Some Aspects of Numerical Modeling in Heterogeneous Mechanics

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a joint work with

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MULTIMAT 2013,

September 2-6, 2013, San Francisco CA, USA

Basic objective: numerical modeling problems of heterogeneous mechanics.

Term "heterogeneous": non-uniform medium that consists of several materials (fractions) with different physical and mechanical properties. Each fraction can be in either gas, liquid, or solid phase.
Liquid and solid fractions can be in continuous, or dispersed phase due to material fracture and fragmentation.

Basic interests: multi-D intensive dynamical processes with large deformation of the medium.

Way of description: Eulerian continual approach with arbitrary moving grids - a portion of grid points serve to track only some peculiarities of the process, as contacts, shocks, detonation waves, etc. Other grid points move in an appropriate way to maintain the initial grid topology.

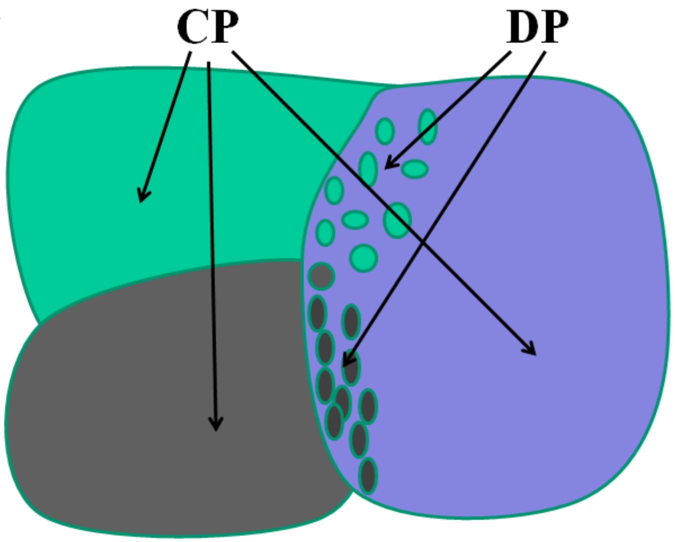
PHYSICAL MODEL

The model to be considered is represented by a **heterogeneous mixture of different materials** (fractions). In general the fractions (or some of them) can be in **two phases**: **continuous (CP) and/or dispersed (DP)** .

Each CP component occupies a part of the domain; its distribution is described by the volume fraction α_k; $k = 1,\dots, n$, where n is the number of components.

The DP component is characterized by the volume fraction β_k, $k = 1,\dots, n$.

The quantity $\beta = \beta_1 + \cdots + \beta_n$ is the total volume fraction of the dispersive phase.
$\alpha = \alpha_1 + \cdots + \alpha_n$ represents the total volume of the continuous phase or porosity, with $\alpha + \beta = 1$.



Previous meetings (MULTIMAT2011, NMH2012): generalization of the Godunov method for calculating shocked flows of 2-ph. fluid/suspended solids mixture.

This time: focus on CP modeling (no DP) with the Prandtl-Reuss elasto-plastic equations and the Von Mises plastic flow rule.

Objective: a numerical approach for modeling the physics of high-rate elasto-plastic deformation processes in multimaterial medium.

Typical: high-velocity impact of solids: large deformations accompanied by
- nonlinear elasto-plastic shock and rarefaction waves;
- strong displacement of free boundaries and contacts between interacting media.

Stress and strain relations: presence of the yield surface: weak discontinuity in functional dependencies.

This results: increased complexity (with respect to g/d) of the wave process:
- loading: one-front elastic, one-front plastic, or two-front elastic-plastic;
- unloading: one-wave elastic, or two-waves elastic-plastic structures.

Therefore: finite deformation in solids requires numerical methods able
- accurately capture variety of waves;
- correctly track the location of deforming contacts and free boundaries.

OUTLINE

1. DISCRETE MODEL
   1.1 GOVERNING EQUATIONS
   1.2 NUMERICAL METHOD
   1.3 WAYS OF SPLITTING IN PHYSICS
2. VALIDATION RESULTS
   2.1 LOADING REGIMES
   2.2 UNLOADING REGIMES
   2.3 2D
3. MODEL VALIDATION (KANEL'S EXPERIMEN)
   3.1 BASIC CALCULATIONS (WITHOUT FRACTURE)
   3.3 ACCOUNTING OF THE FRACTURE MODEL
4. EULERIAN APPROACH FOR MULTIMATERIAL (MM) FLOWS
   4.1 NUMERICAL MODEL
   4.2 ACCOUNTING OF SUB-CELL STRUCTURE
   4.3 1D CALCULATIONS (MM ADVECTION, MM IMPACT)
   4.3 2D CALCULATIONS (SHOCK/BUBBLE, JETTING)
5. CONCLUSIONS AND FUTURE WORK

GOVERNING EQUATIONS

$$\begin{cases} \dfrac{\partial \vec{q}}{\partial t} + \dfrac{\partial \vec{f}_k}{\partial x_k} = 0 \\ \dfrac{dS_{ij}}{dt} - S_{ik}\omega_{jk} - S_{jk}\omega_{ik} + \dfrac{2}{3}\mu \cdot div(\mathbf{u})\delta_{ij} + \mu\left(\dfrac{\partial u_i}{\partial x_j} + \dfrac{\partial u_j}{\partial x_i}\right) + Fm(S_{ij}) = 0 \end{cases}$$

$$\vec{q} = \begin{pmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{pmatrix} \qquad \vec{f}_k = \begin{pmatrix} \rho u_k \\ \rho u_k u_1 - \sigma_{k1} \\ \rho u_k u_2 - \sigma_{k2} \\ \rho u_k u_3 - \sigma_{k3} \\ \rho u_k E - \sigma_{ki} u_i \end{pmatrix}$$

model of Prandtl and Reus :

$$Fm(S_{ij}) = \lambda S_{ij}$$

$$\lambda = \begin{cases} \dfrac{3W}{2Y^2}, & Q = 2Y^2/3 \\ 0, & Q < 2Y^2/3 \end{cases}$$

$$W = \mu S_{ij}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

model of Sokolovskii and Perzyna:

$$Fm(S_{ij}) = \mu \frac{S_{ij}}{\eta} \cdot \frac{\sqrt{Q} - \sqrt{\frac{2}{3}}Y}{\sqrt{Q}} H\left(\sqrt{Q} - \sqrt{\frac{2}{3}}Y\right)$$

$$Q = S_{ij}S_{ij}$$

Y - yield strength

μ - shear modulus

η - dynamic viscosity

H – Heaviside function

$$\omega_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$ *- spin tensor*

Equation of State:

Two-term (stiffened gas) EOS:

$$P = (\gamma - 1)\rho\xi + c_0^2(\rho - \rho_0)$$

wide-range EOS:

GES library of EOS

Log EOS:

$$\ln\left(\frac{\rho}{\rho_0}\right) = \frac{P}{K} - \frac{\alpha}{c_v}(\xi - \xi_0),$$

$$\xi = c_v T$$

Mie-Gruneisen EOS :

$$P(\rho, \xi) = \rho_0, a_0^2 f(\eta) + \rho_0 \Gamma_0 \xi$$

$$f(\eta) = \frac{(\eta - 1)(\eta - \frac{1}{2}\Gamma_0(\eta - 1))}{(\eta - s(\eta - 1))^2}$$

$$\eta = \frac{\rho}{\rho_0}$$

Basic approach: Splitting in physics

Use the method of splitting by Marchuk and Yanenko:

$$\frac{\partial \mathbf{q}}{\partial t} + \sum_{k=1}^{n} L_k(\mathbf{q}) = 0$$

replace by a set of subsystems:

$$\frac{\partial \mathbf{q}}{\partial t} + L_k(\mathbf{q}) = 0, \quad \mathrm{k=1,2,\ldots,n}$$

and solve for the time step Δt in n stages

$$\mathbf{q}^{(1)} = L_1^h(\Delta t, \mathbf{q}^{(0)}), \quad \mathbf{q}^{(2)} = L_2^h(\Delta t, \mathbf{q}^{(1)}), \ \ldots, \quad \mathbf{q}^{n+1} = L_n^h(\Delta t, \mathbf{q}^{(n-1)})$$

TWO ways of splitting are investigated:

Method of splitting A:

I stage

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho \\ \rho v_i \\ \rho E \\ \rho S_{ij}\end{pmatrix} + \frac{\partial}{\partial x_k}\begin{pmatrix}\rho v_k \\ \rho v_i v_k + P_i \delta_{ik} - S_{ik} \\ \rho E v_k + \sum_{n=1}^{N}\left(P v_n - S_{nk} v_n\right) \\ \rho S_{ij} v_k\end{pmatrix} = \begin{pmatrix}0 \\ 0 \\ 0 \\ 0\end{pmatrix}$$

__Pseudo-hydrodynamical stage:__ frozen deviatoric stress; use of moving grids to track contacts, free boundaries, shocks, etc.; resonant non-strictly hyperbolic system; flux – Rusanov, HLL, Godunov for the uniaxial 1D stress model

II stage

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho \\ \rho v_i \\ \rho E \\ \rho S_{ij}\end{pmatrix} = -\begin{pmatrix}0 \\ 0 \\ 0 \\ +2\mu\rho\frac{\partial v_i}{\partial x_j} - \frac{2}{3}\mu\rho\frac{\partial v_k}{\partial x_k} + S_{ik}\omega_{jk} + S_{jk}\omega_{ik} + \lambda S_{ij}\end{pmatrix}$$

__Constitutive stage__: the grid is frozen in time, and the equations are integrated for each computational cell as a system of ODEs.

The solution vector is updated as $\vec{q}^{\,*} = L_1\left(\Delta t, \vec{q}^{\,n}\right)$; $\vec{q}^{\,n+1} = L_2\left(\Delta t, \vec{q}^{\,*}\right)$

__Operator L_1__ : second-order accurate Godunov discrete operator with a MUSCL-type cell interpolation scheme implemented with an explicit-implicit absolutely stable time marching scheme.

__Operator L_2__ : second-order 2 stage Runge-Kutta explicit scheme.

Method of splitting B:

I stage

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho v_i\\ \rho E\\ \rho S_{ij}\end{pmatrix}+\frac{\partial}{\partial x_k}\begin{pmatrix}\rho v_k\\ \rho v_i v_k + P\delta_{ik}\\ \rho E v_k + \sum_{n=1}^{N}\left(P\delta_{ik}v_n\right)\\ \rho S_{ij}v_k\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\end{pmatrix}$$

Hydrodynamic stage: no effect of the dev.stress; strict hyperbolic system - FVM discretization on moving grids with Godunav type flux appr. (Rusanov, Roe, HLL);

II stage

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho v_i\\ \rho E\\ \rho S_{ij}\end{pmatrix}+\frac{\partial}{\partial x_k}\begin{pmatrix}0\\ -S_{ik}\\ \sum_{n=1}^{N}\left(-S_{nk}v_n\right)\\ \mu\rho v_i\delta_{kj}-\frac{2}{3}\mu\rho v_k\delta_{ij}\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\end{pmatrix}$$

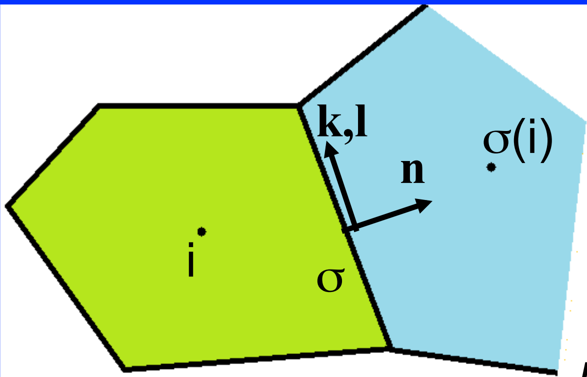
Elastic stage: correction due to elastic stress and updating deviatoric stresses. Strict hyperbolic system in conservative form – FVM with stationary grid, flux: Roe, Rusanov, HLL.

III stage

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho v_i\\ \rho E\\ \rho S_{ij}\end{pmatrix}=-\begin{pmatrix}0\\0\\0\\ S_{ik}\omega_{jk}+S_{jk}\omega_{ik}+\lambda S_{ij}\end{pmatrix}$$

Plastic stage: correcting solution due to plasticity and accounting objectivity of the stress tensor (Yaumann derivative); system of ODEs solved with second-order Runge-Kutta explicit scheme.

Solving stage I: $\vec{q}^{\,*} = L_1\left(\Delta t, \vec{q}^{\,n}\right)$



Moving grid: unstructured, fixed topology: cell-centred control volume method:

$$\frac{dV_i\vec{q}_i}{dt} = -\sum_{\sigma}\left(\vec{f}_k n_k - \vec{q}U_n\right)_{\sigma} S_{\sigma}$$

Normal face velocity U_n : GCL: $\frac{dV_i}{dt} = \sum_{\sigma} U_{n,\sigma} S_{\sigma}$: $U_{n,\sigma} = \frac{\Delta V_{\sigma}}{\hat{S}_{\sigma}\Delta t}$

$\Delta V_{\sigma} = Volume(\sigma(t), \sigma(t+\Delta t))$ - volume swept by the face as *i(t) ->i(t+Δt)*

$\hat{S}_{\sigma} = Aver(\sigma(t), \sigma(t+\Delta t))$ - face average position

$$T = \begin{pmatrix} 1 & & & & 0 \\ & n_1 & n_2 & n_3 & \\ & k_1 & k_2 & k_3 & \\ & l_1 & l_2 & l_3 & \\ & & & & \bullet \\ 0 & & & & 1 \end{pmatrix}$$

Local 1D flux: $\vec{f}_k n_k - \vec{q}U_n = T^{-1}\left(\vec{F} - \vec{Q}U_n\right); \quad \vec{Q} = T\vec{q}$

$$\vec{F} = \left(\rho u_n; \rho u_n^{\,2} - \sigma_{nn}; \rho u_n u_k - \sigma_{nk}; \rho u_n u_l - \sigma_{nl}; \rho u_n E - \sigma_{nn}u_n - \sigma_{nk}u_k - \sigma_{nl}u_l; \rho u_n S\right)$$

Semi-discrete form: $$\frac{dV_i\vec{q}_i}{dt} = -\sum_{\sigma} T_{\sigma}^{-1}\vec{\Phi}_{\sigma} S_{\sigma} \quad : \quad \vec{\Phi} = \vec{F} - U_n\vec{Q}_{\sigma}$$

Solving hydrodynamical stage: numerical flux

$\vec{\Phi} = \vec{\Phi}\left(\lambda, \vec{Q}_i^{\sigma}, \vec{Q}_{\sigma(i)}^{\sigma}\right)$ <u>*σ-values*</u>: accurancy of the scheme: MUSCL approach:

$$\vec{Q}^{\sigma} = \vec{Q}^{n} + T\left(r_k^{\sigma} I - 0.5\Delta t A_k\right)\nabla_k \vec{q}^{\,n} \qquad A_k = \partial \vec{f}_k \big/ \partial \vec{q}$$ - Jacobian

∇_k = operator of limited derivative: $r_k^{\sigma}\nabla_k \varphi_i = C\left(\varphi_{\sigma(i)}, -\varphi_i\right) \quad 0 \le c \le 0.5$

Explicit time integration: second-order scheme:

$$\vec{q}_i^{\,n+1} = \frac{1}{v_i^{n+1}}\left[V_i^n q_i^n - \Delta t \sum_{\sigma} T_{\sigma}^{-1} \Phi_{\sigma} S_{\sigma}\right] = \boxed{S^{(2)}\left(\Delta t, \vec{q}^{\,n}\right)}$$

Stability of the operator $S^{(2)}$: ensured by a CFL condition:

$$\lambda\left(\vec{q}_i^{\,n}\right) = \frac{V_i}{\sum_{\sigma} \rho_{\sigma}^{\Phi} S_{\sigma}} \qquad \Delta t = \max_i \left[\lambda\left(\vec{q}_i^{\,n}\right)\right]$$

Hydrodynamical stage: explicit/implicit scheme

Eliminate the CFL restriction: change to explicit/implicit scheme:

intermediate time level: $t^{\omega} = \omega t^{n} + (1-\omega)t^{n+1}$

$$0 \le \omega \le 1$$

intermediate state vector: $\vec{q}^{\,\omega} = \omega \vec{q}^{\,n} + (1-\omega)\vec{q}^{\,n+1}$

explicit/implicit scheme: $\boxed{\vec{q}^{\,n+1} = S^{(2)}\left(\omega \Delta t, \vec{q}^{\,\omega}\right)}$

absolute stability: ω in each computational cell: $\omega_i = \min_i \left[1, \frac{\lambda\left(\vec{q}_i^{\,\omega}\right)}{\Delta t} \right]$

(I.Menshov, Y.Nakamura: AIAA J., 2004)

solving explicit/implicit scheme: matrix-free LU-SGS :

- two linear sub-systems

  with a lower- and upper- triangular block matrices;

- 2 explicit-type forward and backward sweeps over cells.

Numerical results 1D: loading regimes

Verification: 1D impact problem:

0<x<10 cm, initial velocity $u_0<0$,

$P_0=0$, $S_0=0$

aluminum, Mie-Grunaisen EOS.

