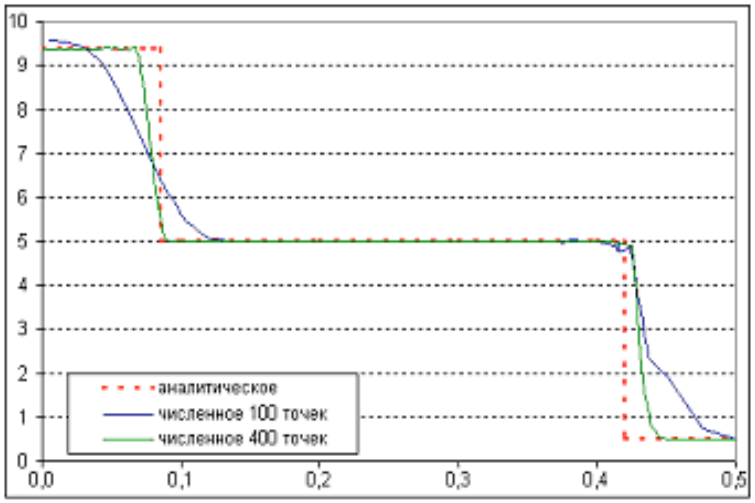
- Method 2: Local adjustments of 3D meshes, that rest upon two operations – partitioning and integration of cells.

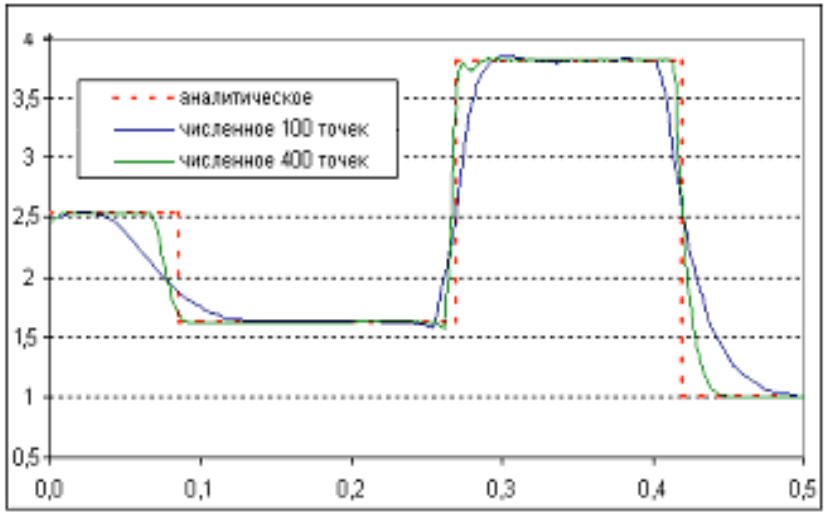
- Method 3 is based upon the process of velocity field smoothing in mesh nodes to suppress high-frequency perturbations.

Examples of Calculations

Decay of an arbitrary discontinuity in gas dynamics settings (TIM)

Let an ideal gas, whose conditions are defined as follows: left – P_I=2.5; u_I=0, right - P_{II}=0.5; u_{II}=-2.8026. ρ=1, γ=*1.4*

