Solid-fluid diffuse interface model

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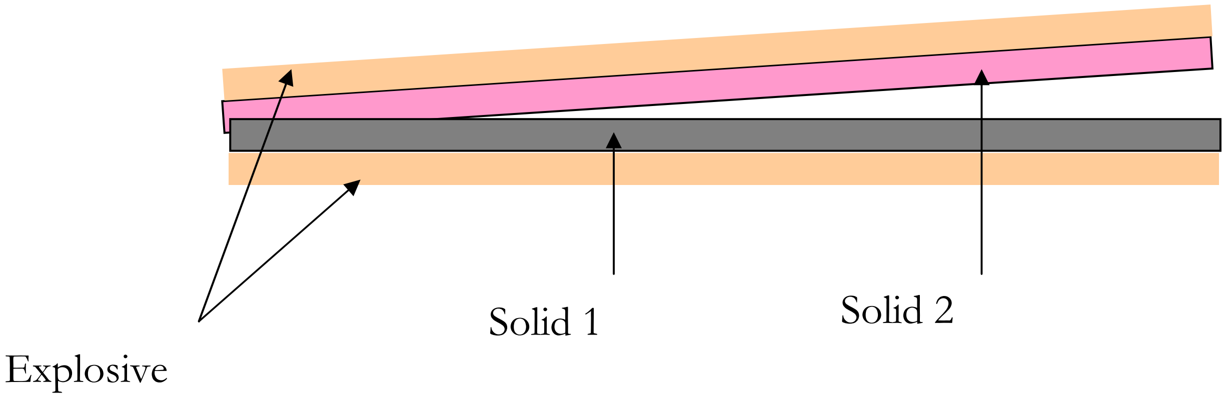
Joint work with N. Favrie, AMU

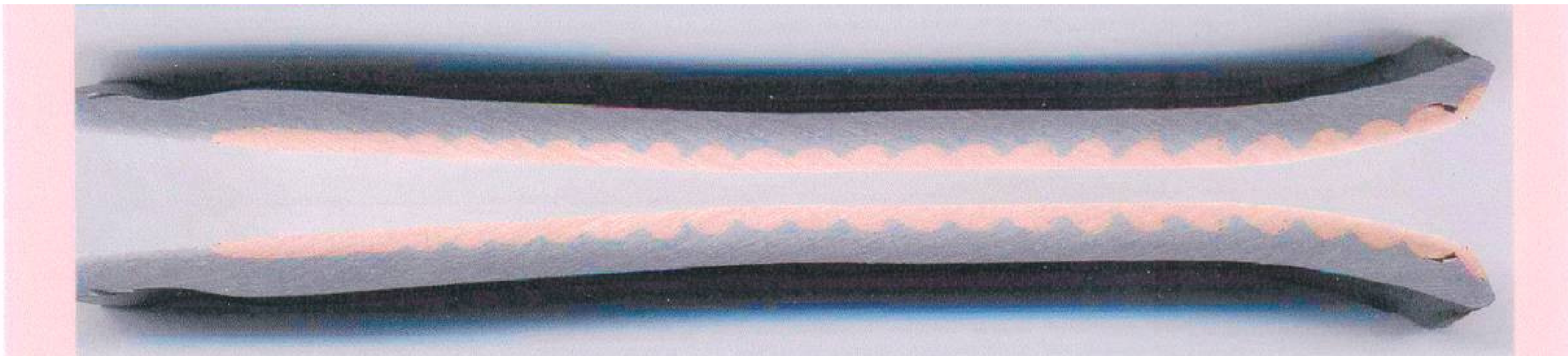
Paris VI, 14-16 February 2011

Motivation

- Explosion welding
- High intensity focused ultrasound

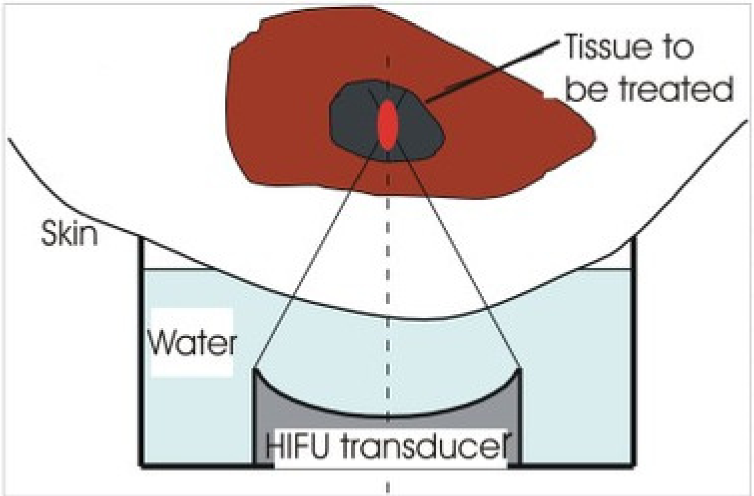
Explosion welding of metals





Experimental results by Professor V. I. Mali (Lavrentyev Institute of Hydrodynamics)

High intensity focused ultrasound (HIFU)



The potential of HIFU as a non-invasive surgical tool has been demonstrated recently for the treatment of tumours of the liver, kidney and pancreas.

The main modeling problem

Two-phase coupling of a good « elastic-plastic model » with Euler equations

Hypoelastic Wilkins's model for elastic-plastic solids (basic model in CTH code of Sandia National Laboratories, USA)

Mass conservation law
$$\frac{\partial \rho}{\partial t} + div(\rho \mathbf{v}) = 0$$

Momentum conservation law
$$\frac{\partial \rho \mathbf{v}}{\partial t} + div(\rho \mathbf{v} \otimes \mathbf{v} + p\mathbf{I} - \mathbf{S}) = 0$$

Energy conservation law
$$\frac{\partial \rho E}{\partial t} + div((\rho E + p)\mathbf{v} - S\mathbf{v}) = 0, \quad E = \varepsilon(\rho,\eta) + \frac{1}{2}|\mathbf{v}|^2 + \frac{S:S}{4\rho\mu(\rho,\eta)}$$

Evolution equation for S
$$\frac{D_J S}{Dt} + \frac{2}{3}\mu\, tr(D) I - 2\mu D = 0, \quad D = \frac{1}{2}\left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right)^T\right)$$

Jaumann derivative
$$\frac{D_J S}{Dt} = \frac{DS}{Dt} + SW - WS, \quad W = \frac{1}{2}\left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right)^T\right)$$

Material derivative
$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$$

Entropy equation
$$T\frac{D\eta}{Dt} = \frac{S:S}{2(\rho\mu)^2}\frac{D(\rho\mu)}{Dt}$$