Theory:

$0<|u_0|<u_Y^+$ - 1-wave elastic,

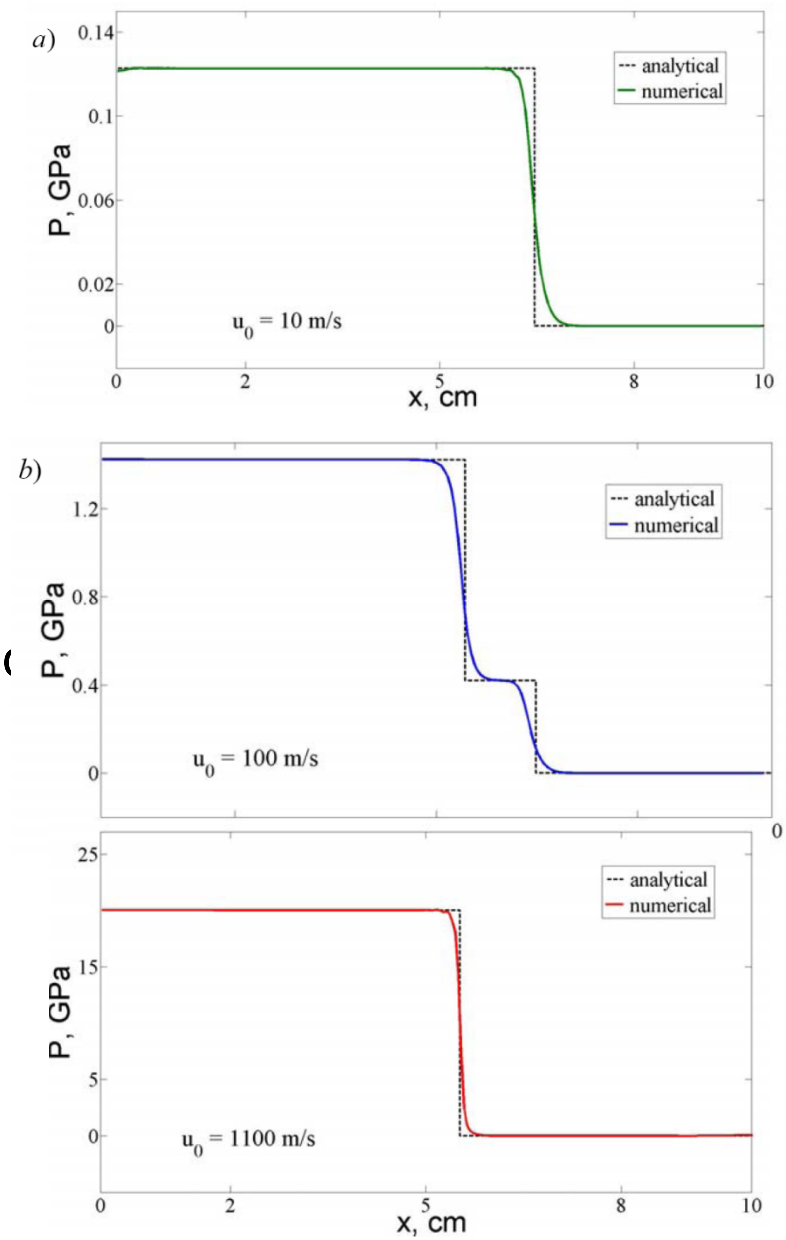
$u_Y^+ \le |u_0| < (u_0)_*$ - 2-wave elastic-plasti

$|u_0| > (u_0)_*$ - 1-wave plastic:

$(u_0)_Y^+ = 33.99\,\mathrm{m/s}$, $(u_0)_* = 990.98\,\mathrm{m/s}$

Calculations:

$$u_0 = 10, 100, 1100\,\mathrm{m/s}$$



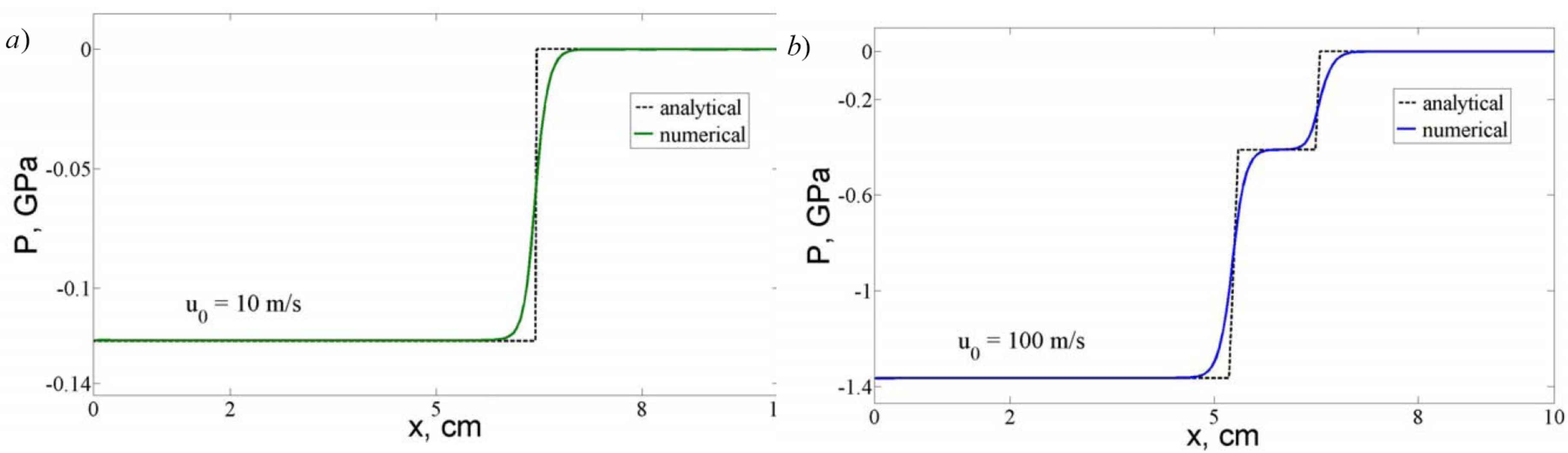
Numerical results 1D: unloading regimes

<u>Verification</u>: $0<x<10$ cm, initial velocity $u_0>0$,

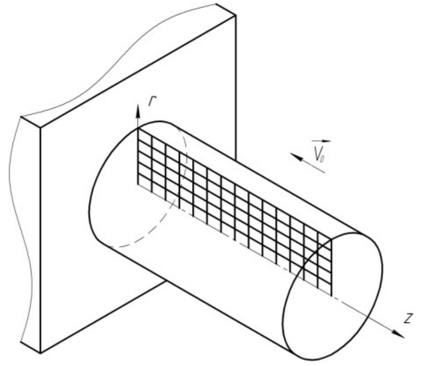
$P_0=0$, $S_0=0$, aluminum, Mie-Grunaisen EOS.

<u>Theory</u>: $0 < u_0 \le (u_0)_Y^-$: 1-wave elastic, $u_0 \ge (u_0)_Y^-$: 2-wave elastic-plastic,

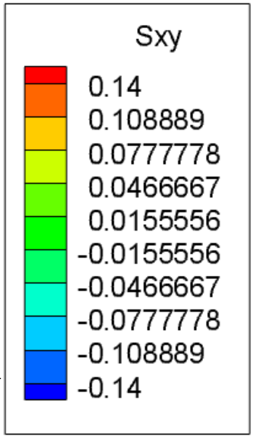
$(u_0)_Y^- = 33.82\ \mathrm{m/s}$ *<u>Calculations</u>*: $u_0 = 10\ \mathrm{m/s}$, $u_0 = 100\ \mathrm{m/s}$



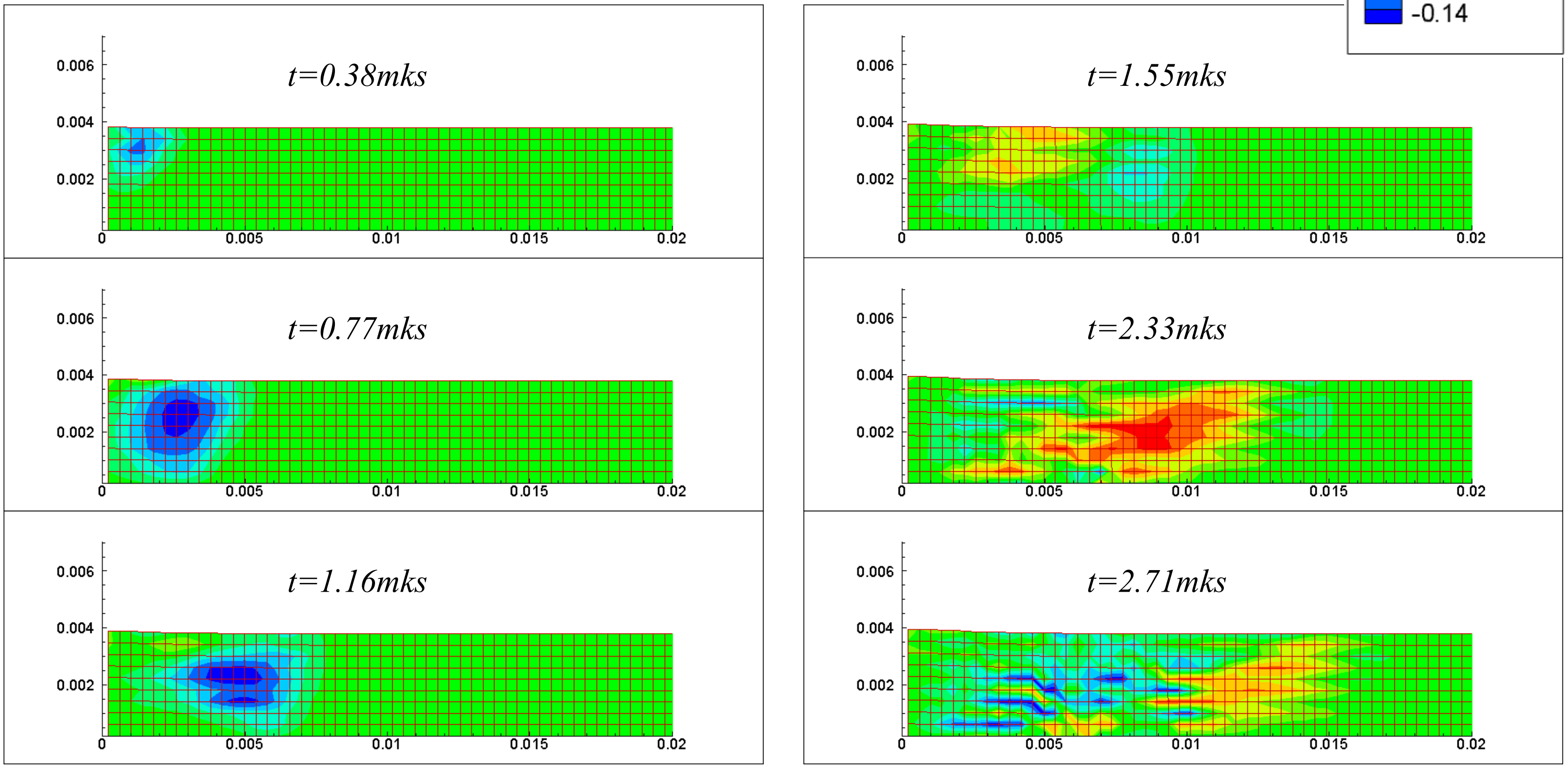
2D *Taylor impact problem: instability of method A*



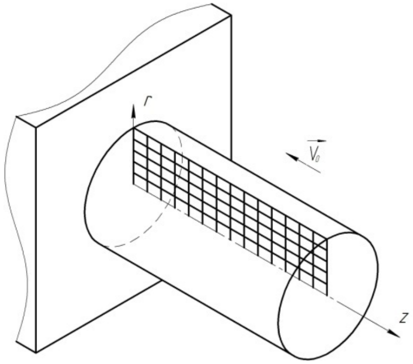
material - Al
Impact velocity – 100m/sec
Geometry:
L = 4cm r = 0,4cm
Splitting method A



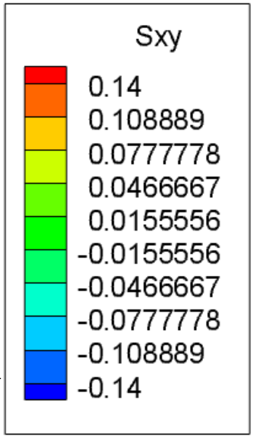
Shear stress distribution:



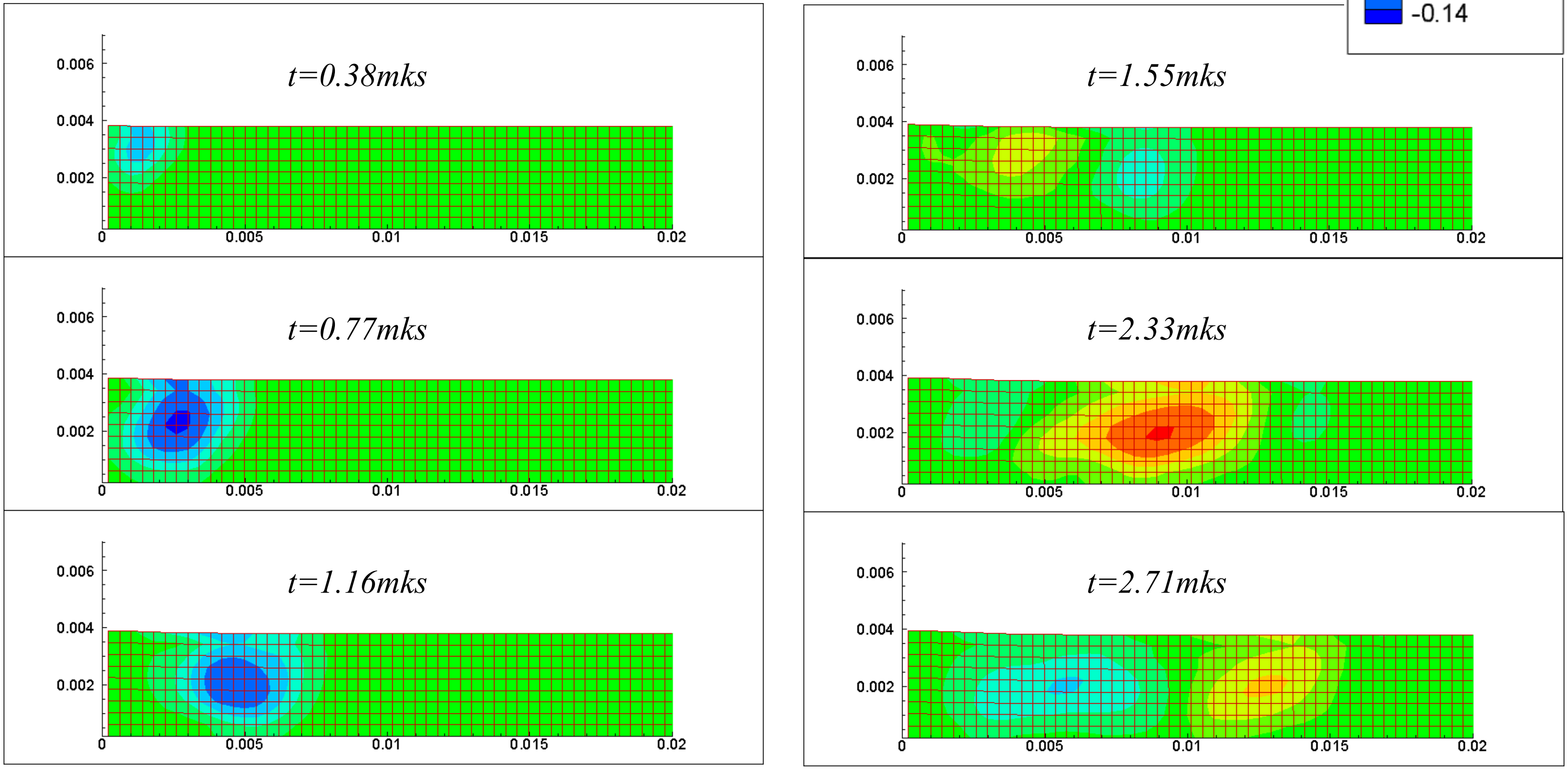
2D *Taylor impact problem: splitting method B*



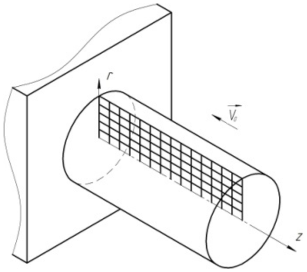
material - Al
Impact velocity – 100m/sec
Geometry:
L = 4cm r = 0,4cm
Splitting method B (3 stages)



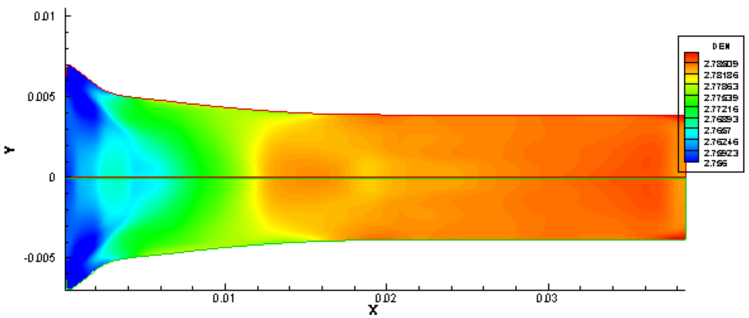
Shear stress distribution:

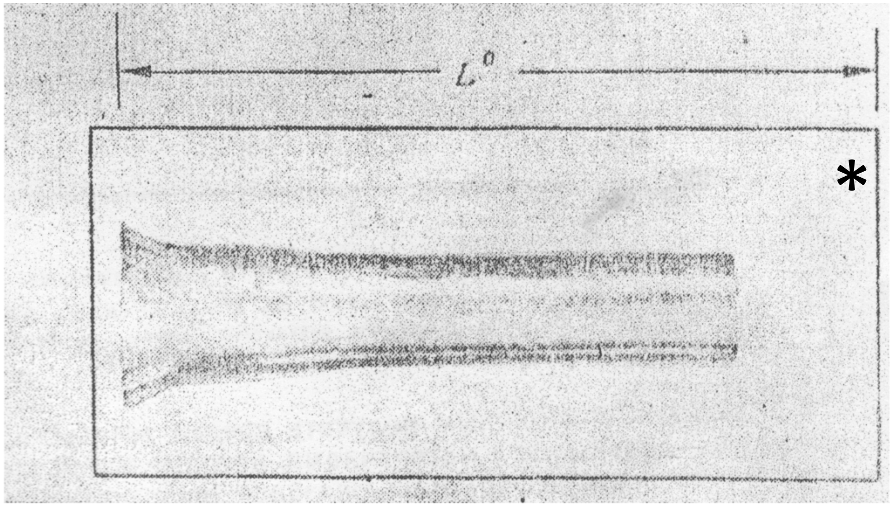


Validation: splitting method B.