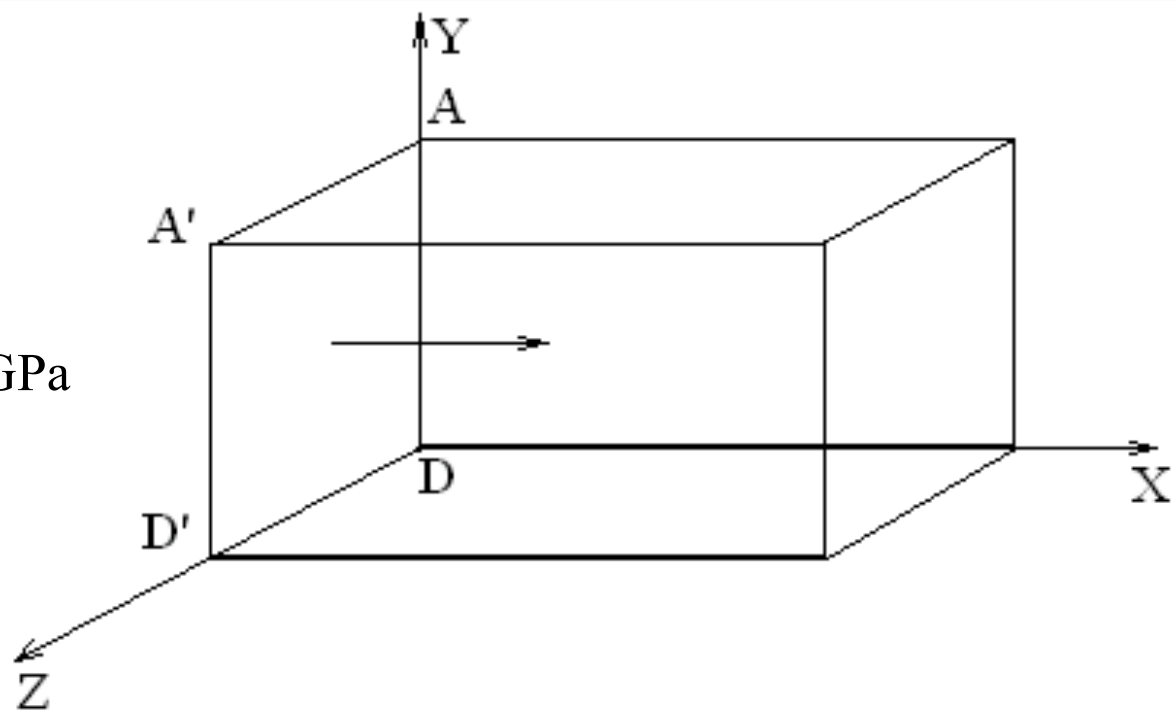




Pressure and density distribution at t=0.24

The plane stress wave problem (TIM)

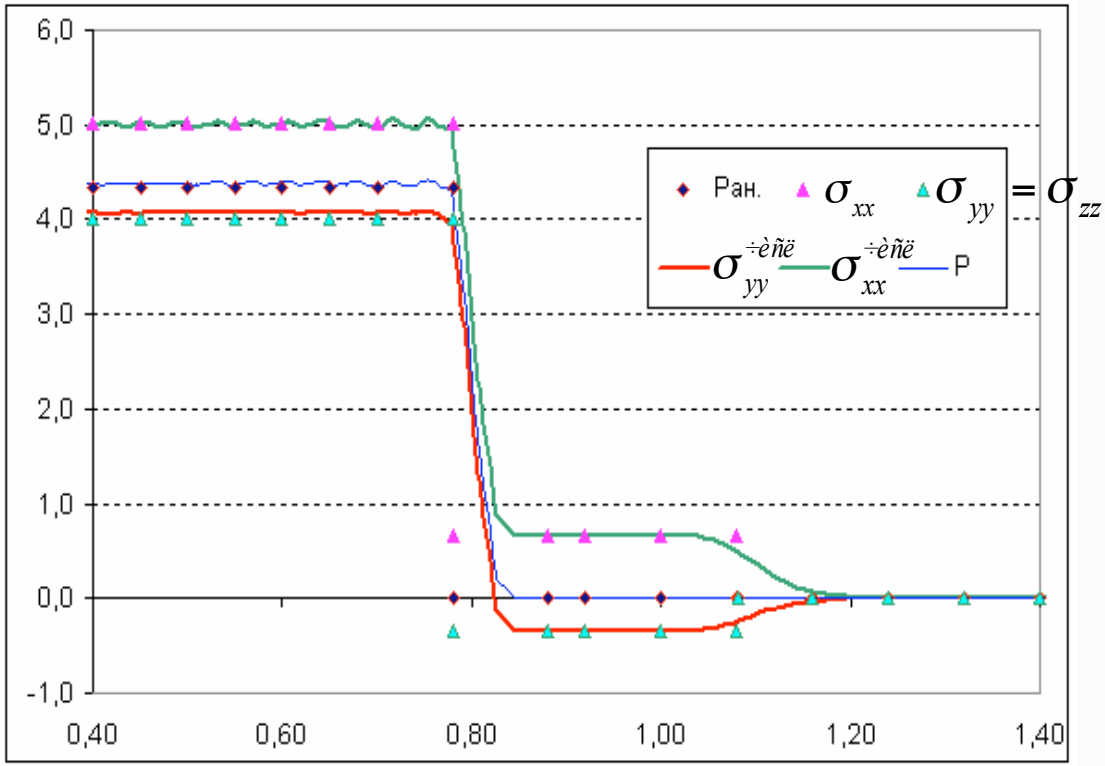
P_{rp} = 5 GPa



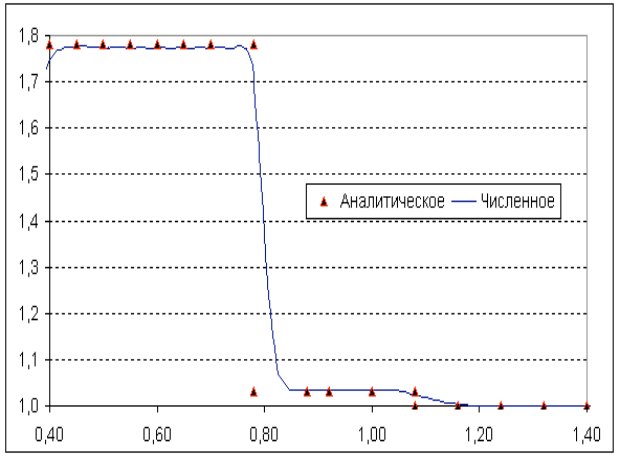
ρ_0=1. g/cm^3, =0, E_0= P_0=Sx_iy_j =0. , G = 15 GPa, Y_0=1 GPa.