Plan

I. Hyperelastic model (Godunov, 1978, Miller and Colella, 2001)

II. Extension to diffuse solid-fluid interfaces

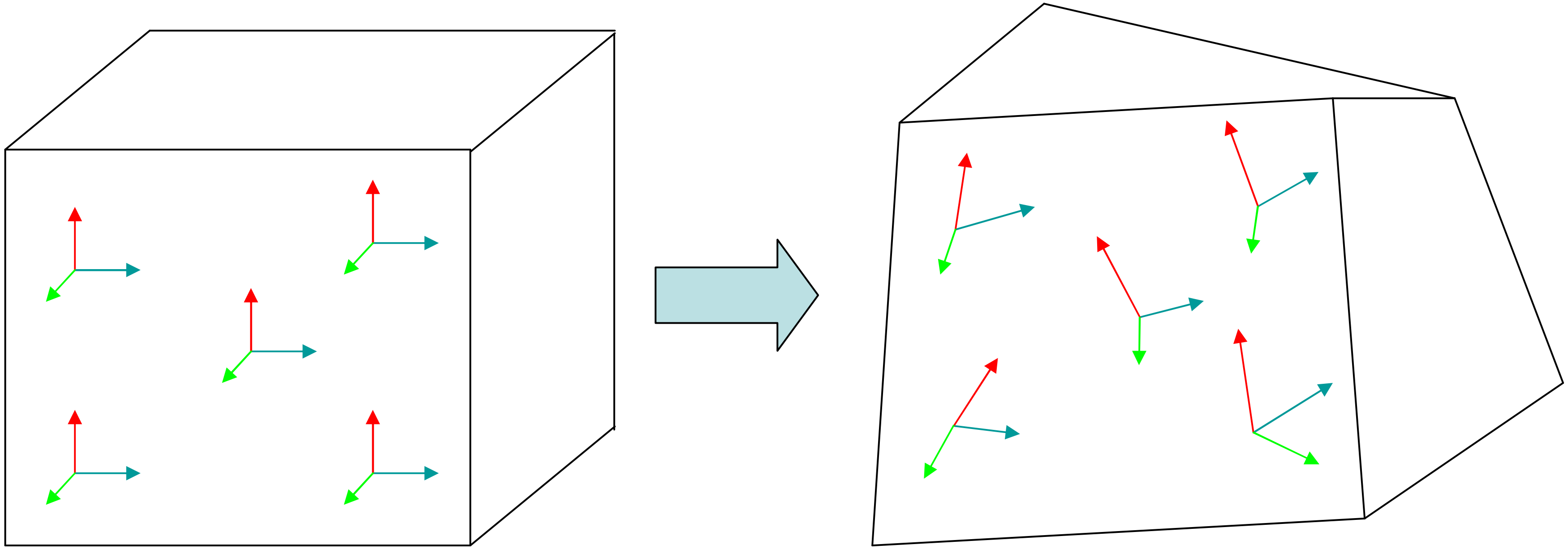
III. Visco-plasticity

IV. Numerical examples

I. Hyperelastic model (modified)

A material is *hyperelastic* if the stress tensor is defined in terms of a stored energy function.

Basic idea



- Use a local cobasis at each point of the solid.
- Determine evolution equations for the cobasis vectors.
- Link the stress tensor to the cobasis vectors.

Definitions

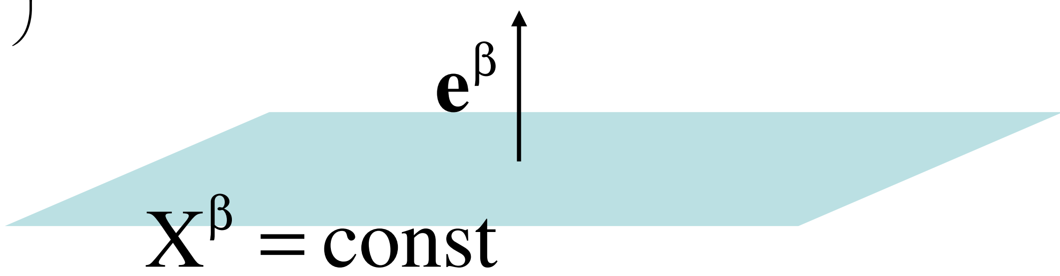
Deformation gradient $\mathbf{F} = \dfrac{\partial \mathbf{x}}{\partial \mathbf{X}}$

$\mathbf{X}$ Lagrangian coordinates

$\mathbf{x}$ Eulerian coordinates

Cobasis $\left(\mathbf{F}^{-1}\right)^{\mathrm{T}} = \left(\mathbf{e}^1 \quad \mathbf{e}^2 \quad \mathbf{e}^3\right) = \left(\nabla \mathrm{X}^1, \nabla \mathrm{X}^2, \nabla \mathrm{X}^3\right)$

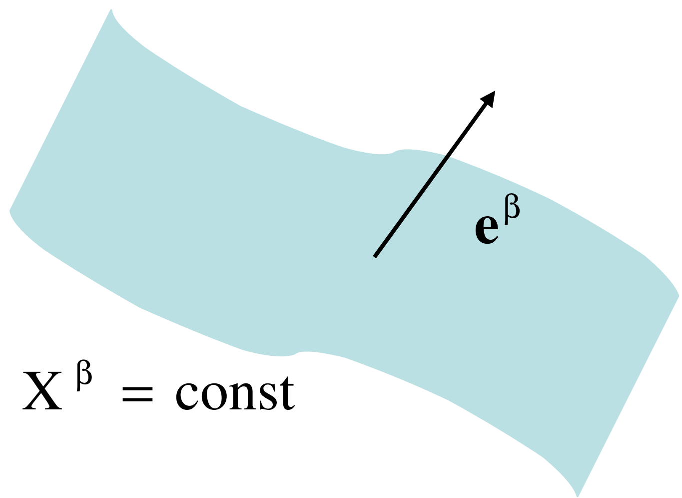
$$\mathbf{X} = \begin{pmatrix} X^1 \\ X^2 \\ X^3 \end{pmatrix}, \qquad \mathbf{x} = \begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix}$$



Evolution of the local cobasis

Evolution of the Lagrangian coordinates $\dfrac{DX^{\beta}}{Dt} = 0, \; \dfrac{D}{Dt} = \dfrac{\partial}{\partial t} + \mathbf{v} \cdot \nabla,$

Evolution of the local cobasis $\nabla\left(\dfrac{DX^{\beta}}{Dt}\right) = 0 \Longrightarrow \dfrac{\partial \mathbf{e}^{\beta}}{\partial t} + \nabla(\mathbf{v} \cdot \mathbf{e}^{\beta}) = 0, \quad \mathrm{rot}\,\mathbf{e}^{\beta} = 0$



Definitions

Finger tensor (inverse of the left Cauchy - Green tensor) $\mathbf{G} = \left(\mathbf{F}^{\mathrm{T}}\right)^{-1}\mathbf{F}^{-1} = \sum_{\beta=1}^{3} \mathbf{e}^{\beta} \otimes \mathbf{e}^{\beta}$