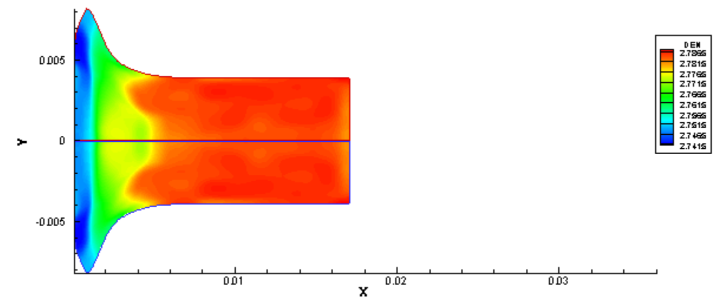


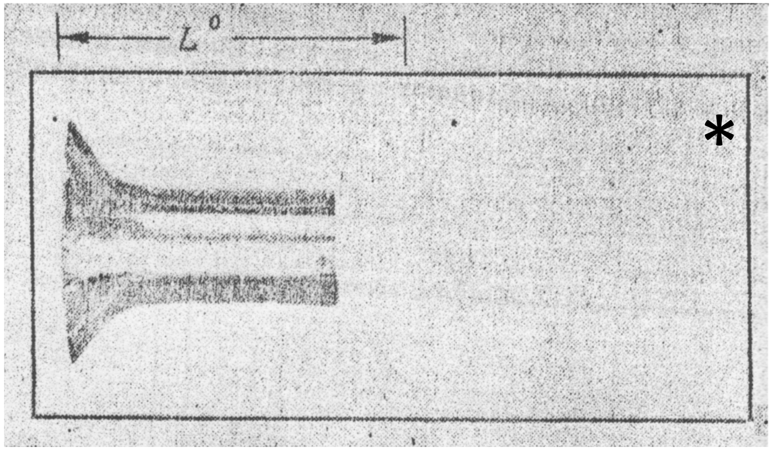
material - Al
Impact velocity – 273m/sec
Geometry:
L = 4.694cm r = 0,392cm





material - Al
Impact velocity – 373m/sec
Geometry:
L = 2.382cm r = 0,392cm

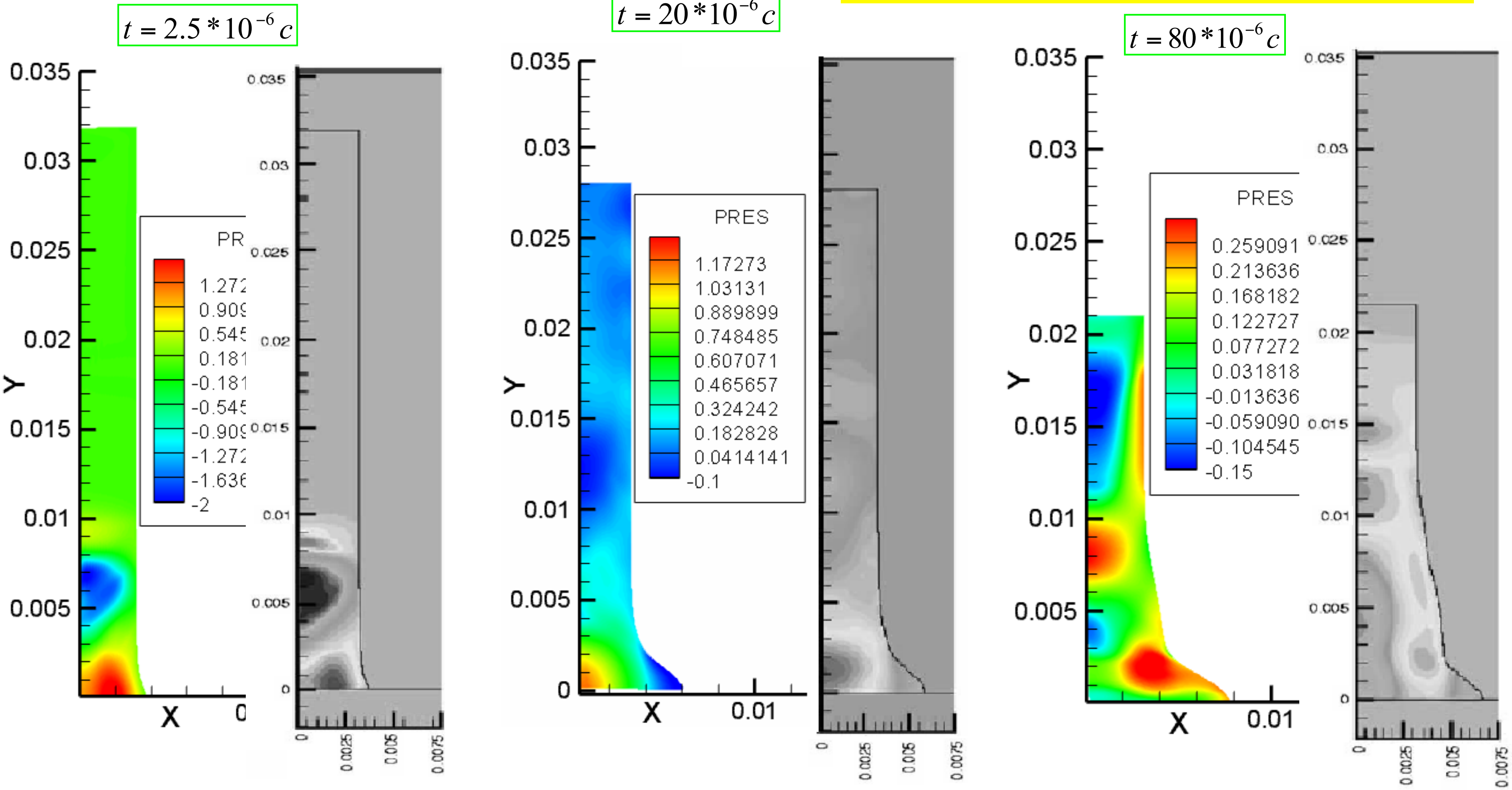




*| *Wilkins M.L., Guinan M.W.* Impact of cylinders on a rigid boundary // J. Appl. Phys. 1973. V. 44. № 3. P. 1200-1216.

Validation: splitting method B

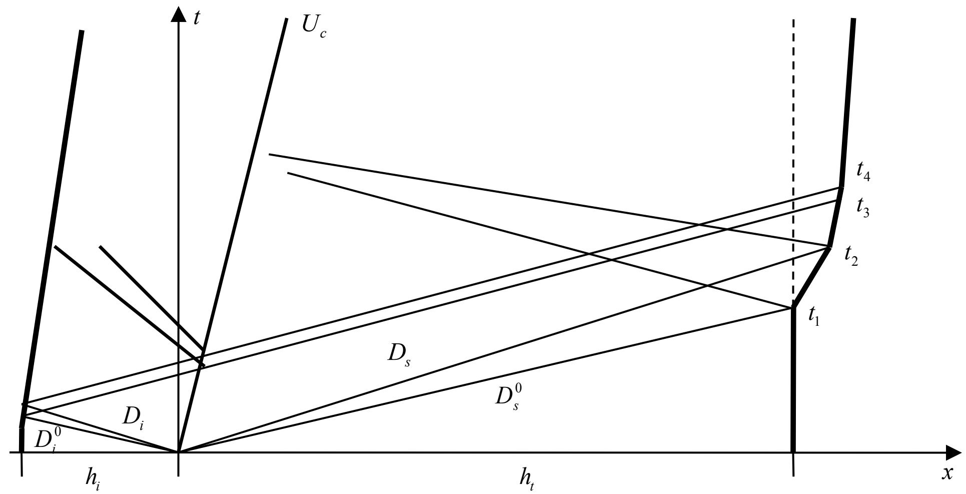
material - Cu
impact velocity – 227m/sec
geometry : L = 3.25cm r = 0,325cm



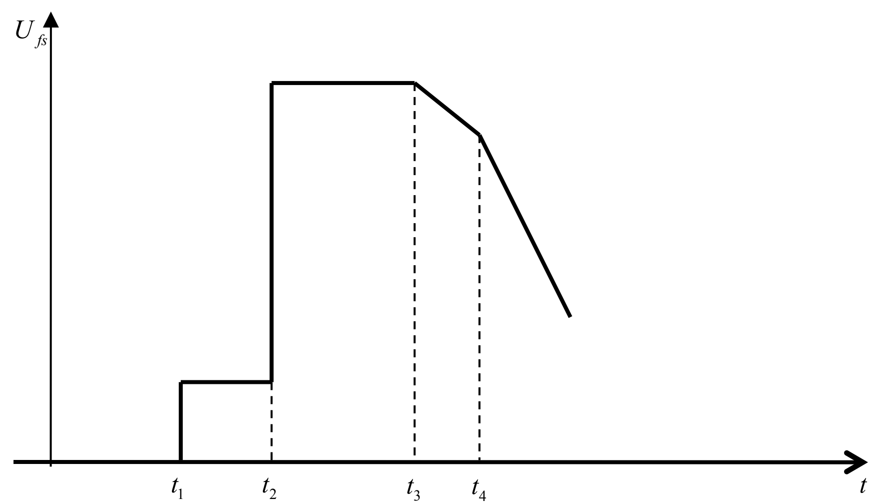
*| H.S. Udaykumar, L. Tran, D.M. Belk, K.J. Vanden, «An Eulerian method for computation of multimaterial impact with ENO shock-capturing and sharp interfaces» Journal of Computational Physics 186 (2003) 136–177

Model Validation Tests (G. Kanel)

To **validate the model**: experimental data for the shock loading of aluminum and titan samples (G. Kanel). Plate impact is a 1D problem of interaction of 2 solid samples: target that is initially at rest and flyer plate (impactor)



Basic wave processes: 2F shock structure in target and impactor, reflection shocks from free surfaces, formation of 2F unloading waves, reflection of unloading waves at the target free surf.



Free surf. velocity time history – image of wave processes in the target:

- t_1 – elastic precursor;
- t_2 – plastic shock wave;
- t_3 – leading unloading wave;
- t_4 – secondary unloading wave.

Model Validation Tests (G. Kanel)

2 cases of "impactor-target" configuration are considered:

Parameters	Case 1 Al-Al	Case 2 Al-Ti
h_i mm	0,85	2
h_t mm	4,1	10
U_i m/sec	630	705
U_c km/sec	315	261,7
D_{i0} km/sec	6,4	6,4
D_{t0} km/sec	6,4	6,15
D_i km/sec	5,3975	5,4452
D_t km/sec	5,3975	5,165
t_1 mks	0,61	1,56
t_2 mks	0,72	1,843
t_3 mks	0,884	2,21
t_4 mks	1,03	2,58

Model Validation Tests (G. Kanel)

Calculations are done for 3 models:

- the **basic model** of Prandtl-Reus: $\dot{S} + \lambda S = \frac{4}{3}\mu \dot{e} \quad |S| \leq \frac{2}{3}Y \quad Y = Y_0$

- **relaxation model**: accounting finite time of elastic to plastic transition:

$$\dot{S} = \frac{4}{3}\mu \dot{e} - \psi(S)\frac{S}{\tau} \qquad \psi(S) = \begin{cases} 0, & \text{при } |S| < \frac{2}{3}Y \\ \dfrac{|S| - \frac{2}{3}Y}{|S|}, & \text{при } |S| \geq \frac{2}{3}Y \end{cases}$$

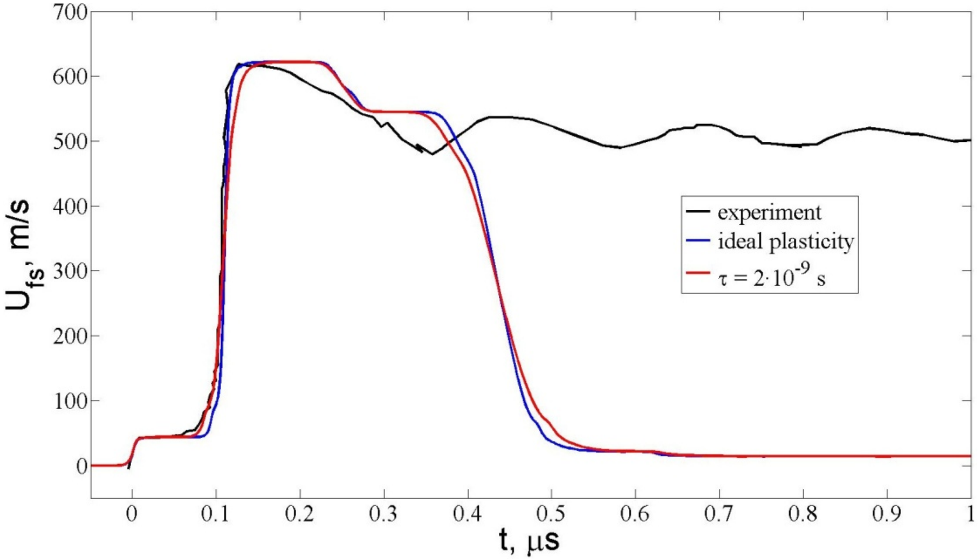
τ = relaxation time, if τ -> 0 - the basic Prandtl-Reuss model.

- **stress hardening model**: increase in flow resistance in plastic deformation

$$Y = Y_0 + Y_1 \varepsilon_u^p \qquad \varepsilon_u^p = \int_{t_0}^{t} \sqrt{\frac{2}{3}(\dot{e}^p : \dot{e}^p)} = |\varepsilon^p|$$ - equivalent plastic strain

fracture model: 2-parametric kinetic damage model with integral dissipative energy criteria for fracture (A. Kisilev, M. Yumashev, 1990, J.Ap.Math.Tech.Phys.)

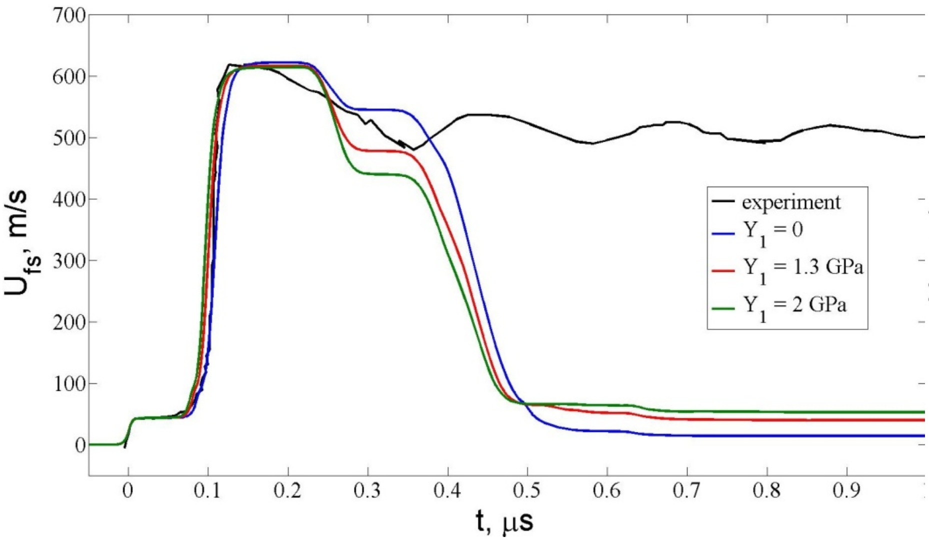
Model Validation Tests (G. Kanel): Case 1