The plane stress wave problem (TIM)

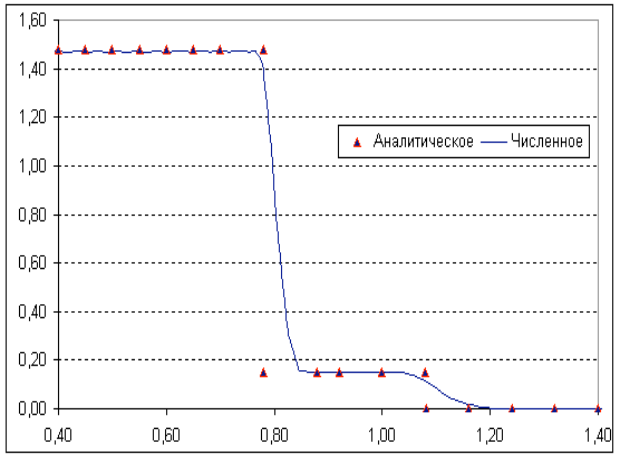
T=0.24



Pressure and stress profiles

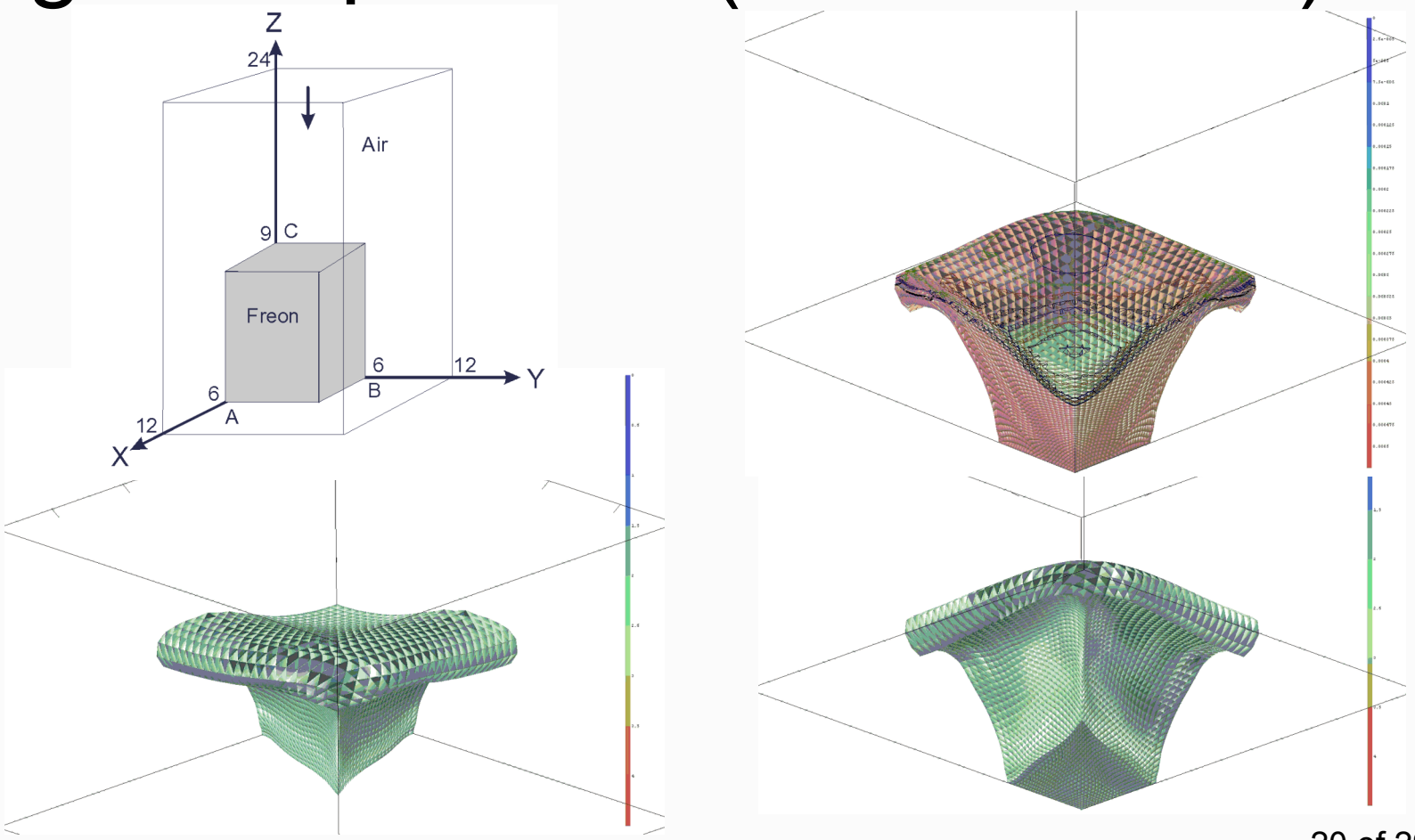


Velocity profiles



Density distribution profiles

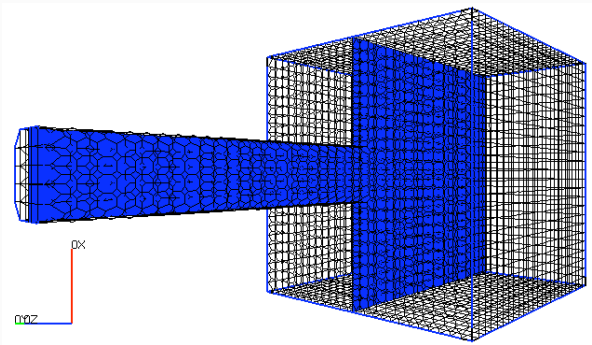
The Richtmyer-Meshkov instability growth problem (MEDUZA-3D)



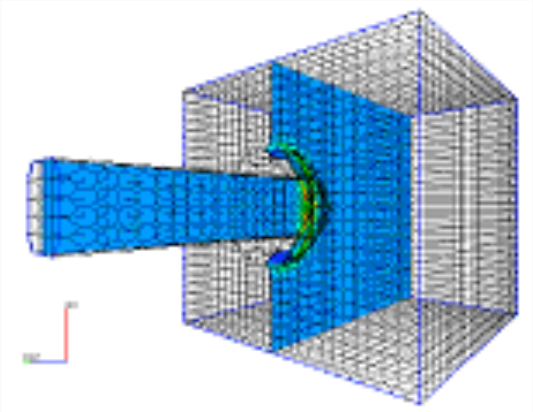
The shape of Freon and the pressure field for the point of time t=0.764 ms