Evolution equation for the Finger tensor $\frac{\mathrm{D}\,\mathbf{G}}{\mathrm{Dt}} + \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right)^{\mathrm{T}} \mathbf{G} + \mathbf{G}\,\frac{\partial \mathbf{v}}{\partial \mathbf{x}} = 0$

Alternative equations $\frac{\partial \mathbf{e}^{\beta}}{\partial t} + \nabla(\mathbf{v} \cdot \mathbf{e}^{\beta}) = 0, \quad \mathrm{rot}\,\mathbf{e}^{\beta} = 0, \quad \beta = 1,2,3.$

Isotropic solids

The specific internal energy $e(\mathbf{G},\eta)$ is supposed to be an isotropic function of $\mathbf{G}$

$$e = e(J_1, J_2, J_3, \eta), \quad J_i = \mathrm{tr}(\mathbf{G}^i)$$

Stress tensor (Murnaghan):

$$\sigma = -2\rho \frac{\partial e}{\partial \mathbf{G}} \mathbf{G} = -2\rho \left(\frac{\partial e}{\partial J_1} \mathbf{I} + 2 \frac{\partial e}{\partial J_2} \mathbf{G} + 3 \frac{\partial e}{\partial J_3} \mathbf{G}^2 \right) \mathbf{G} = [\sigma_{ij}], \ \sigma = \sigma^T$$

Conservative model of elasticity

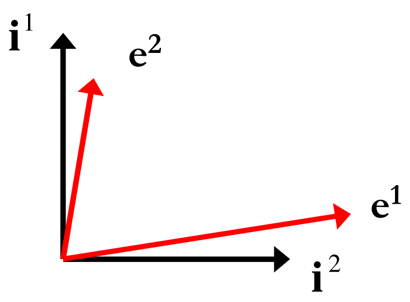
Mass equation $\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \mathbf{v}) = 0$

Momentum equation $\frac{\partial \rho \mathbf{v}}{\partial t} + \mathrm{div}(\rho \mathbf{v} \otimes \mathbf{v} - \boldsymbol{\sigma}) = 0$

Energy equation $\frac{\partial \rho E}{\partial t} + \mathrm{div}(\rho E \mathbf{v} - \boldsymbol{\sigma} \cdot \mathbf{v}) = 0, \quad E = e + \frac{|\mathbf{v}|^2}{2}$

Cobasis $\frac{\partial \mathbf{e}^\beta}{\partial t} + \nabla(\mathbf{v} \cdot \mathbf{e}^\beta) = 0$ and $\mathrm{rot}(\mathbf{e}^\beta) = 0$

with $\mathbf{e}^\beta\big|_{t=0} = \mathbf{i}^\beta$ where $\mathbf{i}^\beta$ are the vector of the Cartesian base



Equation of state (EOS)

Separate form

$$e = \underbrace{e^h(\rho,\eta)}_{\text{Hydrodynamic}} + \underbrace{e^e(\mathbf{g})}_{\text{Shear}} \quad \text{with} \quad \mathbf{g} = \frac{\mathbf{G}}{|\mathbf{G}|^{1/3}}$$

$$e^h(\rho,p) = \frac{p+\gamma p_\infty}{\rho(\gamma-1)}$$

$$e^e(\mathbf{g}) = \frac{\mu_s}{4\rho_0}\,\mathrm{tr}\left((\mathbf{g}-\mathbf{I})^2\right)$$

The stress tensor can be written as:

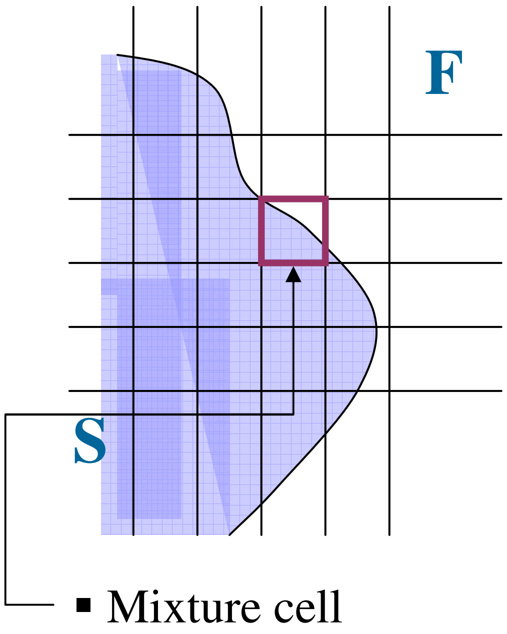
$$\boldsymbol{\sigma} = -2\rho\frac{\partial e}{\partial \mathbf{G}}\mathbf{G} = -p\mathbf{I} + \mathbf{S} = -p\mathbf{I} - \mu_s\left[\frac{\mathbf{G}^2 - \frac{J_2}{3}\mathbf{I}}{|\mathbf{G}|^{1/6}} - \left(\mathbf{G} - \frac{J_1}{3}\mathbf{I}\right)|\mathbf{G}|^{1/6}\right]$$

$$J_i = \mathrm{tr}\left(\mathbf{G}^i\right)$$

Hyperbolicity

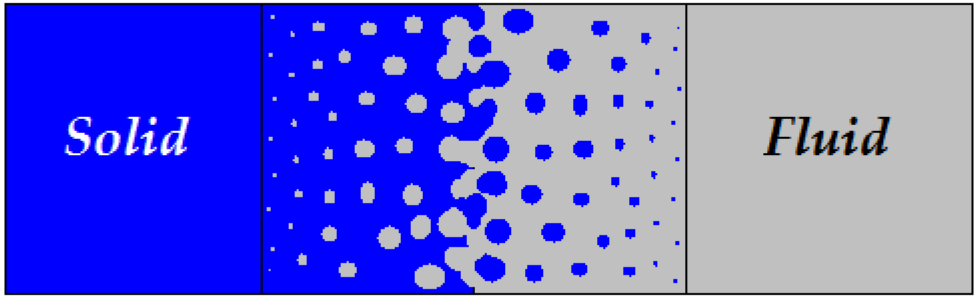
In 1D case the equations are hyperbolic in all domain of parameters

II. Modeling solid-fluid interfaces



What equation of state should we use in the mixture cells ?