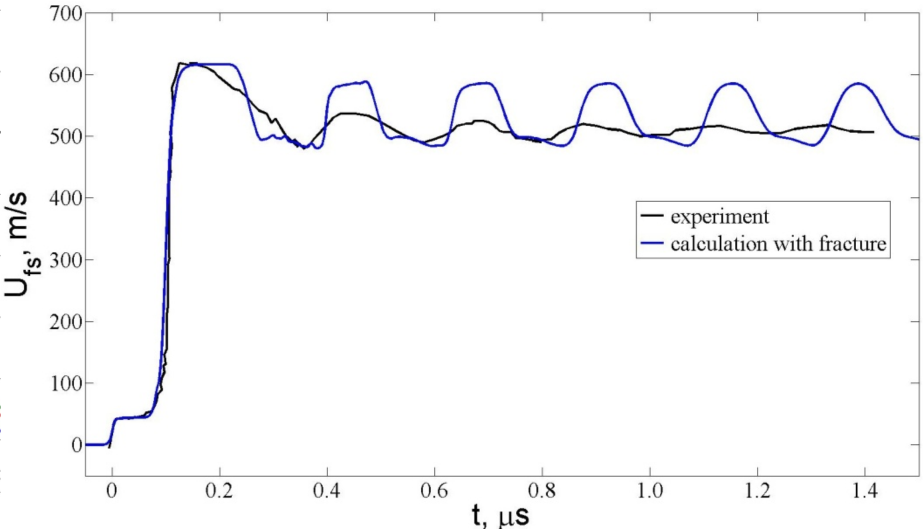


Parameters	Case 1 Al-Al
h_i mm	0,85
h_t mm	4,1
U_i m/sec	630

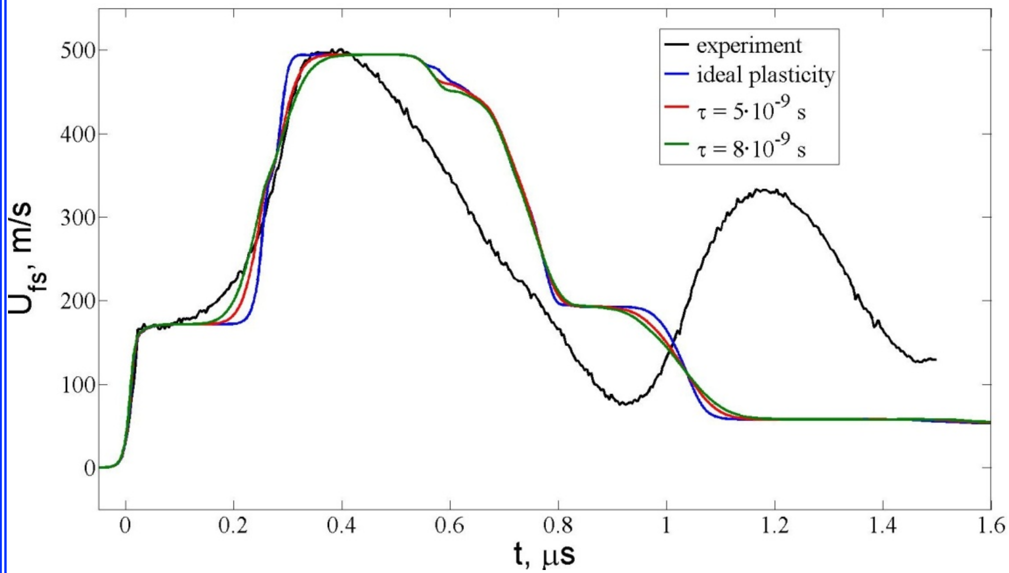
no fracture

with fracture model



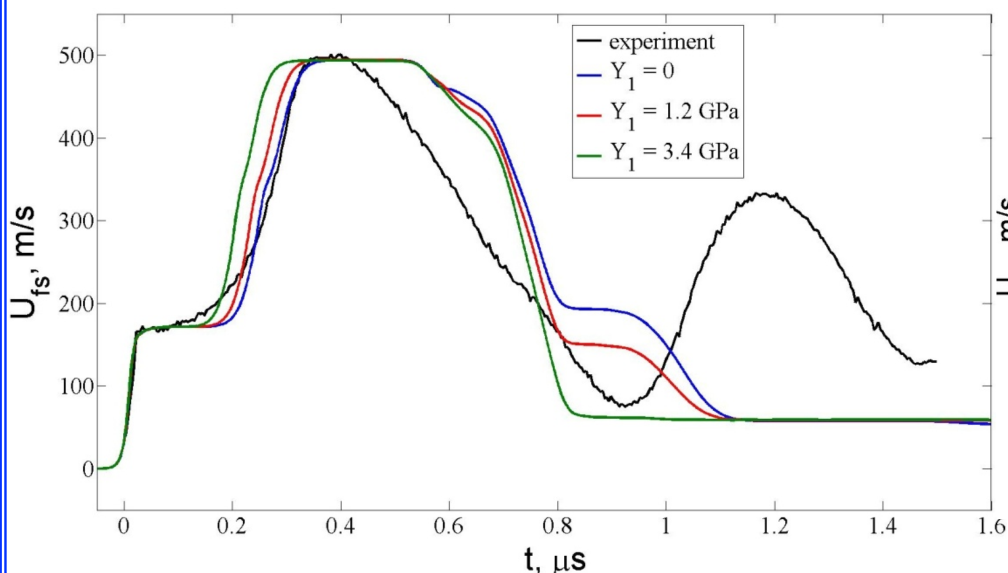


Model Validation Tests (G. Kanel): Case 2

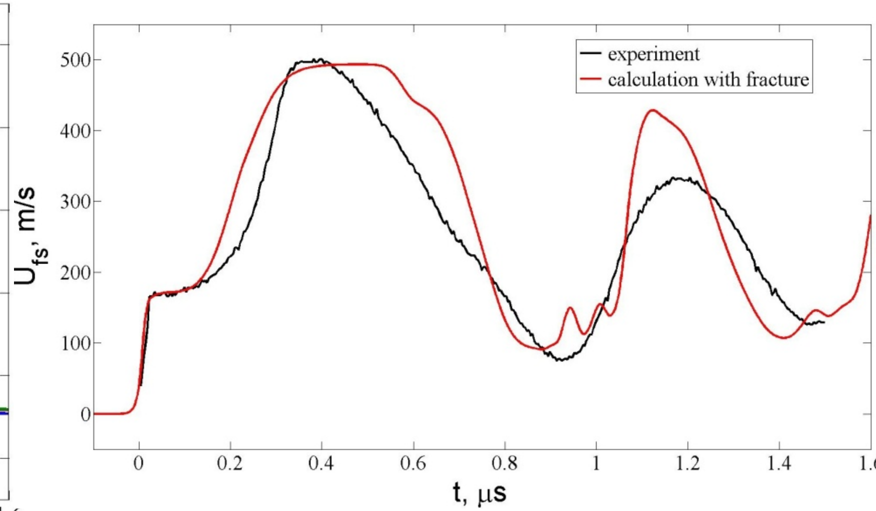


Parameters	Case 2 Al-Ti
h_i mm	2
h_t mm	10
U_i m/sec	705

no fracture



with fracture model



MULTIMATERIAL (MM) FLOW

- Eulerian approach: system of equations describing motion of multimaterial medium: equilibrium in velocity, pressure, and temperature:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}_1(\mathbf{q})}{\partial x} + \frac{\partial \mathbf{f}_2(\mathbf{q})}{\partial y} + \frac{\partial \mathbf{f}_3(\mathbf{q})}{\partial z} = 0$$

$$\mathbf{q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho\varepsilon \\ \rho\beta_1 \\ \cdots \\ \rho\beta_N \end{pmatrix}, \mathbf{f}_1 = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (\rho\varepsilon + p)u \\ \rho u\beta_1 \\ \cdots \\ \rho u\beta_N \end{pmatrix}, \mathbf{f}_2 = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho uv \\ (\rho\varepsilon + p)v \\ \rho v\beta_1 \\ \cdots \\ \rho v\beta_N \end{pmatrix}, \mathbf{f}_3 = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (\rho\varepsilon + p)w \\ \rho w\beta_1 \\ \cdots \\ \rho w\beta_N \end{pmatrix}$$

MIXTURE EQUATIONS of STATE (MEOS)

$$e = \sum_{i=1}^{N} \beta_i e_i(p,T) = e(p,T,\beta_1,\ldots,\beta_N)$$

$$1 \equiv \sum_{i=1}^{N} \alpha_i = \sum_{i=1}^{N} \beta_i \frac{\rho}{\rho_i^o(p,T)}$$

CONVENTIONAL GODUNOV METHOD: NUMERICAL INTERFACE DIFFUSION

- Godunov method can be directly extended for MM flow equations:
  - by solving the Riemann problem calculate the cell interface state vector

$$\mathbf{q}_{\mathrm{e}} = (\rho_{\mathrm{ek}} \;\; u_{\mathrm{z}} \;\; v_{\mathrm{k}} \;\; w_{\mathrm{k}} \;\; p_{\mathrm{z}} \;\; \beta_{1\mathrm{k}} \ldots \beta_{N\mathrm{k}} \;)$$

  - define the interface flux $\mathbf{F}$ as follows:

$$\mathbf{F} = \mathbf{F}(\mathbf{q}_{\mathrm{e}}) = (\; \rho_{\mathrm{ek}} u_{\mathrm{z}} \quad \ldots \; (\rho_{\mathrm{e}} \varepsilon + p_{\mathrm{z}}) u_{\mathrm{z}} \;\; \rho_{\mathrm{e}} u_{\mathrm{z}} \beta_{1\mathrm{k}} \quad \ldots \quad \rho_{\mathrm{e}} u_{\mathrm{z}} \beta_{N\mathrm{k}} \;\;)$$

- This approach suffers from excessive numerical diffusion: it doesn't take into account heterogeneity of the medium in mixed cells, i.e., presence of interphase boundaries; there is no difference between homogeneous and heterogeneous mixture.

- To reduce numerical diffusion: account sub-cell structure when calculating the flux at the cell interface separating mixed and pure cells

SPLITTING of PRIMITIVE STATE VECTOR

- Let's consider primitive state vector in a mixed cell

$$\mathbf{q} = (\ \rho\ \ u\ \ v\ \ w\ \ p\ \ \beta_1 \ldots \beta_j \ldots \beta_N\ )\ ,\ \ \forall\ \beta_j\ < 1$$

- For arbitrary *j*–th component such that $\beta_j \neq 0$, we define two primitive state vectors $\mathbf{q}_1$ and $\mathbf{q}_2$

$$\mathbf{q}_1 = (\ \rho^0_j\ \ u\ \ v\ \ w\ \ p\ \ \beta_1 = 0\ \ \ldots\ \ \beta_j\ = 1\ \ \ldots\ \ \beta_N = 0\ )$$
$$\mathbf{q}_2 = (\ \rho^*\ \ u\ \ v\ \ w\ \ p\ \ \ \beta^*_1\ \ \ldots \beta^*_j = 0\ \ \ldots\ \ \ \beta^*_N\ \ )$$

- ρ^0_j – actual density of *j*-th component
- Parameters ρ^*, β^*_i are defined as follows:

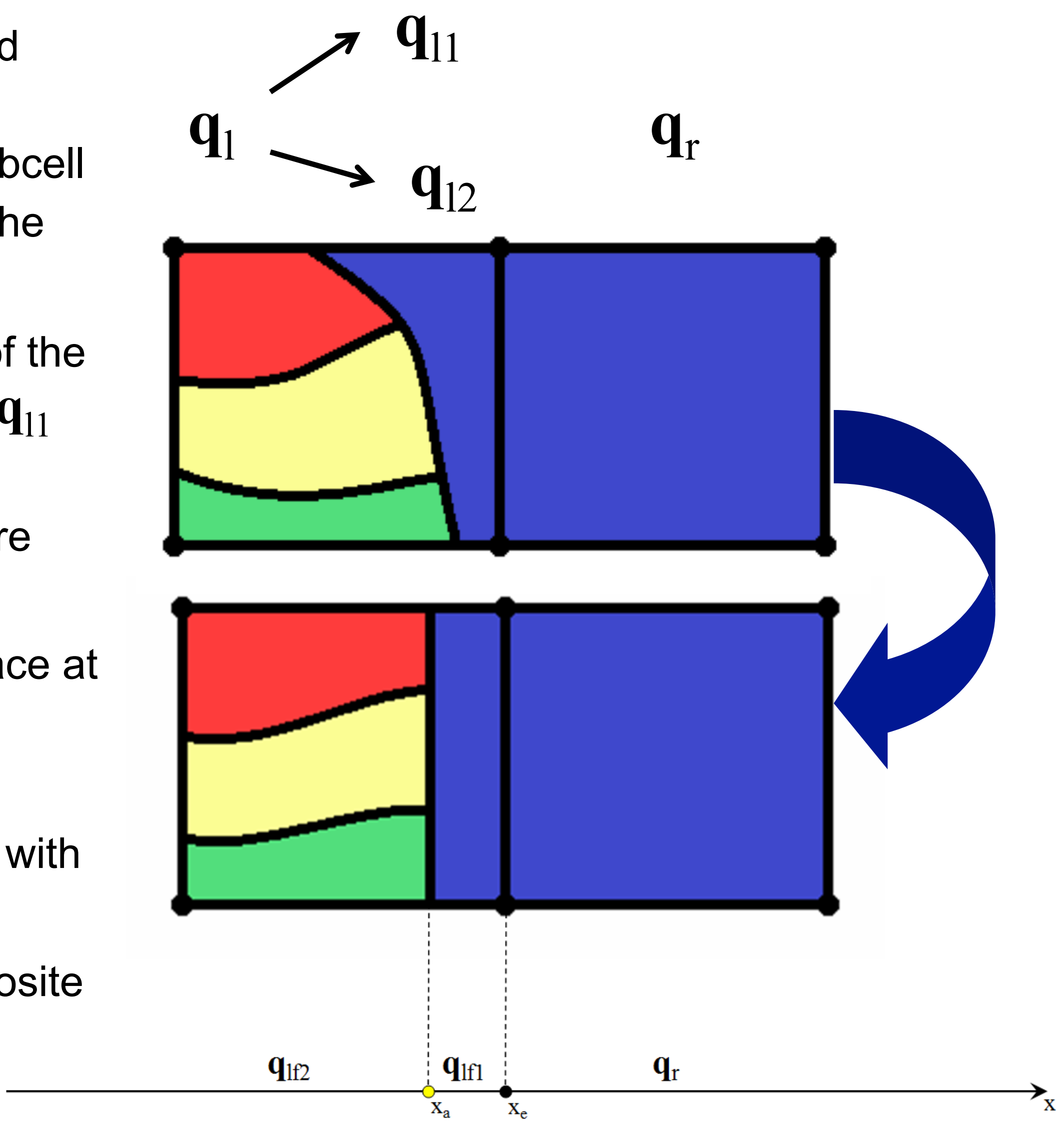
$$\rho^* = (1 - \beta_j)\rho\rho^0_j\,/(\rho^0_j - \rho\beta_j\ )$$
$$\beta^*_i\ = \beta_i/\,(1 - \beta_j)\ ,\ i \neq j$$

and characterize average density and mass fractions of the mixture without j-th component.

- $\mathbf{q}_1$ and $\mathbf{q}_2$ - state vectors of pure j-th component and the rest of the mixture

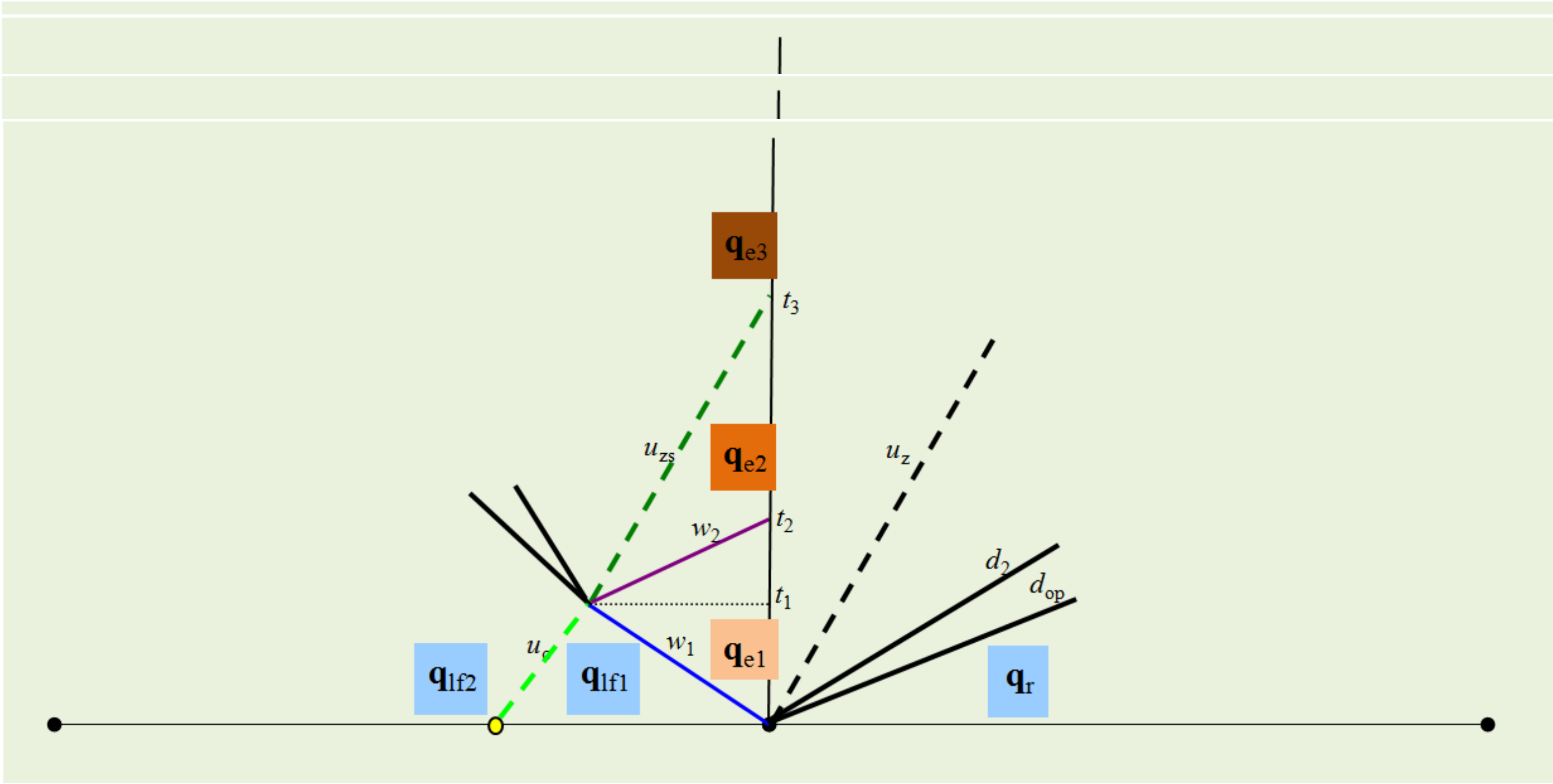
BOUNDARY REPRESENTATION COMPOSITE RIEMANN PROBLEM

- Let a cell interface separates mixed and pure cells. Calculating the flux at the interface we want to account for the subcell structure in the mixed cell. To do this, the following procedure is proposed:
- In the mixed cell, split the component of the pure cell calculating split state vectors $\mathbf{q}_{l1}$ and $\mathbf{q}_{l2}$.
- Calculate the volume fraction of the pure component in the mixed cell.
- Locate the boundary parallel the interface at a distance to be defined by the volume fraction.
- Solve 1D composite Riemann problem with initial data $\mathbf{q}_{l1}$, $\mathbf{q}_{l2}$, and $\mathbf{q}_r$
- Use this solution to calculate the composite numerical flux at the interface.