The problem of bar impact against a wall – Gas dynamics simulation (TIM and TMK)

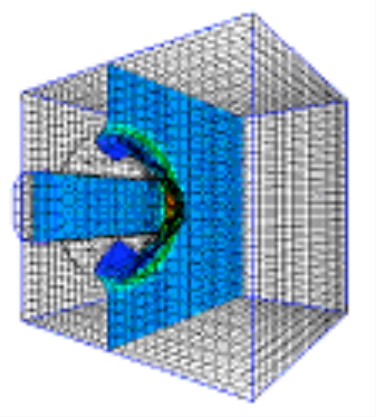
t



initial geometry



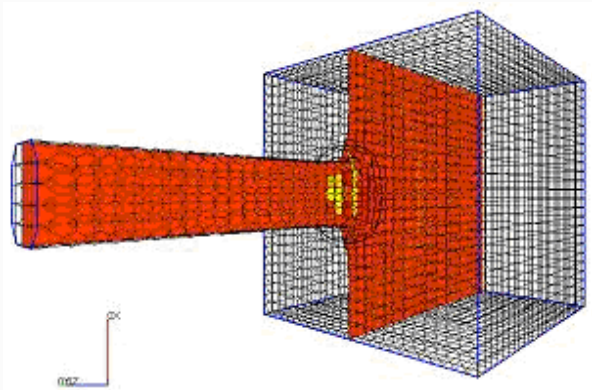
t=7 μsec



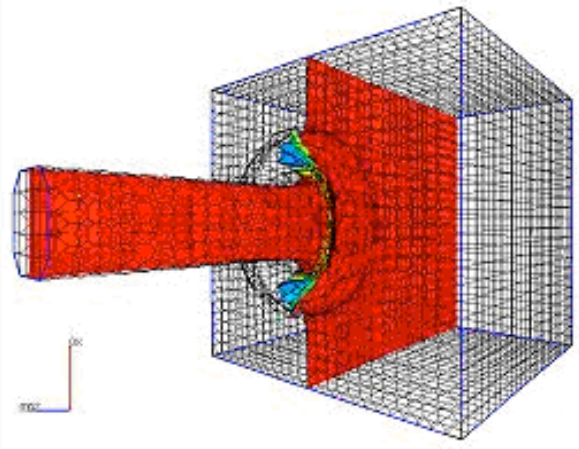
t=3.5 μsec

- Material – ideal gas with γ=1.4; ρ_0=7.8 g/cm^3
- Projectile – 2 x 2 x 10 cm parallelepiped, cube having a 10-cm edge
- mesh having 31,400 computational cells Dirichlet-Voronoi
- The projectile travels at a velocity of 10 km/s.