Mixture cell as a multiphase continuum



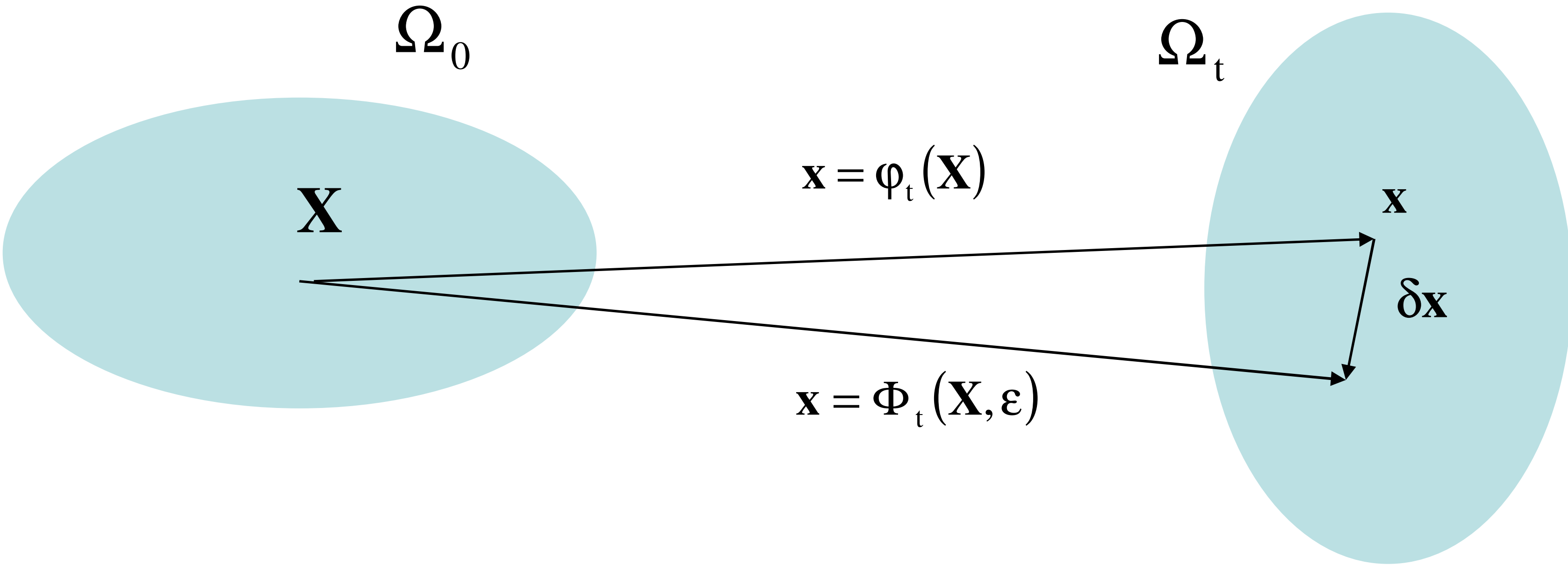
New state variable – volume fraction.

Fluid-fluid interfaces : Karni, Abgrall, Saurel,…

How do we obtain the model?

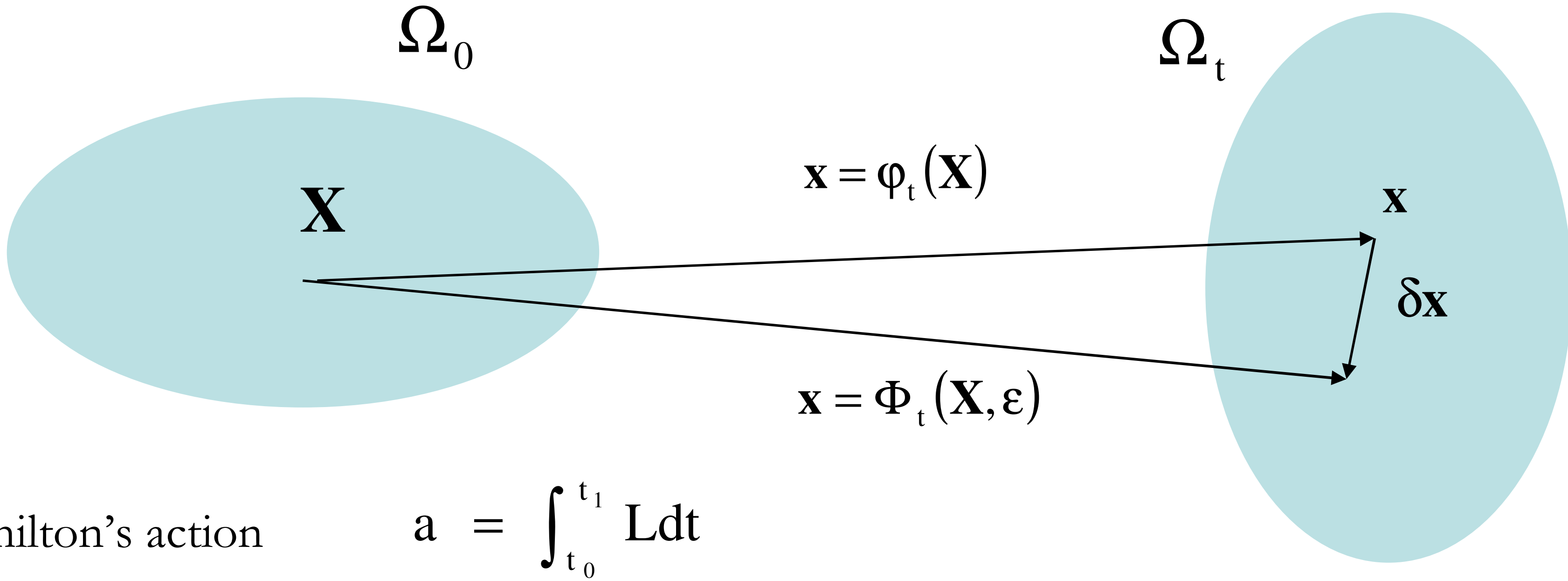
- The equilibrium model is obtained through Hamilton's principle
- The non-equilibrium model is constructed which is compatible with the entropy inequality.

Hamilton's principle (1)



Virtual displacement $$\delta\mathbf{x} = \left.\frac{\partial}{\partial\varepsilon}\Phi_t(\mathbf{X}, \varepsilon)\right|_{\varepsilon=0}$$

Hamilton's principle (2)



Hamilton's action $\quad a = \int_{t_0}^{t_1} L dt$

Hamilton's principle : $\quad \delta a = 0 \quad$ for any virtual displacement vanishing at the boundary $\partial([t_0, t_1] \times \Omega_t)$

Hamilton's principle (3)

Lagrangian $$L = \int_{\Omega_t} \left(\rho \frac{|\mathbf{v}|^2}{2} - \rho e \right) d\Omega$$

$$e = Y_s \left(e_s^h(\rho_s, \eta_s) + e_s^e\left(\frac{G}{|G|^{1/3}} \right) \right) + Y_f e_f(\rho_f, \eta_f), \quad G = \sum_\beta \mathbf{E}^\beta \otimes \mathbf{E}^\beta$$

Constraints $$\frac{DY_s}{Dt} = 0, \quad \frac{DY_f}{Dt} = 0, \quad Y_s = \frac{\alpha_s \rho_s}{\rho}, \quad Y_f = \frac{\alpha_f \rho_f}{\rho}, \quad \rho = \alpha_s \rho_s + \alpha_f \rho_f, \quad \alpha_f + \alpha_s = 1$$

$$\frac{D\eta_s}{Dt} = 0, \quad \frac{D\eta_f}{Dt} = 0, \quad \frac{\partial \mathbf{E}^\beta}{\partial t} + \nabla(\mathbf{v} \cdot \mathbf{E}^\beta) = 0, \quad \mathrm{rot}\mathbf{E}^\beta = 0, \quad \rho = \rho_0 (\det(\mathbf{G}))^{1/2}$$