COMPOSITE RIEMANN SOLVER

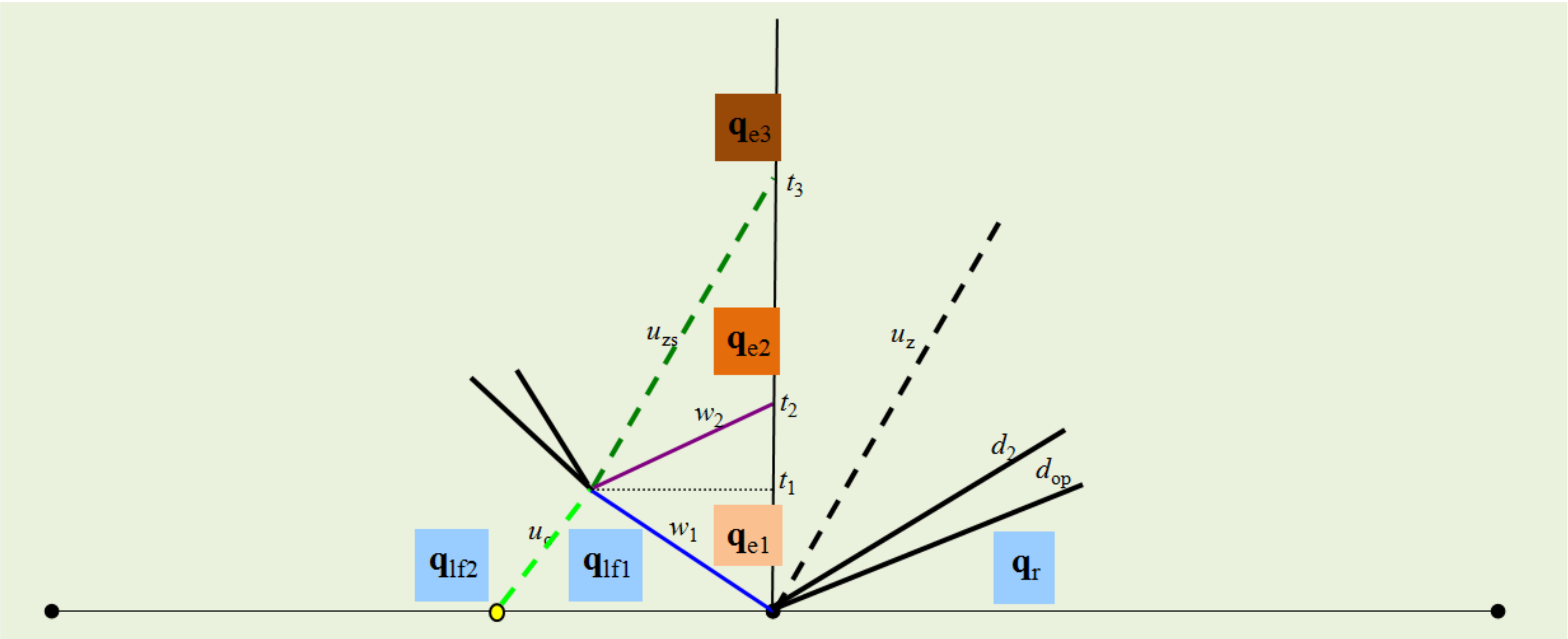
MIXED PURE



- U_C = normal velocity in the mixed cell; U_Z = contact velocity in primery R.S.
- $\mathbf{q}_{e1}$, $\mathbf{q}_{e2}$, $\mathbf{q}_{e3}$ = composite solution at the interface

COMPOSITE FLUX CALCULATION: Uz>0

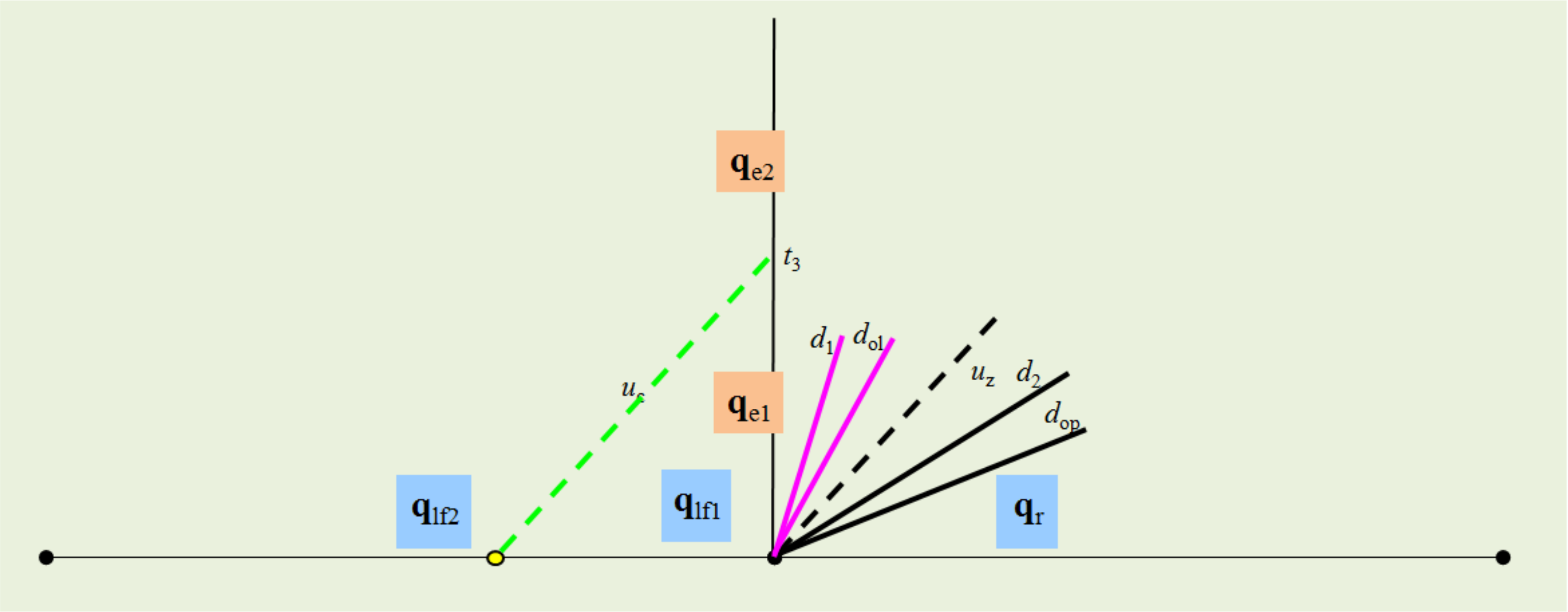
SUBSONIC CASE



- Number of terms in sum depends on times ratio:
  - $\Delta t \leq t_2$: $\lambda_1 \cdot \mathbf{F}(\mathbf{q}_{e1})$
  - $t_2 < \Delta t \leq t_3$: $\lambda_1 \cdot \mathbf{F}(\mathbf{q}_{e1}) + \lambda_2 \cdot \mathbf{F}(\mathbf{q}_{e2})$
  - $\Delta t > t_3$: $\lambda_1 \cdot \mathbf{F}(\mathbf{q}_{e1}) + \lambda_2 \cdot \mathbf{F}(\mathbf{q}_{e2}) + \lambda_3 \cdot \mathbf{F}(\mathbf{q}_{e3})$
- State $\mathbf{q}_{e3}$ **differs** from states $\mathbf{q}_{e1}$, $\mathbf{q}_{e2}$ in mass components

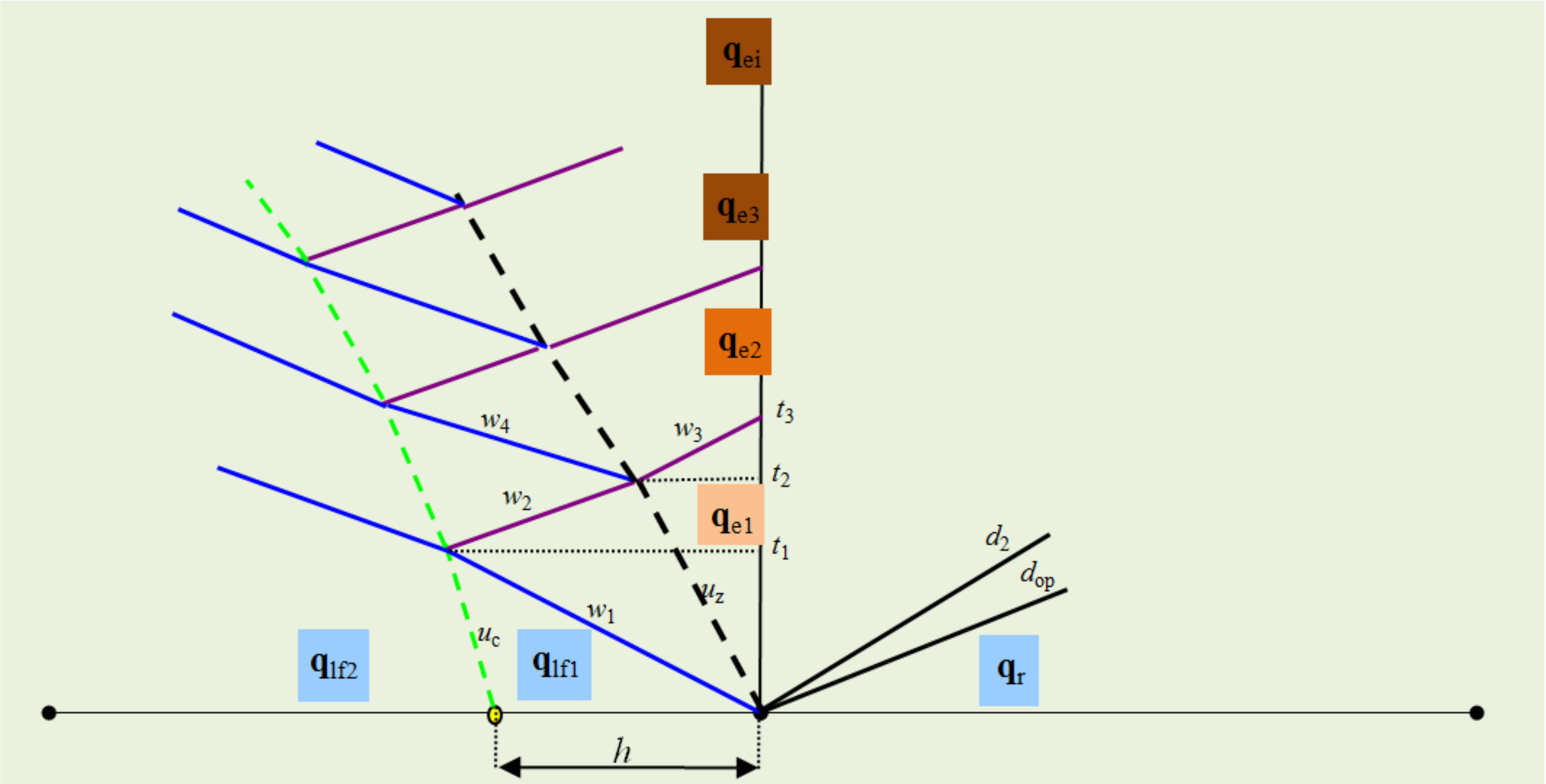
COMPOSITE FLUX CALCULATION: Uz>0

SUPERSONIC CASE



- $\mathbf{q}_{e1} = \mathbf{q}_{lf1}$; $\mathbf{q}_{e2} = \mathbf{q}_{lf2}$
- Number of terms in sum depends on times ratio:
  - $\Delta t \leq t_3$: $\lambda_1 \cdot \mathbf{F}(\mathbf{q}_{e1})$
  - $\Delta t > t_3$: $\lambda_1 \cdot \mathbf{F}(\mathbf{q}_{e1}) + \lambda_2 \cdot \mathbf{F}(\mathbf{q}_{e2})$
- State $\mathbf{q}_{e2}$ **differs** from $\mathbf{q}_{e1}$ in mass components

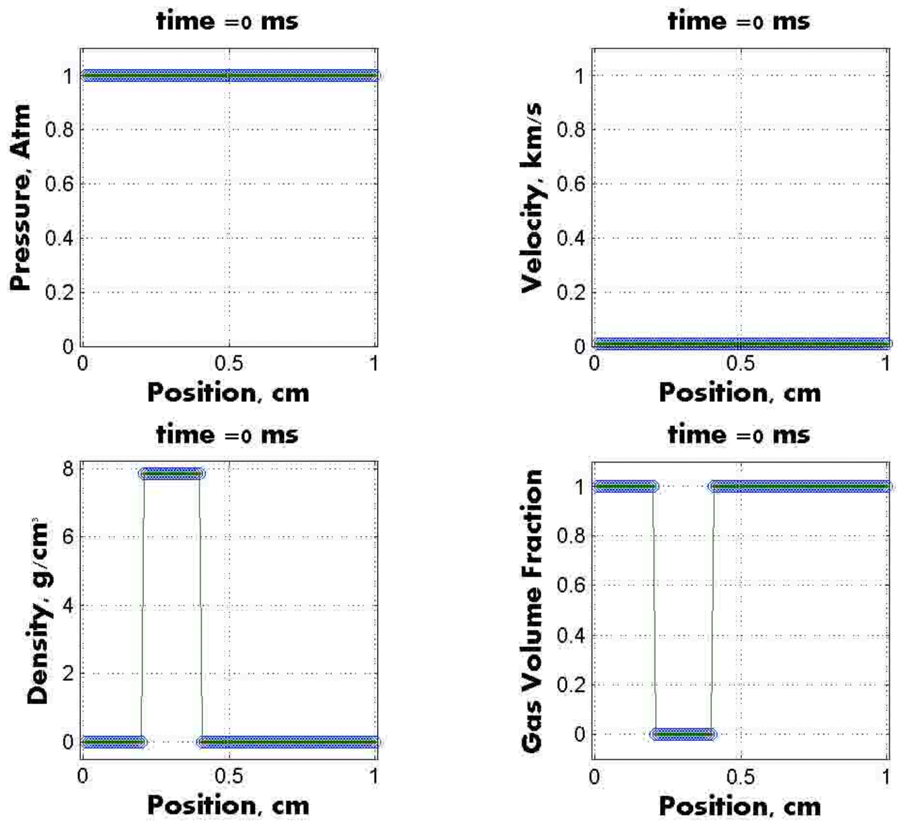
COMPOSITE FLUX CALCULATION: Uz<0

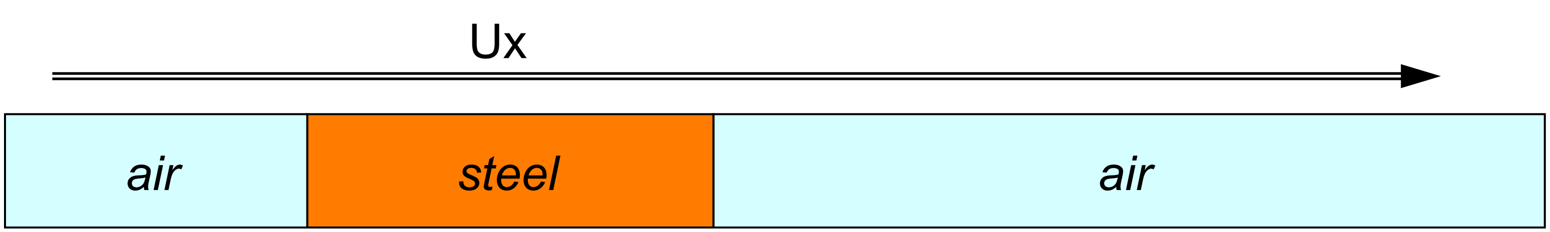


- States $\mathbf{q}_{ei}$ **do not differ** in mass components
- Number of terms in sum depends on times ratio; in case of small h number of terms could be very big; in our calculations we limit number of terms to two