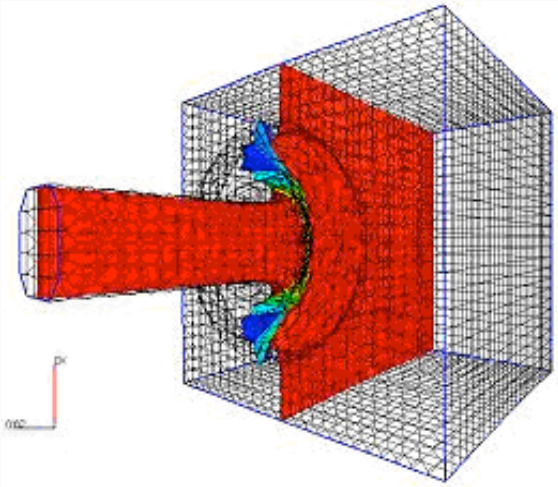
The problem of bar impact against a wall – Elastoplastic simulation (TIM and TMK)



t=10 μsec



t=30 μsec



t=40 μsec

Material – steel (Mie-Gruneisen equation of state).

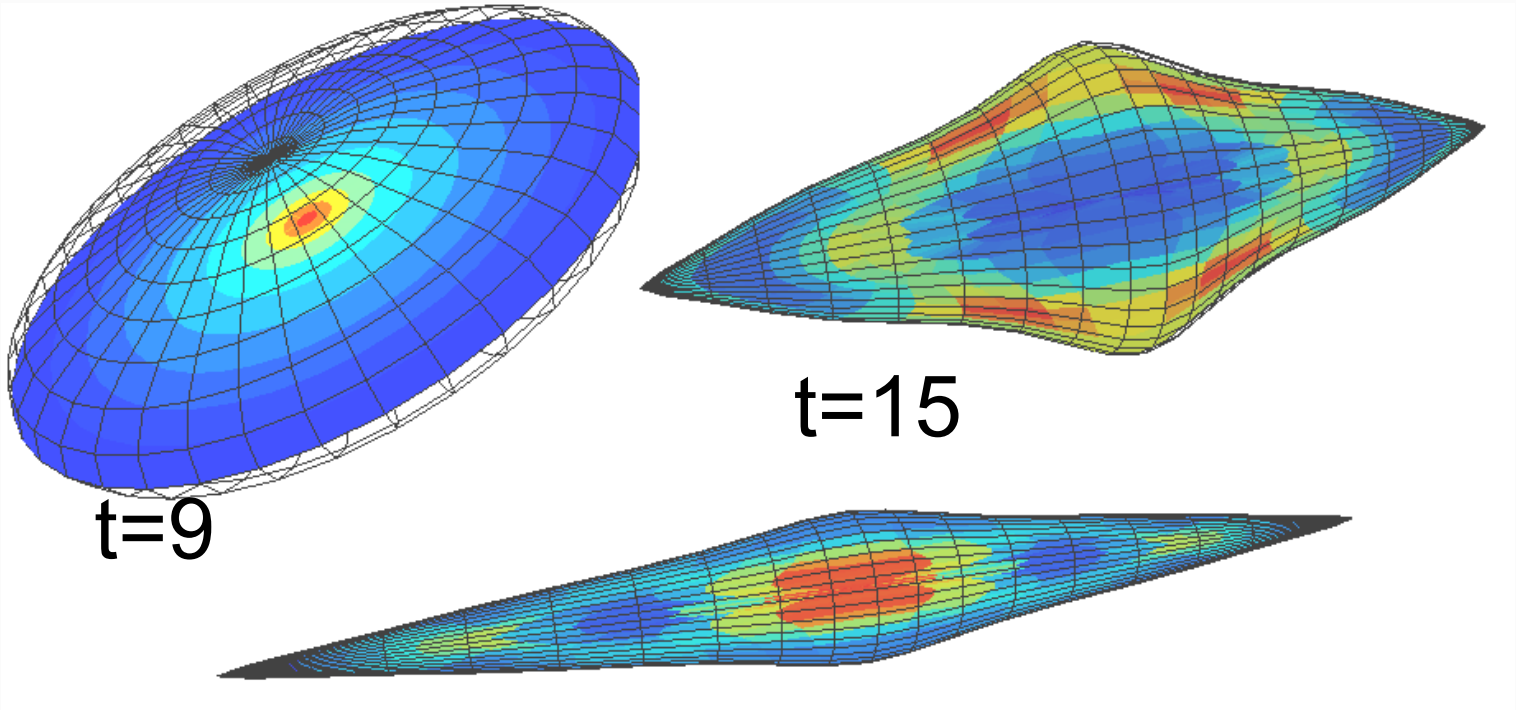
ρ_0=7.8 g/cm^3 c $_0$=4.9 km/s n=5, Γ=1.66;

δ_s=-2.5 GPa; G=81 GPa; Y=1.05 GPa

The projectile travels at a velocity of 1 km/s.