Hamilton's principle (4)

1. Lagrangian variations in terms of virtual (infinitesimal) displacements :

$$\delta\rho = -\rho \,\mathrm{div}(\delta\mathbf{x}), \quad \delta\mathbf{v} = \frac{D\delta\mathbf{x}}{Dt}, \quad \delta\mathbf{E}^{\beta} = -\left(\frac{\partial\delta\mathbf{x}}{\partial\mathbf{x}}\right)^{T}\mathbf{E}^{\beta},$$

$$\delta G = \delta\left(\sum \mathbf{E}^{\beta}\otimes\mathbf{E}^{\beta}\right) = -\left(\frac{\partial\delta\mathbf{x}}{\partial\mathbf{x}}\right)^{T} G - G\left(\frac{\partial\delta\mathbf{x}}{\partial\mathbf{x}}\right), \quad \delta\eta_{\beta} = 0, \quad \delta Y_{\beta} = 0, \quad \beta = s, f$$

2. Variation of the volume fraction

Equilibrium solid-fluid diffuse interface model

Cobasis $$\frac{\partial \mathbf{E}^{\beta}}{\partial t} + \nabla\left(\mathbf{E}^{\beta}\mathbf{v}\right) = -\mathrm{rot}\left(\mathbf{E}^{\beta}\right) \wedge \mathbf{v}, \quad \mathrm{rot}\mathbf{E}^{\beta} = 0$$

Mass $$\frac{\partial \alpha_f \rho_f}{\partial t} + \mathrm{div}\left(\alpha_f \rho_f \mathbf{v}\right) = 0 \qquad \frac{\partial \alpha_s \rho_s}{\partial t} + \mathrm{div}\left(\alpha_s \rho_s \mathbf{v}\right) = 0$$

Momentum $$\frac{\partial \rho \mathbf{v}}{\partial t} + \mathrm{div}\left(\rho \mathbf{v} \otimes \mathbf{v} - \left(\alpha_s \boldsymbol{\sigma}_s + \alpha_f \boldsymbol{\sigma}_f\right)\right) = 0, \quad \rho = \alpha_s \rho_s + \alpha_f \rho_f$$

Total energy $$\frac{\partial \rho E}{\partial t} + \mathrm{div}\left(\rho E \mathbf{v} - \left(\alpha_s \boldsymbol{\sigma}_s + \alpha_f \boldsymbol{\sigma}_f\right)\mathbf{v}\right) = 0, \quad E = Y_s e_s + Y_f e_f + \frac{1}{2}\left|\mathbf{v}\right|^2$$

Volume fraction $$p_s - p_f = 0$$

Entropies $$\frac{d\eta_s}{dt} = 0, \quad \frac{d\eta_f}{dt} = 0$$

Non-equilibrium solid-fluid diffuse interface model

Dissipation functional

$$V = \int_{\Omega} \frac{1}{2\mu_0} \left(\frac{D\alpha_s}{Dt} \right)^2 d\Omega$$

Relaxation equation

$$p_s - p_f = \frac{\delta V}{\delta\left(\frac{D\alpha_s}{Dt} \right)} = \frac{1}{\mu_0} \frac{D\alpha_s}{Dt}$$

Non-equilibrium solid-fluid diffuse interface model

Cobasis
$$\frac{\partial \mathbf{E}^{\beta}}{\partial t} + \nabla\left(\mathbf{E}^{\beta}\mathbf{v}\right) = -\mathrm{rot}\left(\mathbf{E}^{\beta}\right)\wedge \mathbf{v}$$

Mass
$$\frac{\partial \alpha_g \rho_g}{\partial t} + \mathrm{div}\left(\alpha_g \rho_g \mathbf{v}\right) = 0 \qquad \frac{\partial \alpha_s \rho_s}{\partial t} + \mathrm{div}\left(\alpha_s \rho_s \mathbf{v}\right) = 0$$

Momentum
$$\frac{\partial \rho \mathbf{v}}{\partial t} + \mathrm{div}\left(\rho \mathbf{v} \otimes \mathbf{v} - \left(\alpha_s \boldsymbol{\sigma}_s + \alpha_g \boldsymbol{\sigma}_g\right)\right) = 0$$

Total energy
$$\frac{\partial \rho E}{\partial t} + \mathrm{div}\left(\rho E \mathbf{v} - \left(\alpha_s \boldsymbol{\sigma}_s + \alpha_g \boldsymbol{\sigma}_g\right)\mathbf{v}\right) = 0$$

Volume fraction
$$\frac{D\alpha_s}{Dt} = \mu_0\left(p_s - p_g\right)$$

Energies
$$\frac{\partial \alpha_s \rho_s e_s}{\partial t} + \mathrm{div}\left(\alpha_s \rho_s e_s \mathbf{v}\right) - \mathrm{tr}\left(\alpha_s \boldsymbol{\sigma}_s \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right) = \mu_0 p_I (p_s - p_g)$$

$$\frac{\partial \alpha_f \rho_f e_f}{\partial t} + \mathrm{div}\left(\alpha_f \rho_f e_f \mathbf{v}\right) - \mathrm{tr}\left(\alpha_f \boldsymbol{\sigma}_f \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right) = \mu_0 p_I (p_f - p_s)$$

Wellposedness

1. The entropy inequality is satisfied
2. In 1D case the equations are hyperbolic under natural convexity conditions (Godunov, Friedrichs, Lax).

III. Visco-plasticity : generic form

Mass equation $$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \mathbf{v}) = 0$$

Momentum equation $$\frac{\partial \rho \mathbf{v}}{\partial t} + \mathrm{div}(\rho \mathbf{v} \otimes \mathbf{v} - \boldsymbol{\sigma} \mathbf{v}) = 0$$

Energy equation $$\frac{\partial \rho E}{\partial t} + \mathrm{div}(\rho E \mathbf{v} - \boldsymbol{\sigma} \cdot \mathbf{v}) = 0$$