1D TRANSMISSION

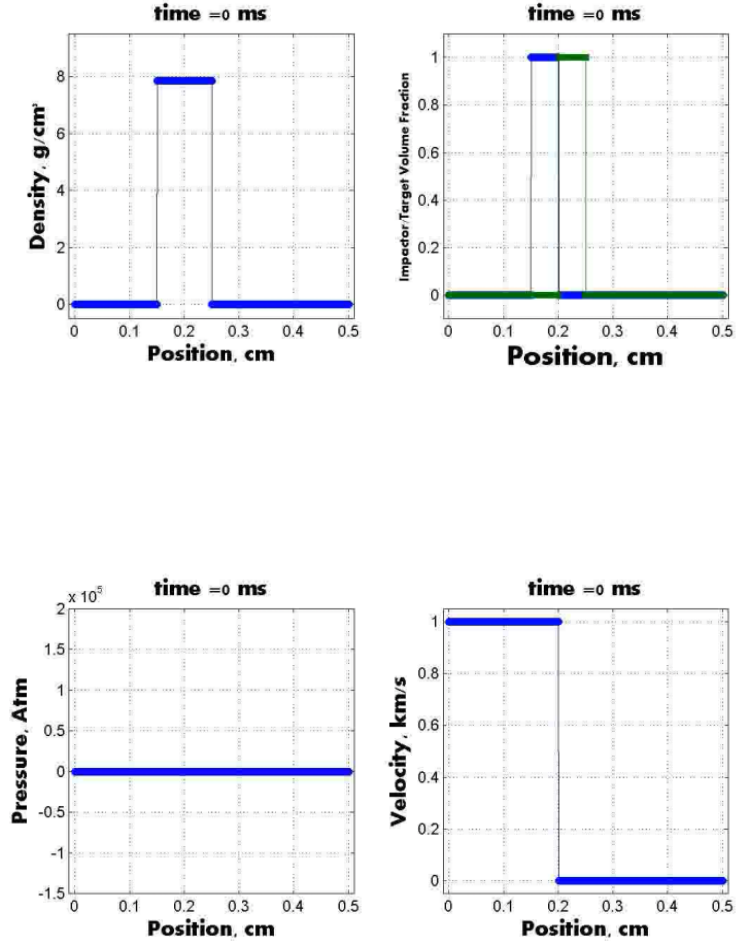
- Problem statement:
  - densities- 7.85 g/cm3 ; 0.001 g/
  - Initial pressure - 1 Atm
  - EOS – ideal gas; Mi-Grunaisen
  - Domain size - 1.0 cm
  - Steel: 0.2 cm < x < 0.4 cm;
  - velocity – 0.1 km/s
  - Number of computational cells
  - - 100
  - CFL = 0.9





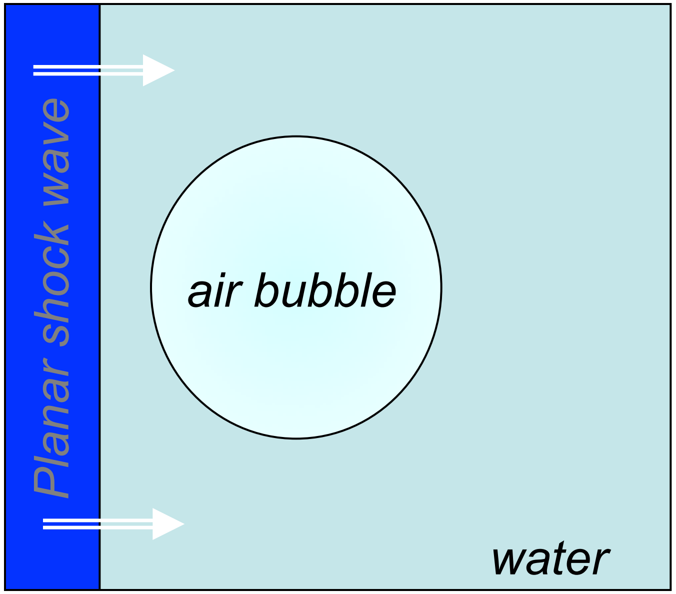
TWO PLATE INTERFACE

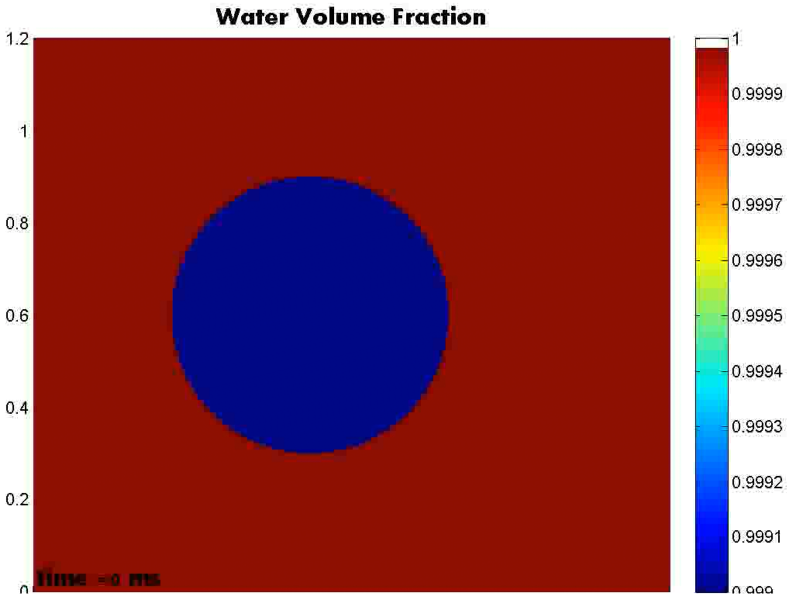
- Problem statement:
  - Densities: - 7.85 g/cm3 ; 0.001 g/cm3
  - Initial pressure - 1 Atm
  - EOS – ideal gas; Mi-Grunaisen EOS
  - Domain size - 0.5 cm
  - Steel impactor: 0.15 cm < x < 0.2 cm;
  - Steel target : 0.2 cm < x < 0.25 cm
  - impact velocity - 1 km/s
  - Number of computational cells - 500
  - CFL = 0.9

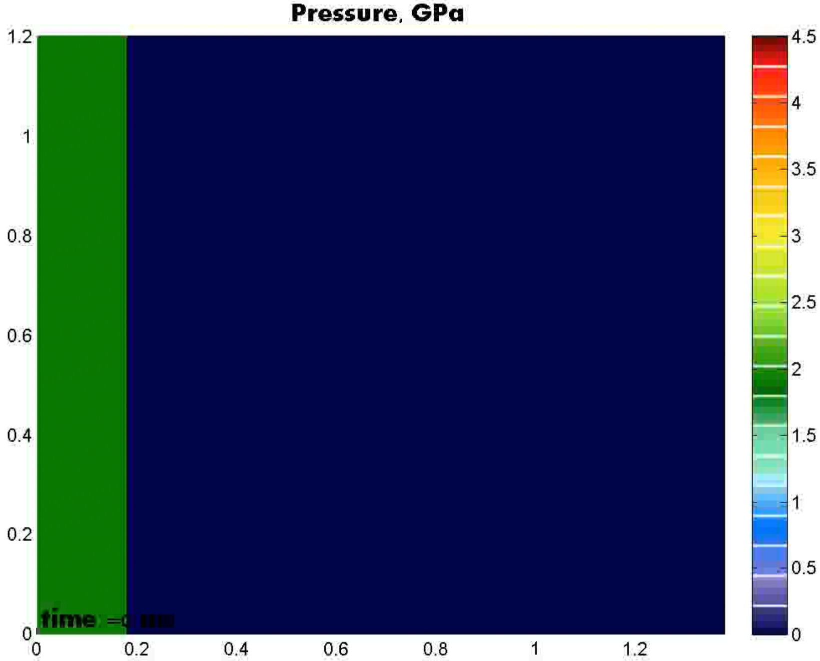


BUBBLE COLLAPSE

- Problem statement:
  - Densities- 1.0 g/cm3 ; air - 0.001 g/cm3
  - Initial pressure - 1 Atm
  - EOS – ideal gas; stiffened gas
  - Planar shock wave: *M=2*
  - Domain size - 1.38 cm*1.2 cm
  - cells – 460*400
  - CFL = 0.9

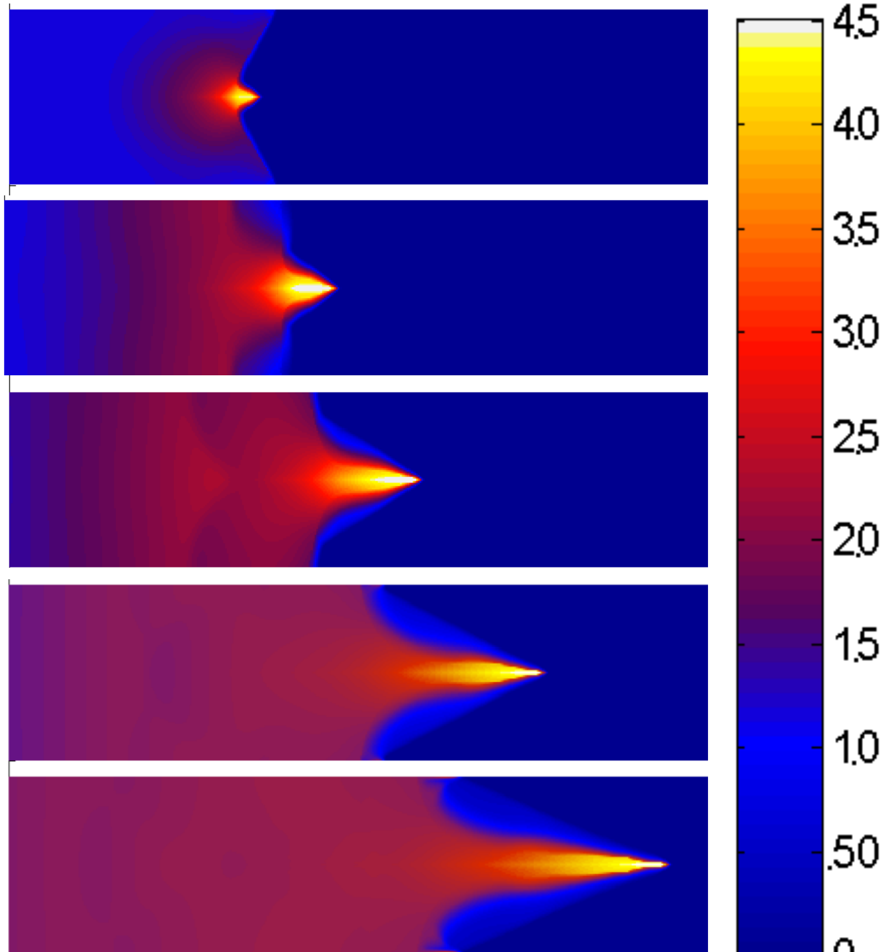




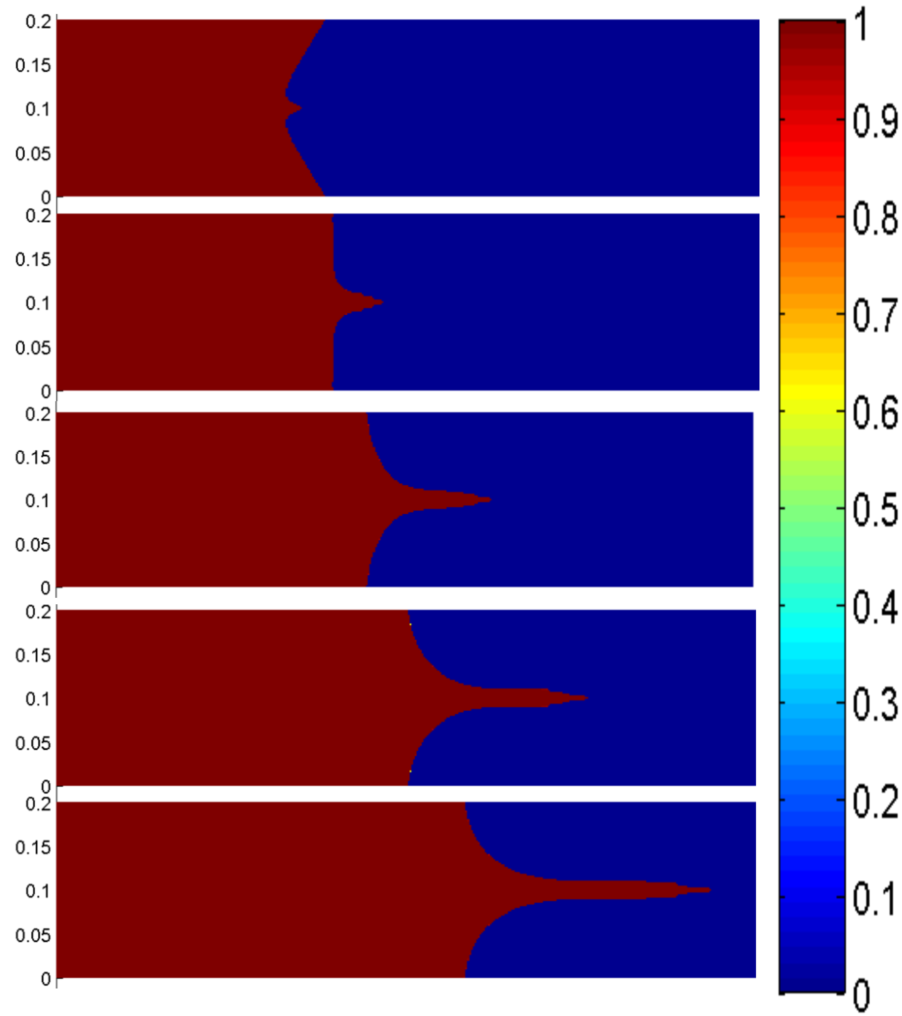


Jetting: Al-Al impact, 2.25 km/sec

velocity Ux, км/sec



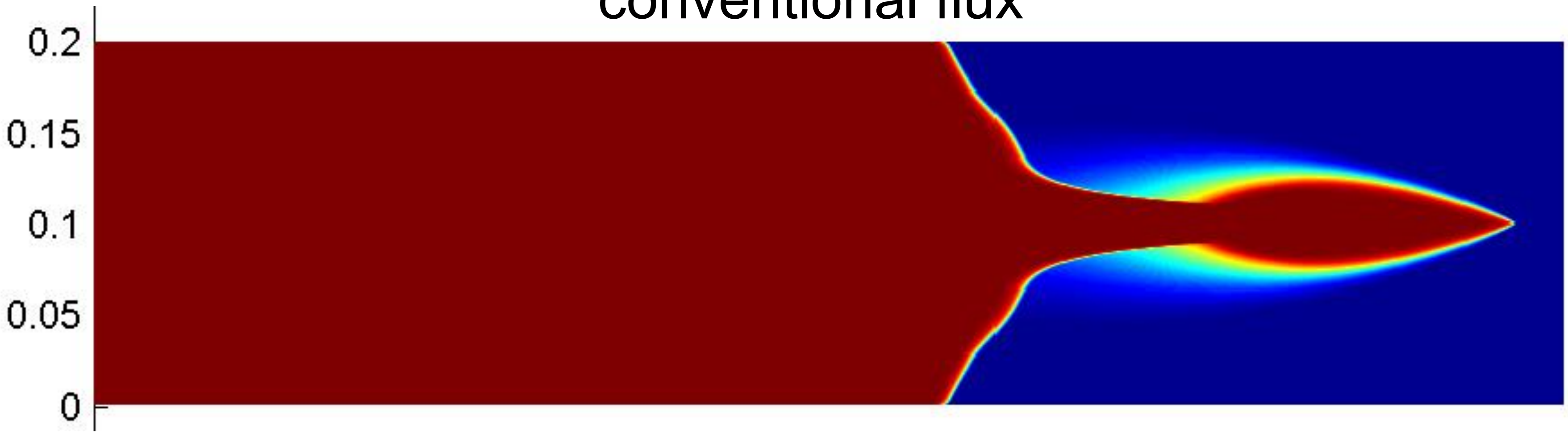
mass fraction of Al



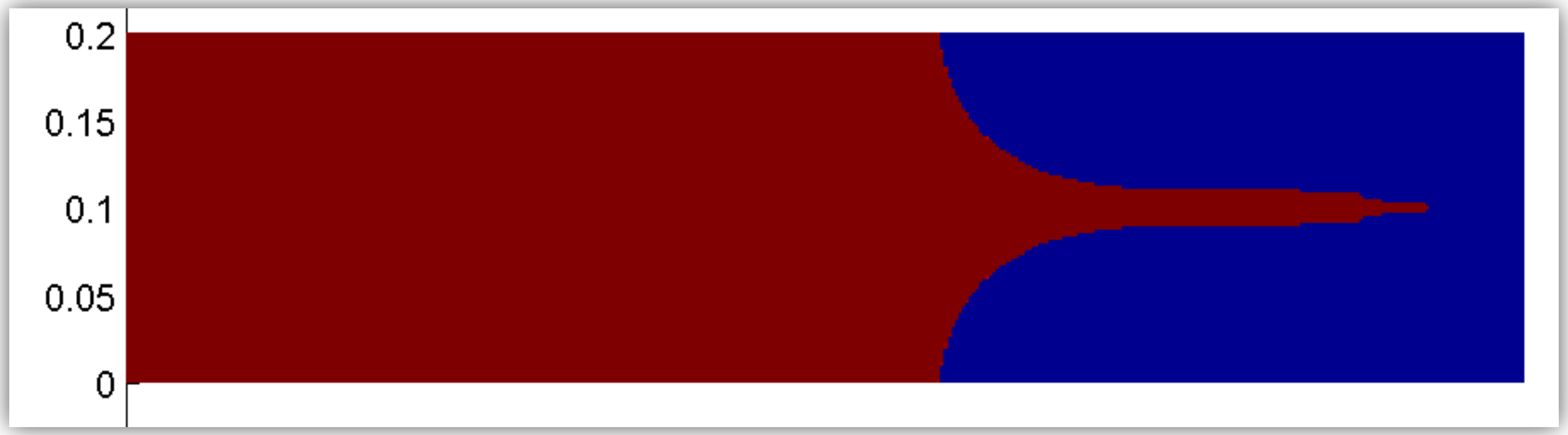
Jetting: Al-Al impact, 2.25 km/sec

Comparison of conventional and composite Godunov's fluxes

conventional flux



composite flux



CONCLUSIONS

2 ways of splitting elasto-plastic equations have been investigated:

- conventional 2-stage splitting results in typical weak instability because of resonant-type of hydro-elastic equations;
- this instability is removed by 3-stage (hydro, elaso, plast.) splitting.