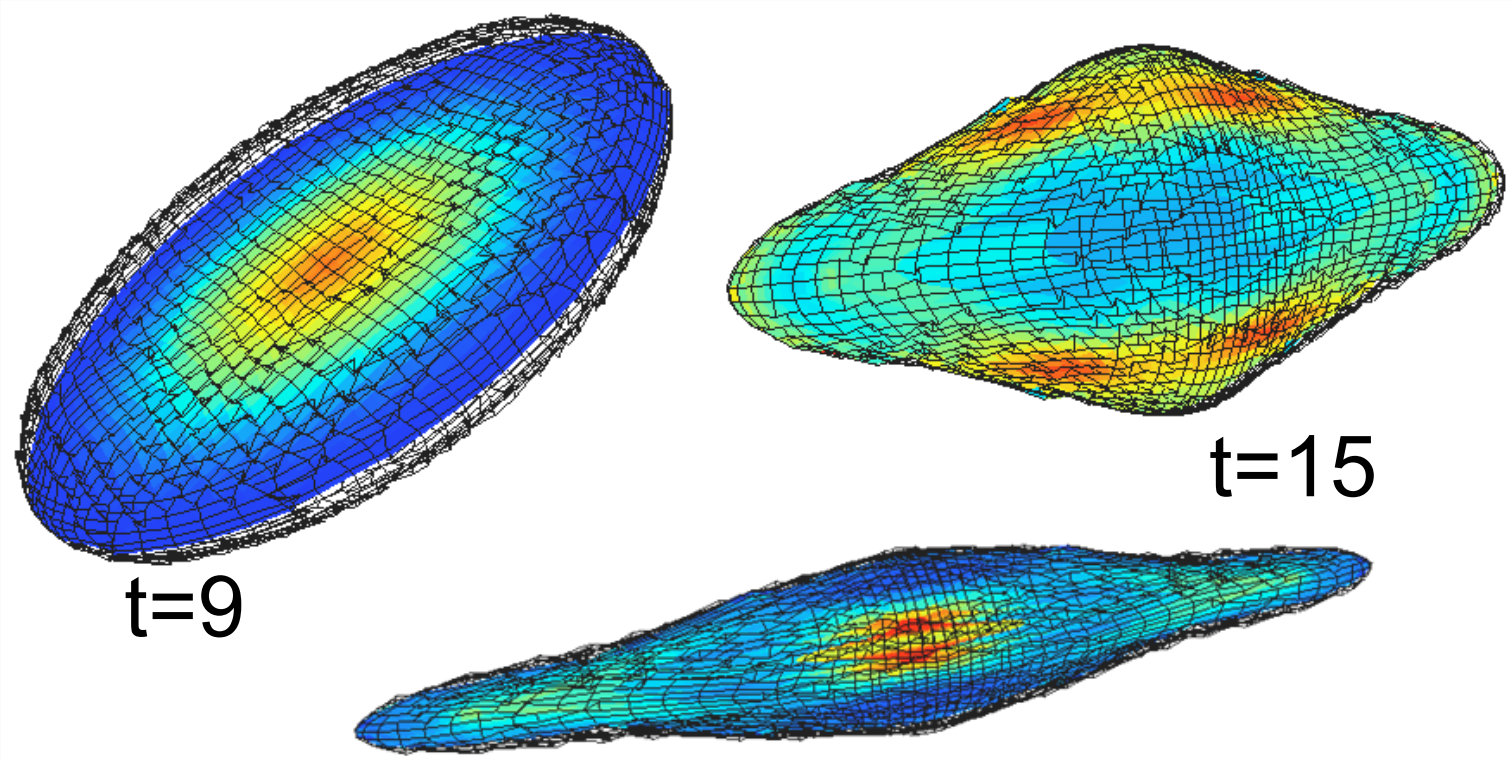
The ellipsoid compression problem (TIM)

Hexahedral mesh (8,000 cells)



The ellipsoid compression problem (TIM)

Polyhedral mesh (22,575 cells)