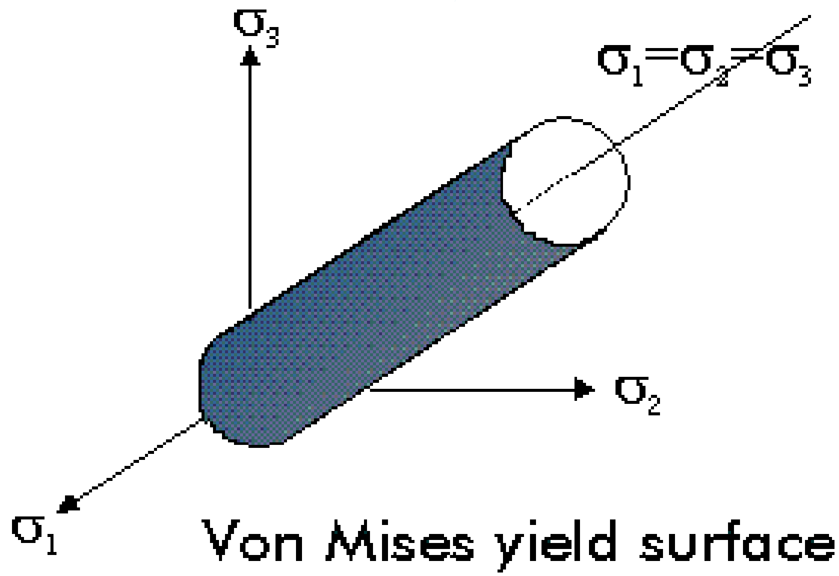
Cobasis equations $$\frac{D\mathbf{e}^{\beta}}{Dt} + \left(\frac{\partial \mathbf{v}}{\partial x}\right)^{T} \mathbf{e}^{\beta} + A^{\beta}{}_{\gamma}\mathbf{e}^{\gamma} = -\frac{1}{\tau_{rel}} \mathbf{R}\mathbf{e}^{\beta}, \quad A^{\beta}{}_{\gamma} = -A^{\gamma}{}_{\beta}$$

« Effective » local cobasis $\mathbf{e}^{\beta}$ and « effective » deformation gradient $\mathbf{F}^{-T} = (\mathbf{e}^{1}, \mathbf{e}^{2}, \mathbf{e}^{3})$

The symmetric tensor $\mathbf{R} = \mathbf{R}^{T}$ should be built in agreement with some basic principles :

- Should be compatible with the mass conservation law
- Should be compatible with the entropy inequality
- The intensity of shear stresses should decrease during the relaxation process
- Should be compatible with the von Mises yield criterion : $\mathbf{S} : \mathbf{S} \leq \frac{2}{3} Y^{2}$

Von Mises yield surface



Mass and entropy compatibility

Compatibility with the mass conservation law $\mathrm{tr}(\mathbf{R}) = 0$

Compatibility with the entropy inequality $\mathrm{tr}(\mathbf{SR}) \leq 0$

A sufficient condition is $\mathbf{R} = -a\mathbf{S}$ with $a > 0$

Lyapunov function

Let us consider the singular value decomposition $\mathbf{F}^{-1} = \mathbf{U}\mathbf{K}\mathbf{V}^{T}$

$\mathbf{V}$ and $\mathbf{U}$ are orthogonal matrices and $\mathbf{K}$ is a diagonal matrix

Hypothesis : The geometry is « frozen » during the relaxation process i.e. $\frac{d\mathbf{U}}{dt} = \frac{d\mathbf{V}}{dt} = 0$

Consequence : $$\frac{d\mathbf{S}:\mathbf{S}}{dt} = \frac{d}{dt}\left(\sum_{\alpha} S_{\alpha}{}^{2}\right) < 0$$

The trajectories are attracted to the yield surface !

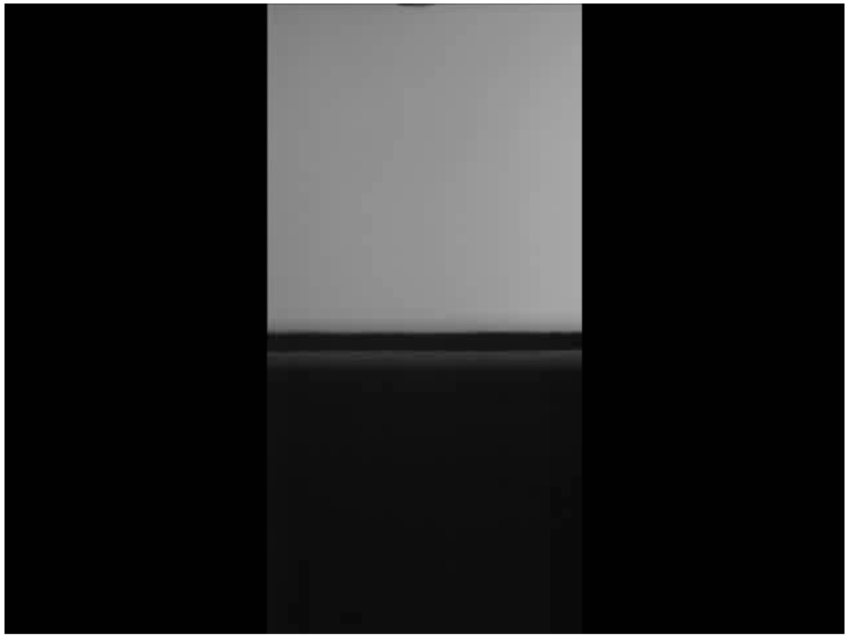
Diffuse solid-fluid interfaces

One can generalize this approach to the case of plastic deformations in solids.