Macroscopic Prandtl-Reus model has been tested by high-speed impact experimens of G. Kanel:

- loading is well matched;
- smooth unloading can not be predicted by the model; it is necessary to account for dynamics and kinetics of microscopic defects (dislocations and microcracks).

Considering subcell structure of mixed cells and implementing composite Godunov's flux can greatly improve accuracy of multimaterial calculations on Euler grids.

Conclusions and future work

A numerical method for calculating elastic-plastic flows on arbitrary moving Eulerian grids has been developed. Conceptual grounds of the method are 1) splitting in physics resulted in two sub-problems for hydrodynamics and material equations, respectively, 2) use of a high-accurate Godunov approach for discretizing the hydrodynamic part on arbitrary moving grids, 3) a hybrid explicit-implicit time marching scheme ensured stable calculations with a physically reasonable time step (not restricted by any specific stability conditions).

A detail analysis of self-similar solutions has been carried out for a simplified 1D model with the assumption of uniaxial deformations. In particular, different shock wave structures in an elasto-plastic material have been obtained depending on shock intensity. These are one-wave elastic, two-wave elasto-plastic, and one-wave plastic shock waves. Analytical solutions for these types of waves have been obtained. Also, self-similar expansion waves have been investigated. It was shown that two types of expansion wave can occur, viz., one-wave elastic and two wave elasto-plastic. Correspondent analytical solutions for these types of expansion have been found.

The present numerical method has verified by computing these analytical solutions, and has applied to calculations of two benchmarks - collapse of a cylindrical beryllium shell and Taylor impact problem. The method has been verified by calculating the problems with presented analytical solutions, and also comparing on some test problems calculated by other authors with different numerical methods.

Analytical solutions

1D model (uniaxial strain):

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}=0\ ; \qquad \frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho u^2-\sigma)}{\partial x}=0\ ; \qquad \frac{\partial(\rho E)}{\partial t}+\frac{\partial(\rho u E-\sigma u)}{\partial x}=0$$

deviatoric stress: $S = S_{11}$ $\quad \sigma = -p + S$

$$S(\rho)=\begin{cases} \frac{2}{3}Y, & \text{if } \rho < \rho_Y^- \\ S_0 - \frac{4}{3}\mu \ln\left(\frac{\rho}{\rho_0}\right), & \text{if } \rho_Y^- \le \rho \le \rho_Y^+ \\ -\frac{2}{3}Y, & \text{if } \rho > \rho^Y \end{cases}$$

Apply to: structures of a shock wave and a self-similar rarefaction wave.

Shock wave structure

Rankine-Hugoniot conditions : $\left[\vec{f}\right] = \bar{D}\left[\vec{q}\right]$

mass flow rate: $\dot{m} = \rho\left(u - D\right) = \rho_0\left(u_0 - D\right)$

Hugoniot adiabate (HA): $e - e_0 = \frac{1}{2}\left(v - v_0\right)\left(\sigma + \sigma_0\right),$

Raleigh-Michelson (RM) line: $\sigma - \sigma_0 = \left(\dot{m}\right)^2\left(v - v_0\right)$

Intersection of HA and RM in $p - v$ plane: shock wave solution.

Important point: HA and RM have a *week discontinuity* at $v = v_Y^+$

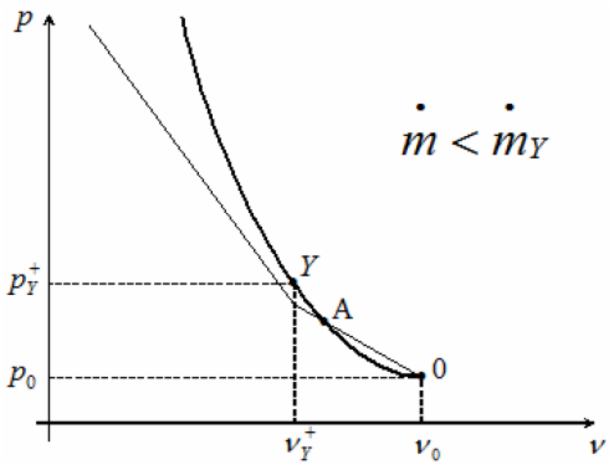
$\dot{m}$: *relative positions* of the HA and RM curves in the $p - v$ plane.

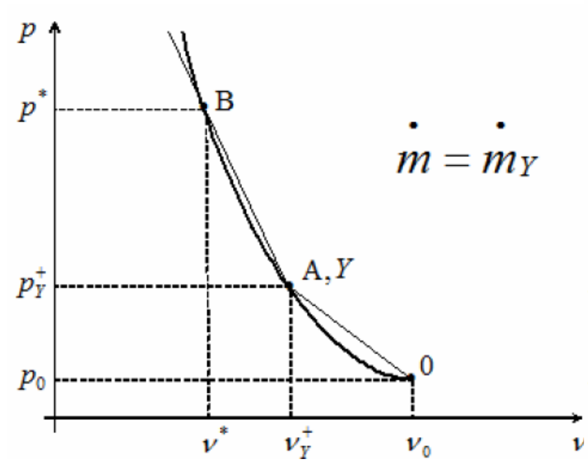
$\left(\dot{m}\right)^2 \geq \left(\dot{m}\right)_0^2 = \rho_0 c_0^2 + \rho_0\left[\frac{4}{3}\mu - \Gamma S_0\right]$: the HA and the RM intersect.

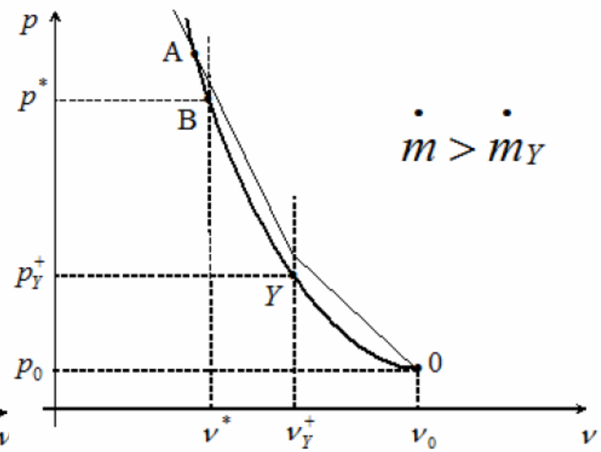
$\dot{m} = \dot{m}_0$: weak shock (a characteristics). HA and RM slopes coincide.

Shock wave structure: one-wave

<u>3 possible cases of intersection</u>:







$\dot{m}$ <u>*just above*</u> $\dot{m}_0$: <u>*one*</u> intersection point HA and RM: A<Y (in $\left[\nu_Y^+, \nu_0\right]$): no Y-condition: <u>*one-wave elastic shock*</u>.

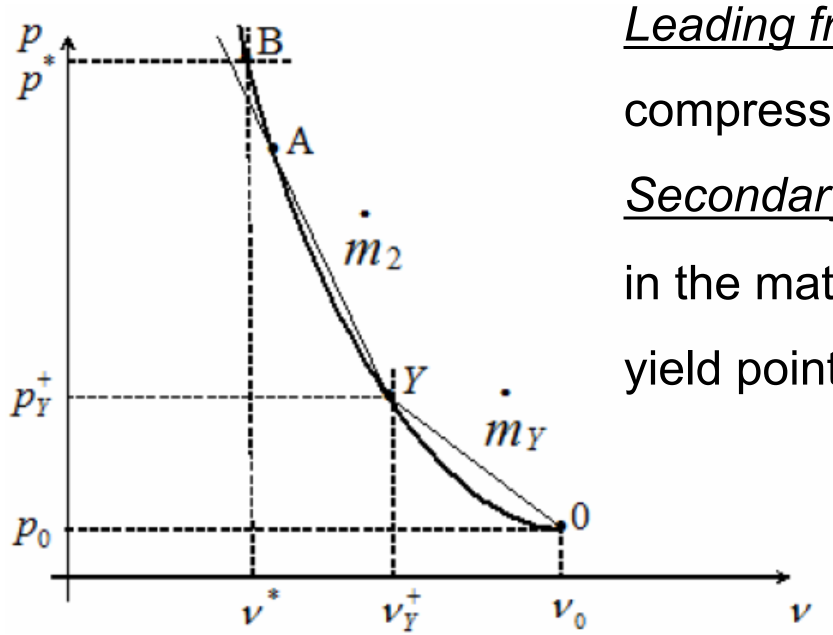
$\dot{m} = \dot{m}_Y$: A=Y: <u>*another solution*</u> B: <u>*two solutions*</u>: weak (A- ν_Y^+, p_Y^+) and strong (B- $\nu^* < \nu_Y^+$, $p^* > p_Y^+$)

$\dot{m} > \dot{m}_Y$: <u>*one*</u> intersection point HA and RM: A>B>Y (in $\nu^* < \nu_Y^+$): <u>*one-wave plastic shock*</u>.

Thus: <u>*no one-wave shock structure found for the middle part*</u> $\nu \in \left[\nu^*, \nu_Y^+\right]$!

Shock wave structure: two-wave

<u>*Middle part*</u> $v \in \left[v^*, v_Y^+\right]$: two-front shock structure:



<u>*Leading front*</u>: elastic precursor: $\dot{m} = \dot{m}_Y$:

compressive yielding: $v = v_Y^+,\ p = p_Y^+$

<u>*Secondary wave*</u>: plastic compressive wave : moves in the material compressed by the precursor to the yield point:

$$\dot{m}_2 = \rho\left(u - D_2\right) = \rho_Y^+\left(u_Y^+ - D_2\right)$$

$$\dot{m}_2^2 \in \left[\dot{m}_{20}^2, \dot{m}_Y^2\right]$$

$\dot{m}_{20}$: RM slope at the Y-point = HA slope at the Y-point for the plastic part.

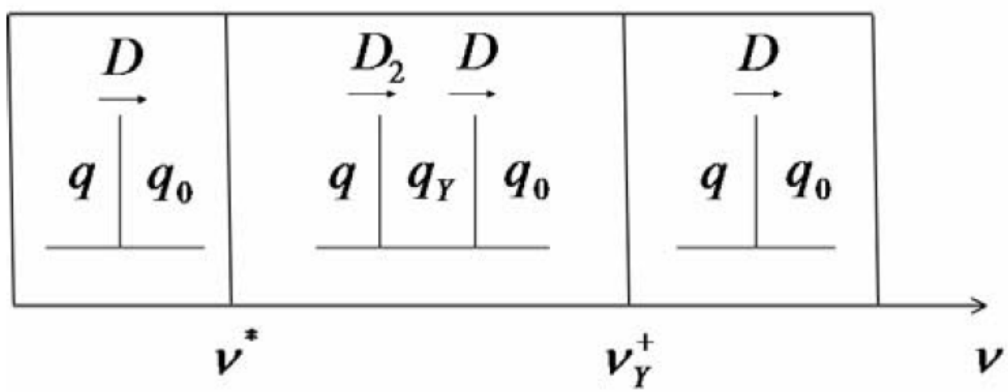
$$\dot{m}_{20}^2 = \left(\rho_Y^+ c_Y^+\right)^2 - \frac{1}{2}\left(S_0 - \frac{2}{3}Y\right)\Gamma_Y^+ \rho_Y^+$$

$\dot{m}_2 = \dot{m}_Y$: elastic precursor and secondary plastic wave coincides:

<u>*one-wave structure*</u> (B).

Shock wave structure

<u>3 types of shock wave structures</u> in elasto-plastic materials: one-front elastic, two-front with an elastic precursor, and one-front plastic.



<u>Illustration</u>: impact problem (uniaxial approximation): impact velocity u_0 , initial parameters $p_0 = S_0 = 0$, EOS Mi-Grunaisen.

	aluminum	copper	berillium
	material constants		
ρ_0, kg/m^3	2780	8930	1845
Γ_0	2.13	2	2
s	1.338	1.49	1.124
a_0, m/s	5330	3970	12870
μ, GPa	27.6	45	151
Y, GPa	0.29	0.09	0.33

	critical parameters		
$(u_0)_Y^+$, m/s	33.99	4.75	18.13
ρ_Y^+, kg/m^3	2794.64	8938.93	1847.02
p_Y^+, GPa	0.419	0.141	0.335
D_Y^+, m/s	6485.88	4745.68	16592.24
$(u_0)_*$, m/s	990.98	708.26	3290.2
ρ_*, kg/m^3	3281.35	10496.52	2301.35
p_*, GPa	17.675	29.955	100.502

Rarefaction wave structure

1D model: self-similar solutions of λ=x/t:

$$\lambda = u \pm a; \quad a v' \pm v u' = 0; \quad a u' \pm v \sigma' = 0$$

$$a^2 = c^2 + v\left(v\dot{S} - \Gamma S\right)$$

σ : $\sigma = \sigma(v)$ - *an isentrope*: defined by integration of $\dfrac{d\sigma}{dv} = \dfrac{c^2}{v^2}$

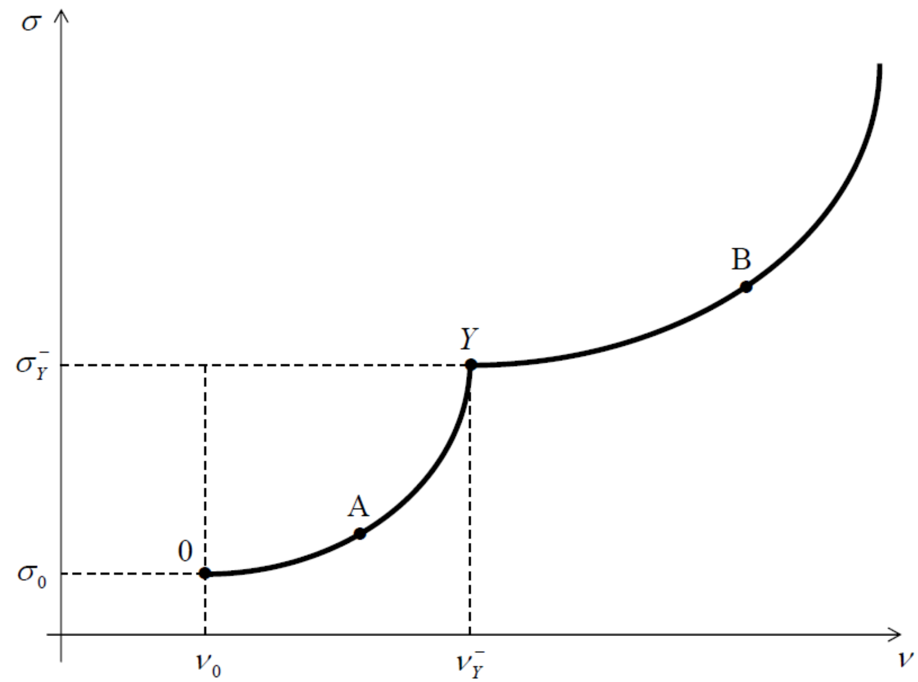
with $\sigma\big|_{v=v_0} = \sigma_0 = -p_0 + S_0$ for $v \ge v_0$

$\sigma = \sigma(v)$: monotonically increasing,

weak discontinuity at the point

of *expansive yielding Y* at $v = v_Y^-$

$$\left.\frac{d\sigma}{dv}\right|_{v=v_Y^-} = \frac{1}{\left(v_Y^-\right)^2}\begin{cases} a^2 - \Gamma S v + \dfrac{4}{3} v\mu, & v = v_Y^-(-0) \\ a^2 - \Gamma S v, & v = v_Y^+(+0) \end{cases}$$