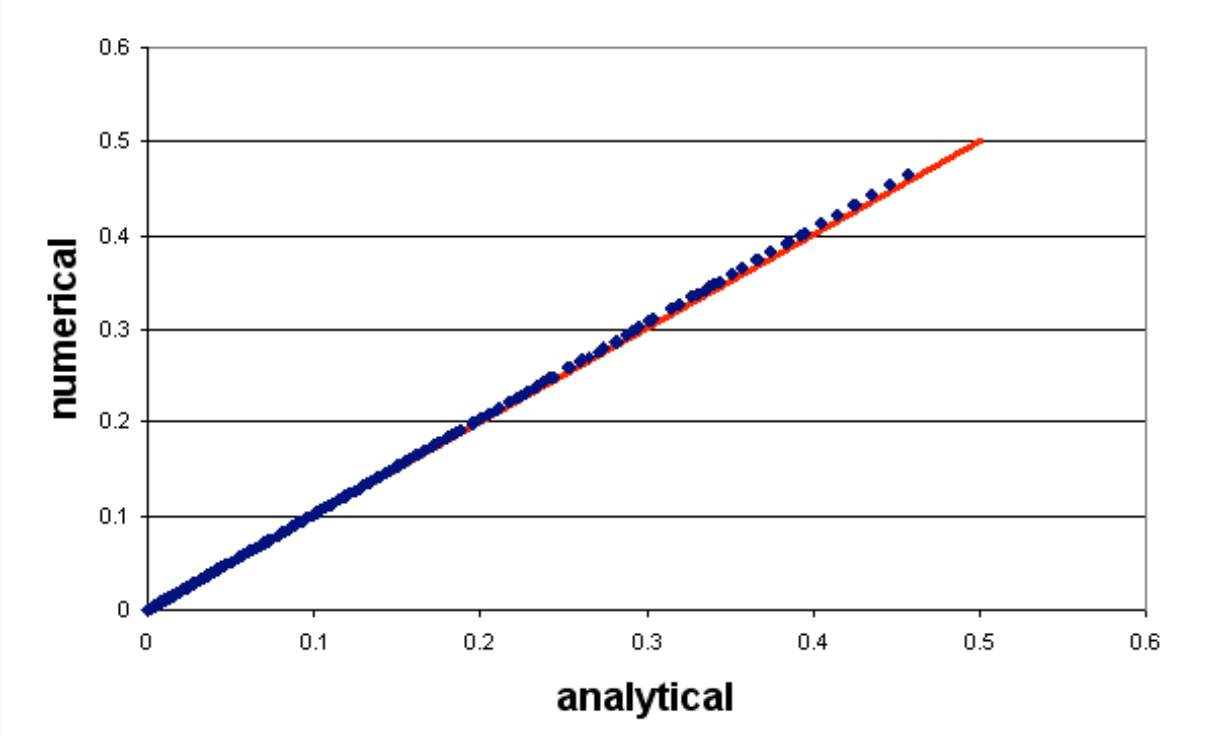
The cooling cube problem (TIM)

- Cube [0,1]x[0,1]x[0,1].
- Temperature within cube is T=1, temperature at its boundary is T=0.
- Analytical solution to the problem:

$$T(x,y,z,t) = f(x,t)f(y,t)f(z,t) \quad f(x,t) = 4\sum_{k=0}^{\infty} \frac{\exp\left(-\pi^2(2k+1)^2 t\right)}{\pi(2k+1)} \sin\left(\pi(2k+1)x\right)$$

- Hexahedral mesh with 20 cells on each direction.
- Time step of 0.0005.

The cooling cube problem (TIM)

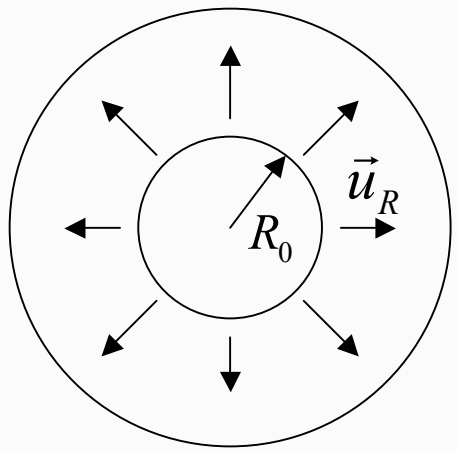


Analytical vs. numerical solution for t=0.05

Problem of a spherical piston in a dipole magnetic field (TIM)