IV. Examples

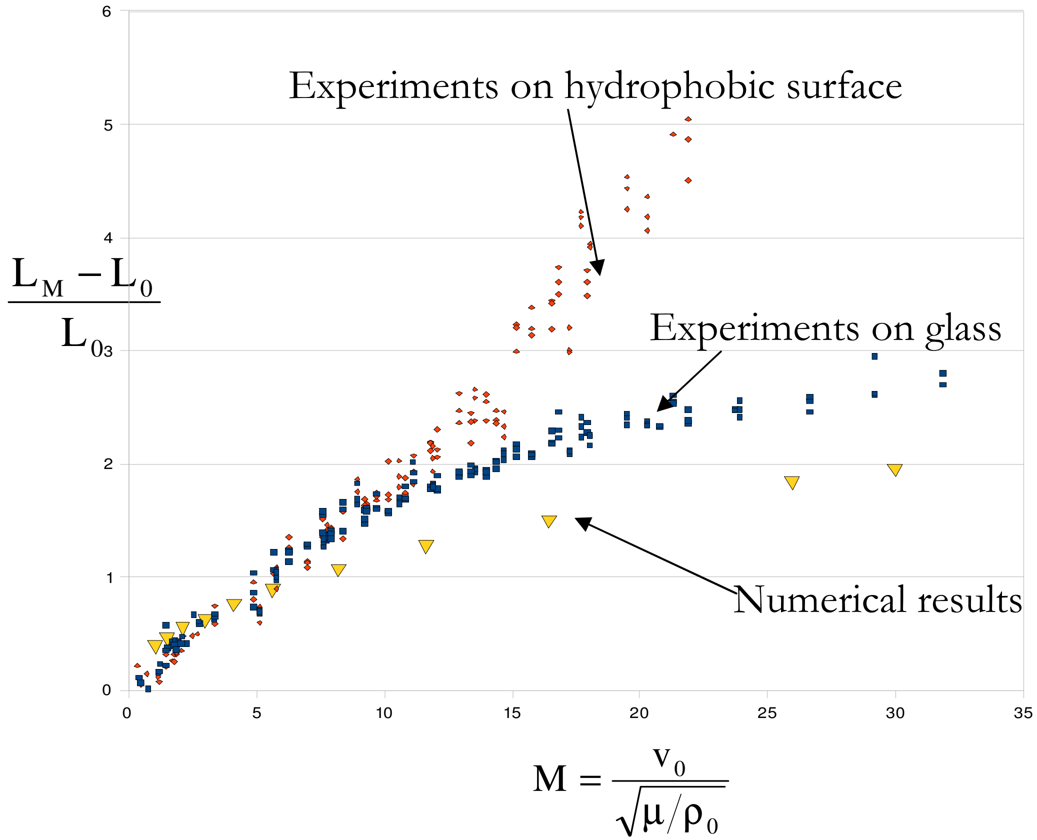
Jelly impact

Impact velocity: 1m/s

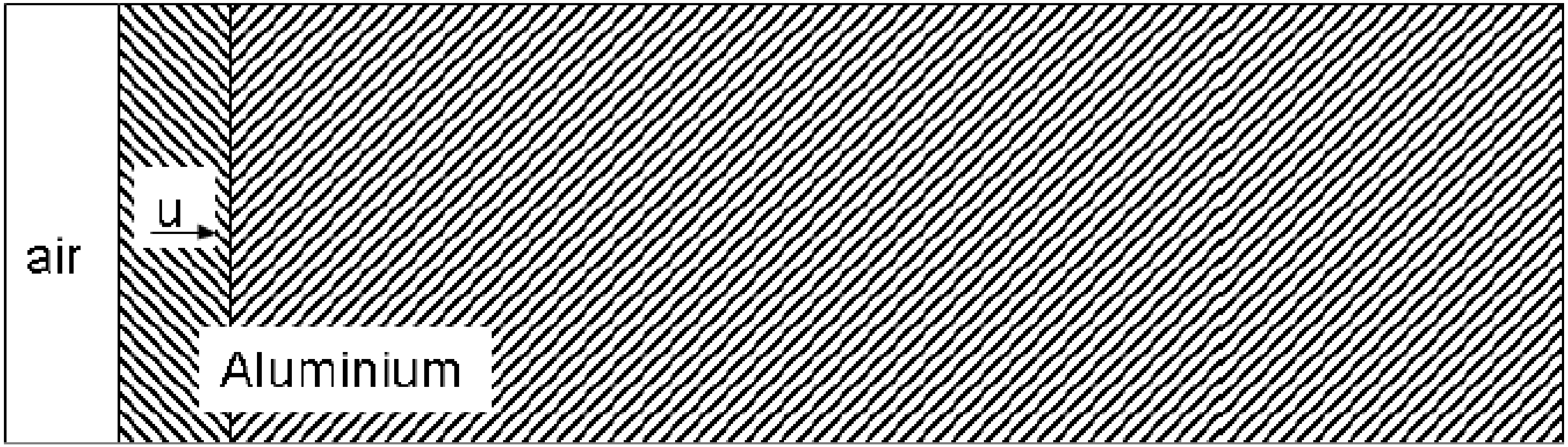


Experiments realized in Marseille (IUSTI) by Li-Hua Luu and Yoël Forterre

Jelly impact

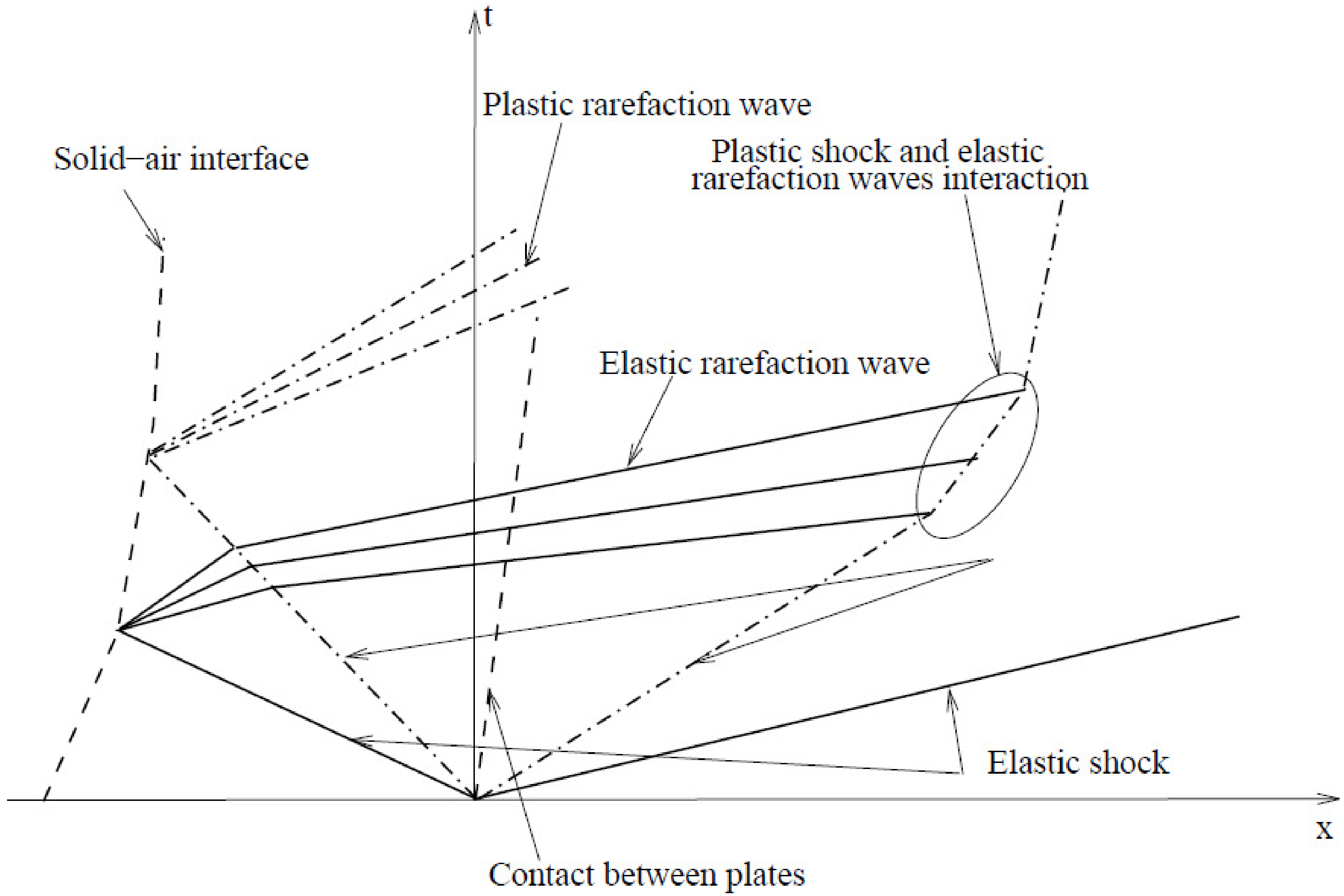