Rarefaction wave structure

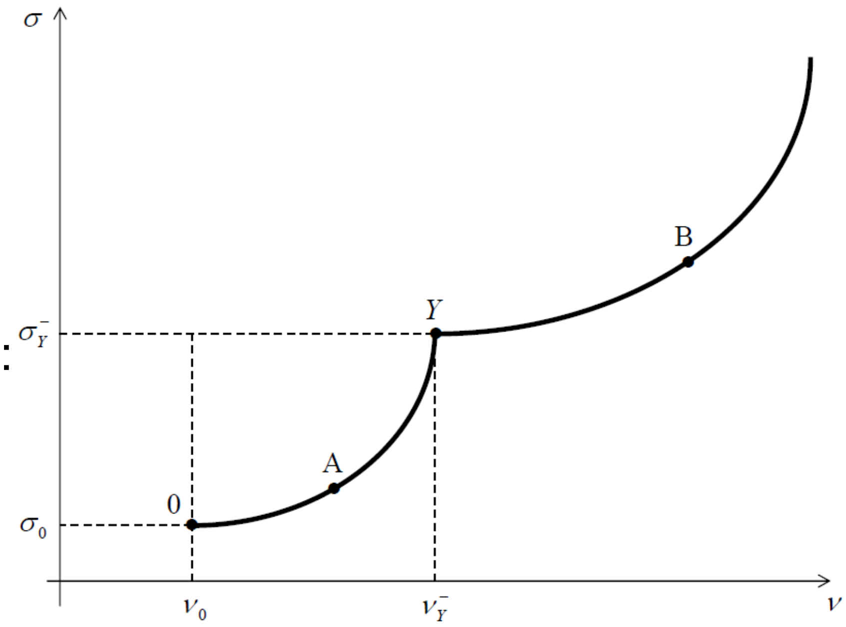
Y point: *two types of wave structures:*

a) *one-front elastic expansion wave*: O->A: $\lambda_A \le \lambda \le \lambda_0$

$$\frac{d\sigma}{d\nu} = \frac{c^2}{\nu^2}; \qquad \sigma\big|_{\nu=\nu_0} = \sigma_0$$

$$\nu_0 \le \nu \le \nu_A$$

$$\frac{du}{d\nu} = \mp\frac{c}{\nu}; \qquad u\big|_{\nu=\nu_0} = u_0$$



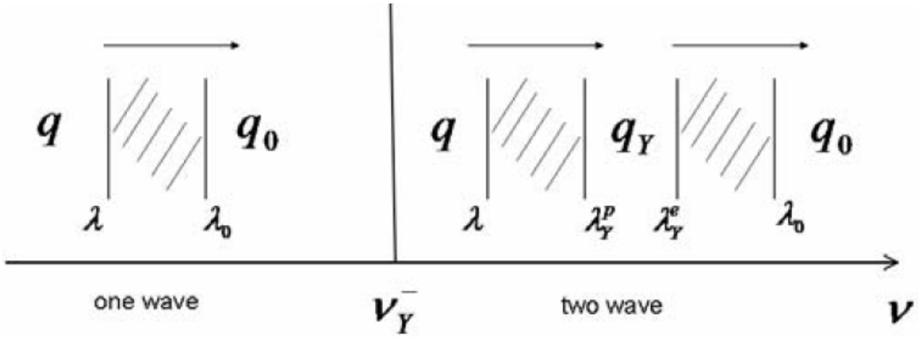
b) *two-wave structure of expansion*: O->Y->B:

elastic precursor : $\lambda_Y^e \le \lambda \le \lambda_0$: O->Y

plastic expansion : $\lambda_B \le \lambda \le \lambda_Y^P$: Y->B

$$\frac{d\sigma}{d\nu} = \frac{c^2}{\nu^2}; \qquad \sigma\big|_{\nu=\nu_Y^-} = \sigma_Y^-$$

$$\frac{du}{d\nu} = \mp\frac{c}{\nu}; \qquad u\big|_{\nu=\nu_Y^-} = u_Y^-$$

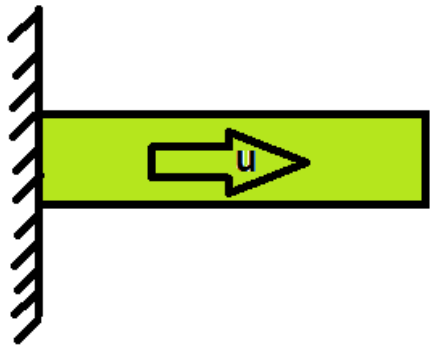


Rarefaction wave structure

Illustration: inverse impact problem (uniaxial approximation):

impact velocity u_0 ,

initial parameters $p_0 = S_0 = 0$, EOS: Mi-Grunaisen.



	aluminum	copper	berillium
critical parameters			
$(u_0)_Y^-$, m/s	33.82	4.73	18.1
ρ_Y^-, kg/m^3	2765.43	8921.07	1842.98
p_Y^-, GPa	-0.410	-0.140	-0.333
σ_Y^-, GPa	0.604	0.200	0.553

Hydrodynamical stage: flux function

Relative system of coordinates that moves with the interface:

$$\vec{Q}_i^{\sigma} \text{ and } \vec{Q}_{\sigma(i)}^{\sigma} \; : \quad u_n \to u_n - U_n$$

Calculate the *relative flux*: $\vec{\Phi}^* = \vec{F}\left(0, \vec{Q}_i^{\sigma}, \vec{Q}_{\sigma(i)}^{\sigma}\right)$

Gas dynamics approaches: Godunov, HLLE, Rusanov,etc.:

$$\vec{\Phi}^* = \frac{1}{2}\left[\vec{F}_i^{\sigma} + \vec{F}_{\sigma(i)}^{\sigma} - \rho_{\sigma}^{F}\left(\vec{Q}_{\sigma(i)}^{\sigma} - \vec{Q}_i^{\sigma}\right)\right]$$

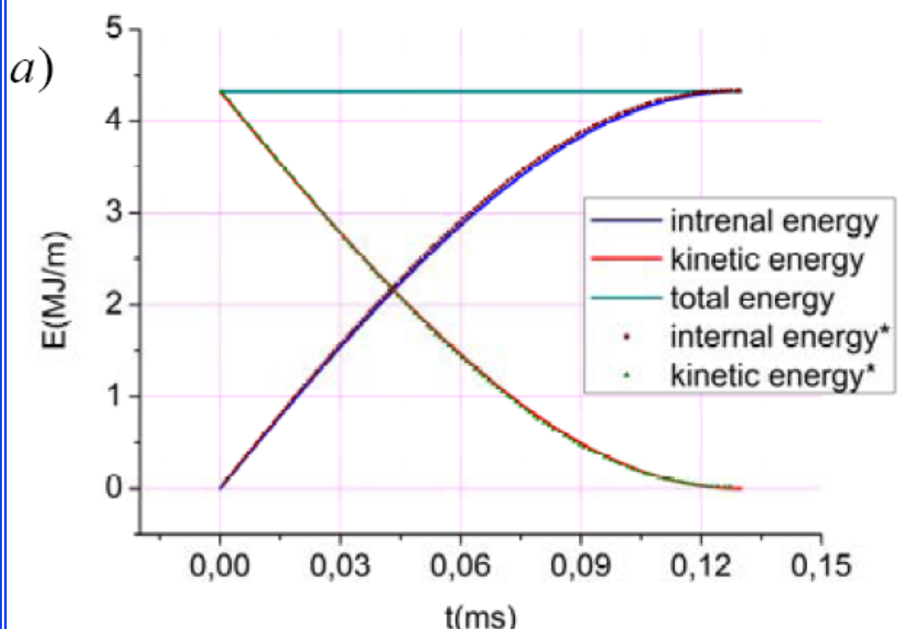
Absolute flux $\vec{\Phi}$: recalculation of the components of the relative flux $\vec{\Phi}^*$

Lagrangian stage: $\dfrac{\partial \vec{q}}{\partial t} = \vec{H}_m$: for $0<t<\Delta t$ with $\vec{q} = \vec{q}^{\,*}$ at $t=0$

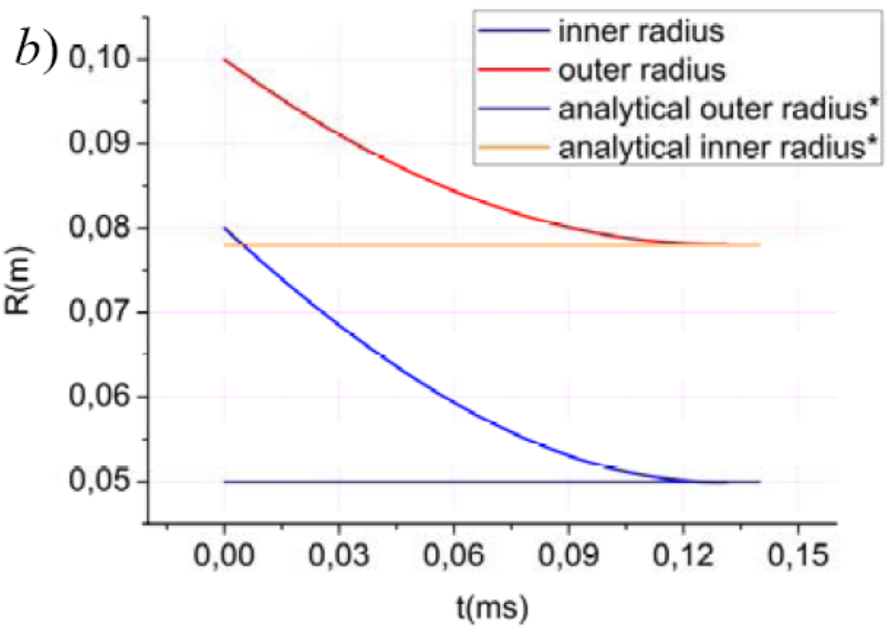
Grid: frozen Calculation $\vec{H}_m$: LSM

Numerical results

Cylindrical beryllium *shell collapse* (B. P. Howell, G. I. Ball: JPC: 2002): converting kinetic energy to internal energy by the mechanism of plastic distortion: moving grid to track radii.



histories of energy distribution



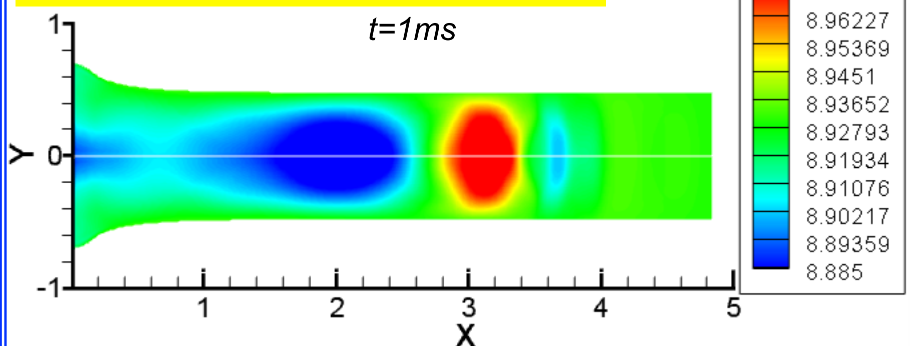
inner and outer radius

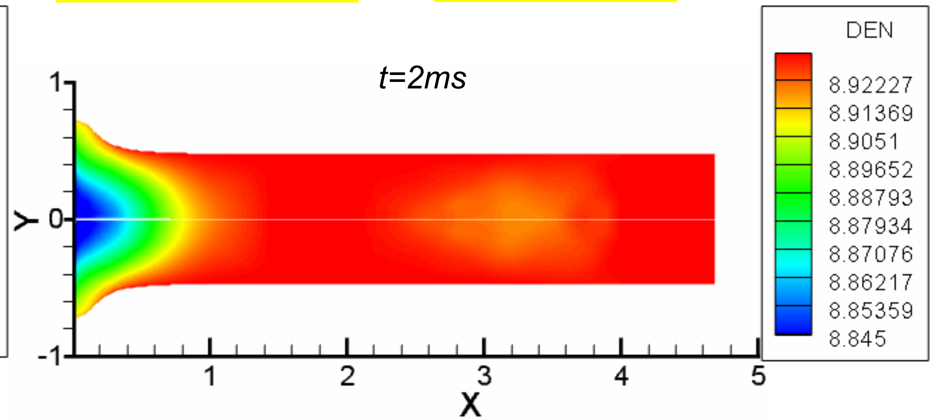
Numerical results: Taylor impact problem

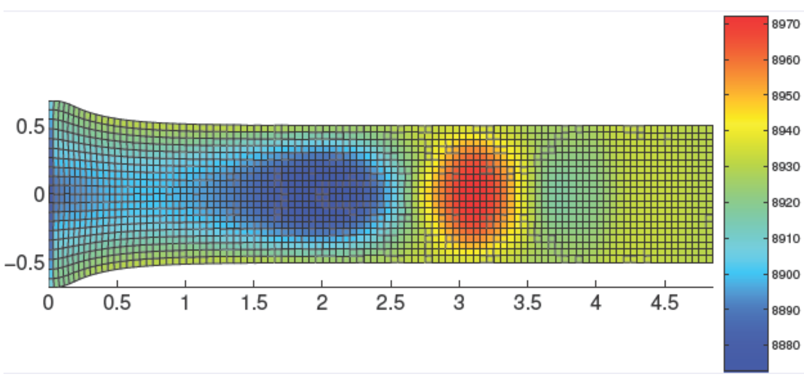
material - Cu
impact velocity- ***150m/s***
time– 0,002 s
size: L = 5m r = 0,5m
EOS – Mie-Gruneisen
model – Prandtl - Reus
numerical flux- Rusanov
moving grid

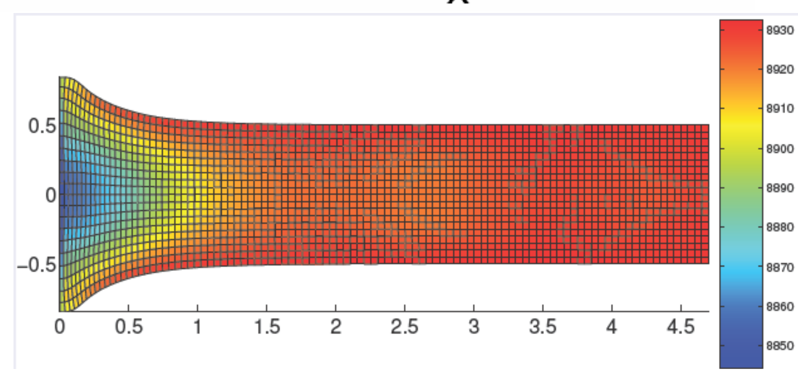
$\rho_0 = 8930 \ кг/м^3$
$P_0 = 0 \ ГПа$
$S_{ij} = 0 \ ГПа$
$a_0 = 3940 \ м/с$

$\Gamma_0 = 2$
$s = 1.49$
$\mu = 45 \ ГПа$
$Y_0 = 90 \ ГПа$









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*| P.-H. Maire, R. Abgrall, J. Breil, R. Loub`ere and B. Rebourcet «A high-order cell-centered Lagrangian scheme for solving two-dimensional elastic-plastic flows» Multimat 2011, September 5-9

Стержень Тейлора

material - Cu
impact velocity - 227м/с
time– 0,00008 с
size : L = 3.25см r = 0,325см
EOS– “log”
model – Prandtl - Reus
numerical flux- Rusanov

$K = 130$

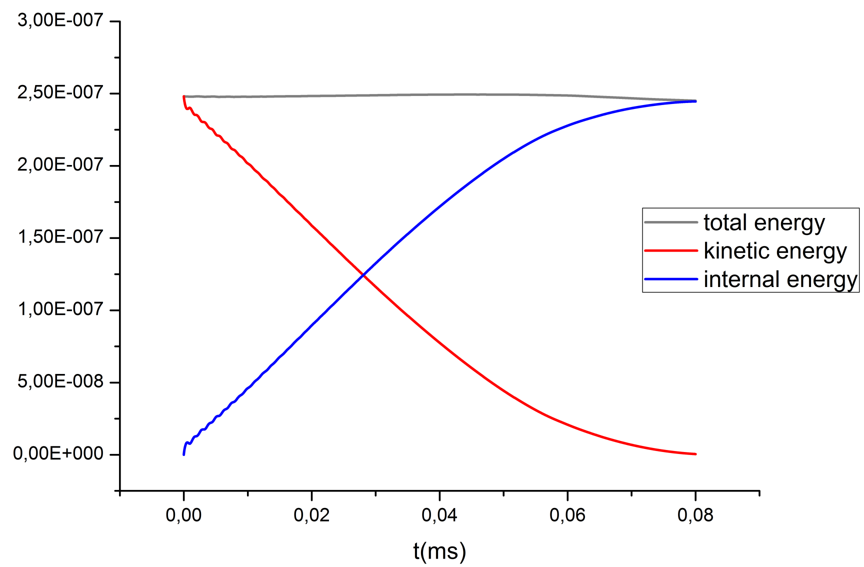
$Y = 0.04$

$\mu = 43.3$

$\alpha = 5.1 * 10^{-5}$

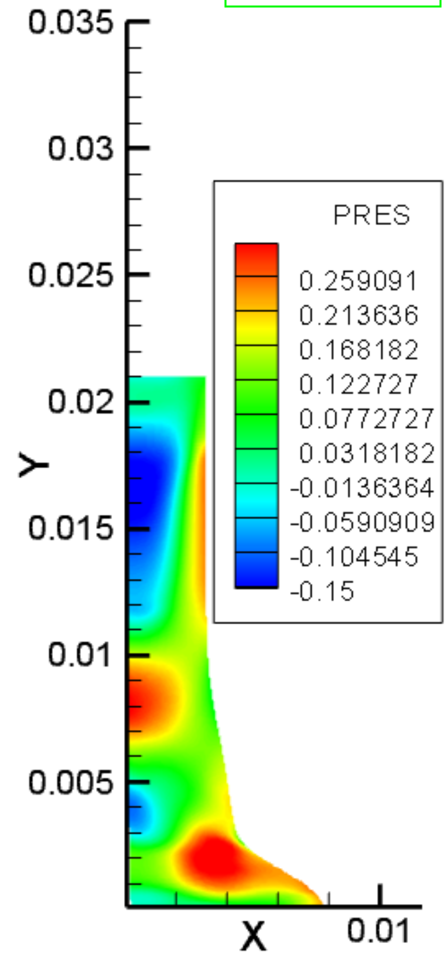
$c_v = 385\,Дж/(кг * K)$

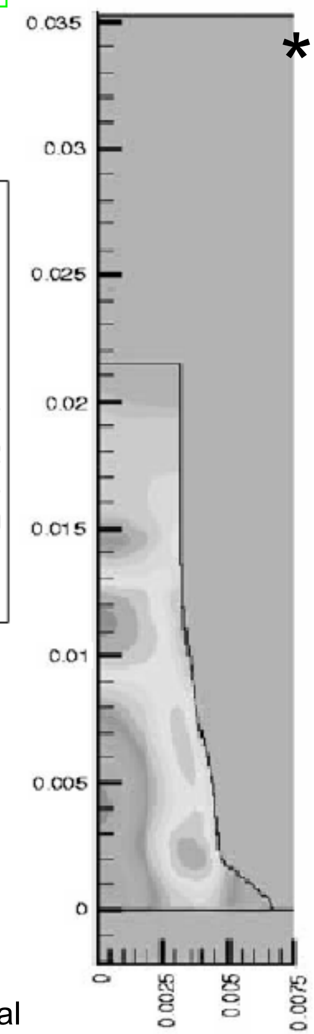
$\rho_0 = 8930\,кг/м^3$



histories of the energy

$t = 80 * 10^{-6} c$





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* H.S. Udaykumar, L. Tran, D.M. Belk, K.J. Vanden, «An Eulerian method for computation of multimaterial impact with ENO shock-capturing and sharp interfaces» Journal of Computational Physics 186 (2003) 136–177