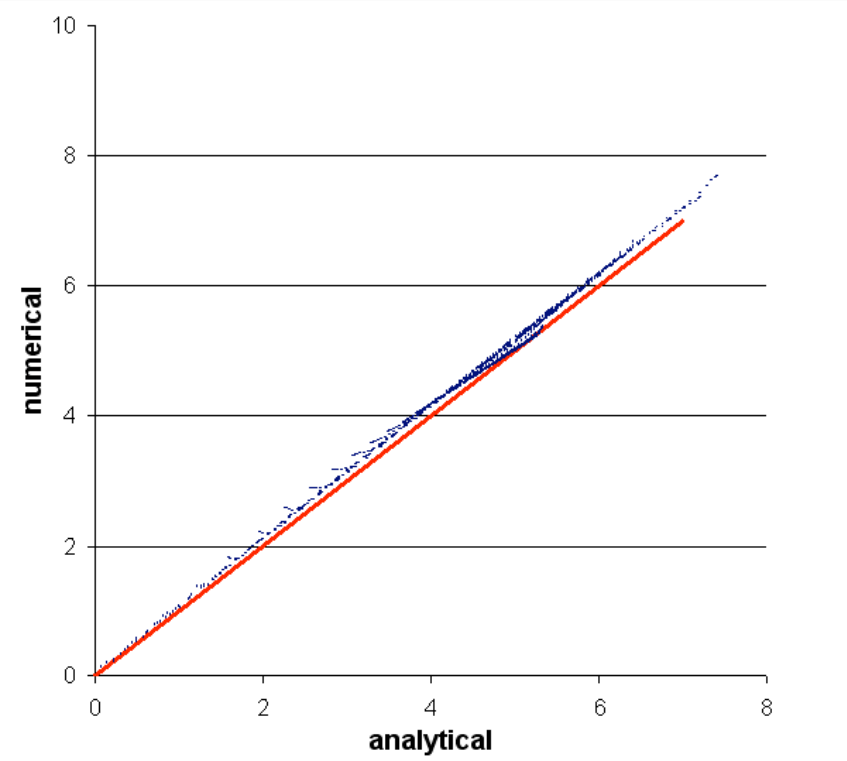
$$H_z = H_0\left(1+\frac{1}{2}\left(\frac{R_0}{R}\right)^3-\frac{3}{2}\left(\frac{R_0}{R}\right)^3\left(\frac{z}{R}\right)^2\right),$$

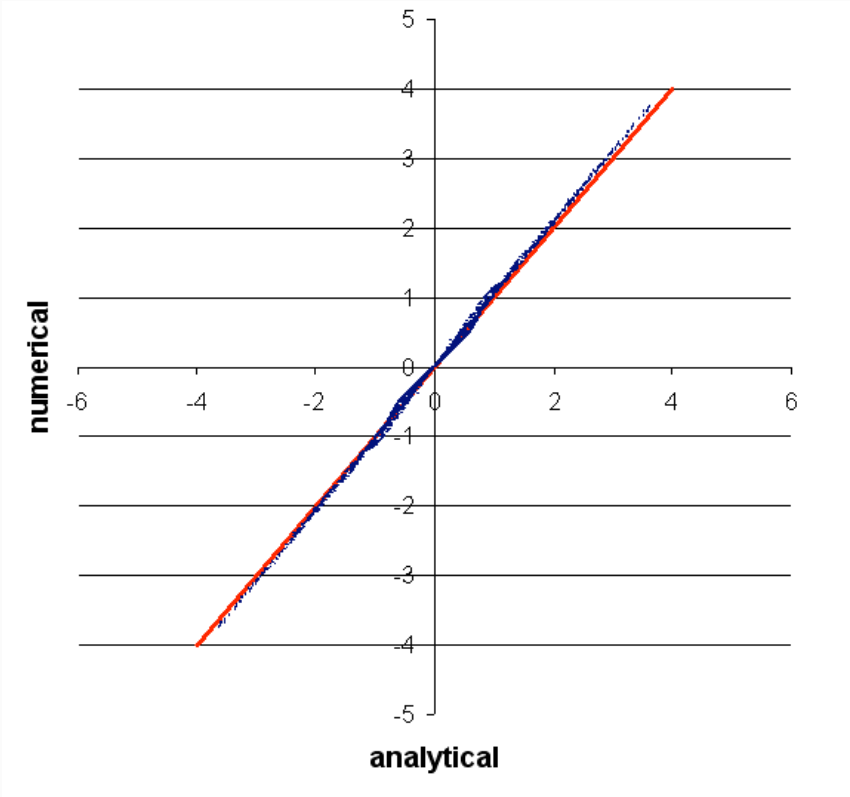
$$H_r = -H_0\cdot\frac{3}{2}\left(\frac{R_0}{R}\right)^3\left(\frac{rz}{R^2}\right)$$



$$H_0 = 5,\ u_R = 0.1,\ R_0 = 0.5$$

Problem of a spherical piston in a dipole magnetic field (TIM)





Values of H_x and H_r at the point of time t=0.31

THANK YOU