Wilkins flying plate problem

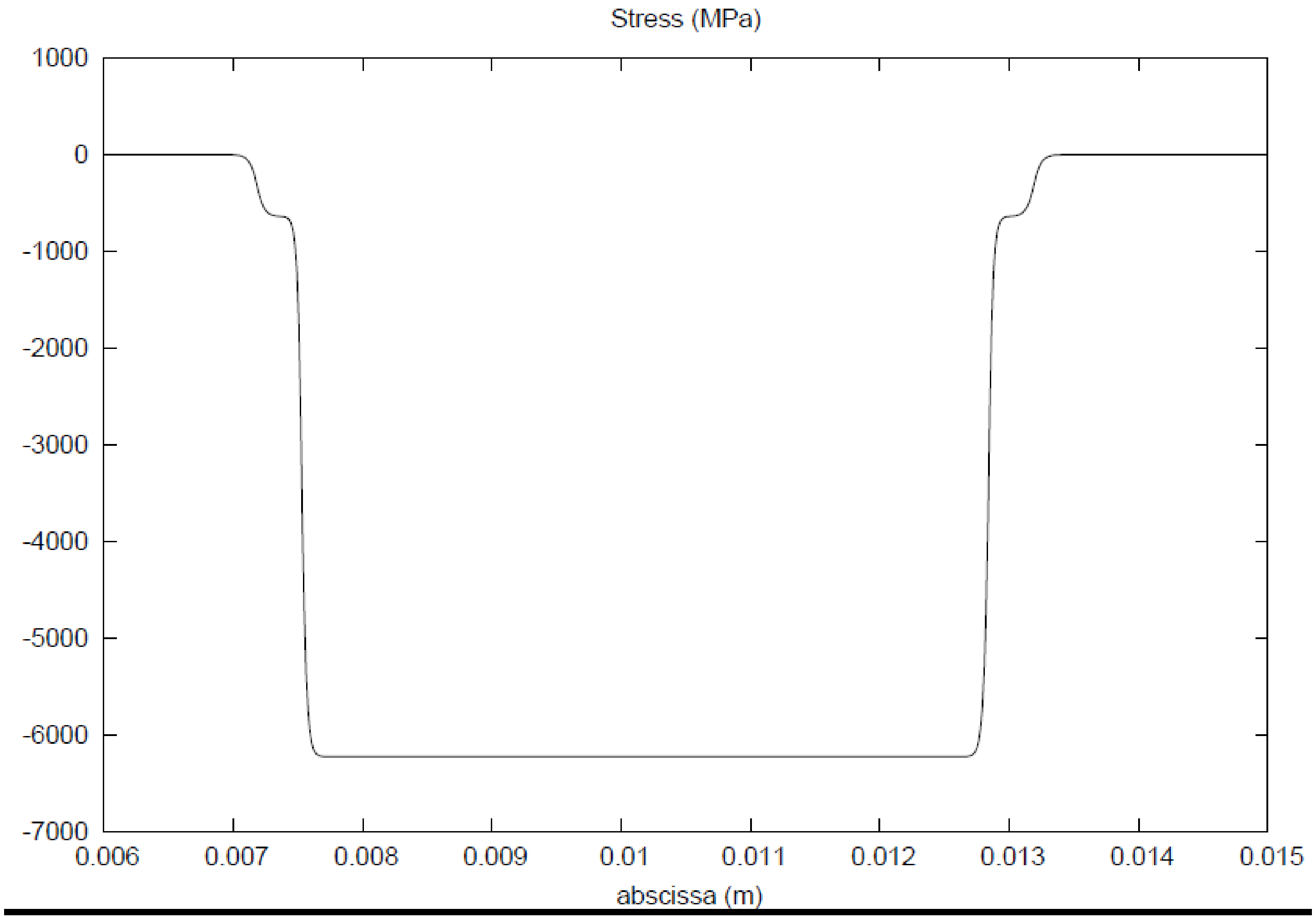


$$u = 800 \ m/s$$

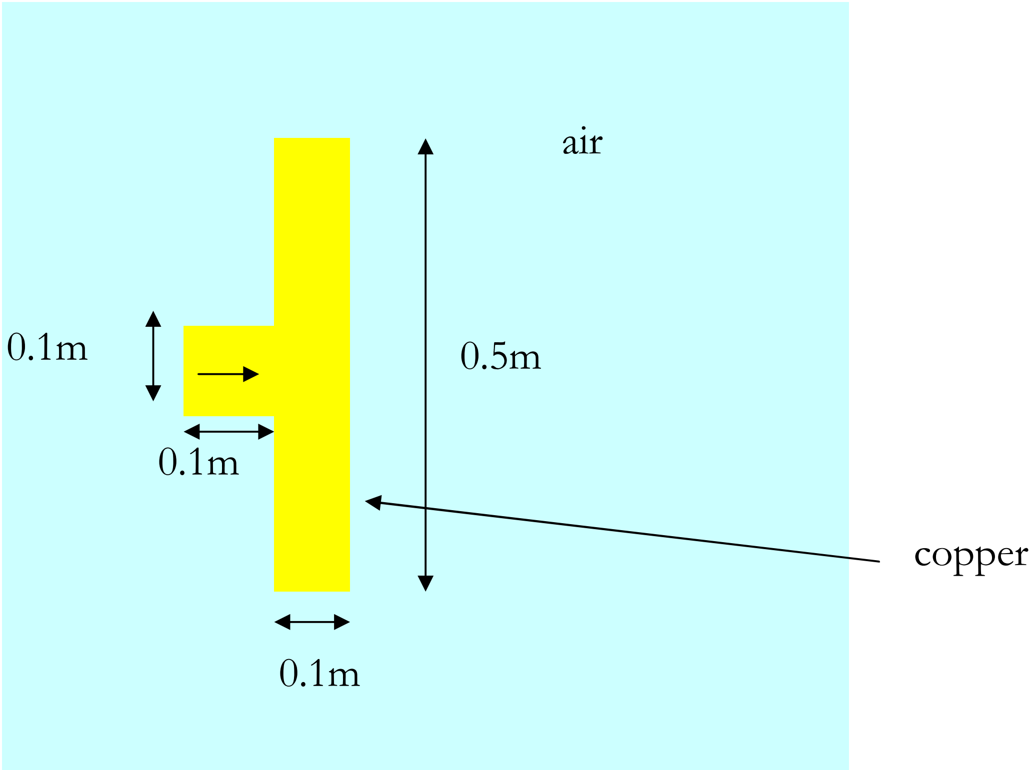
Wave interaction



Stress distribution



2D Impact



$\gamma_s = 4.22$

$p_{\infty s} = 34.2\ \text{GPa}$

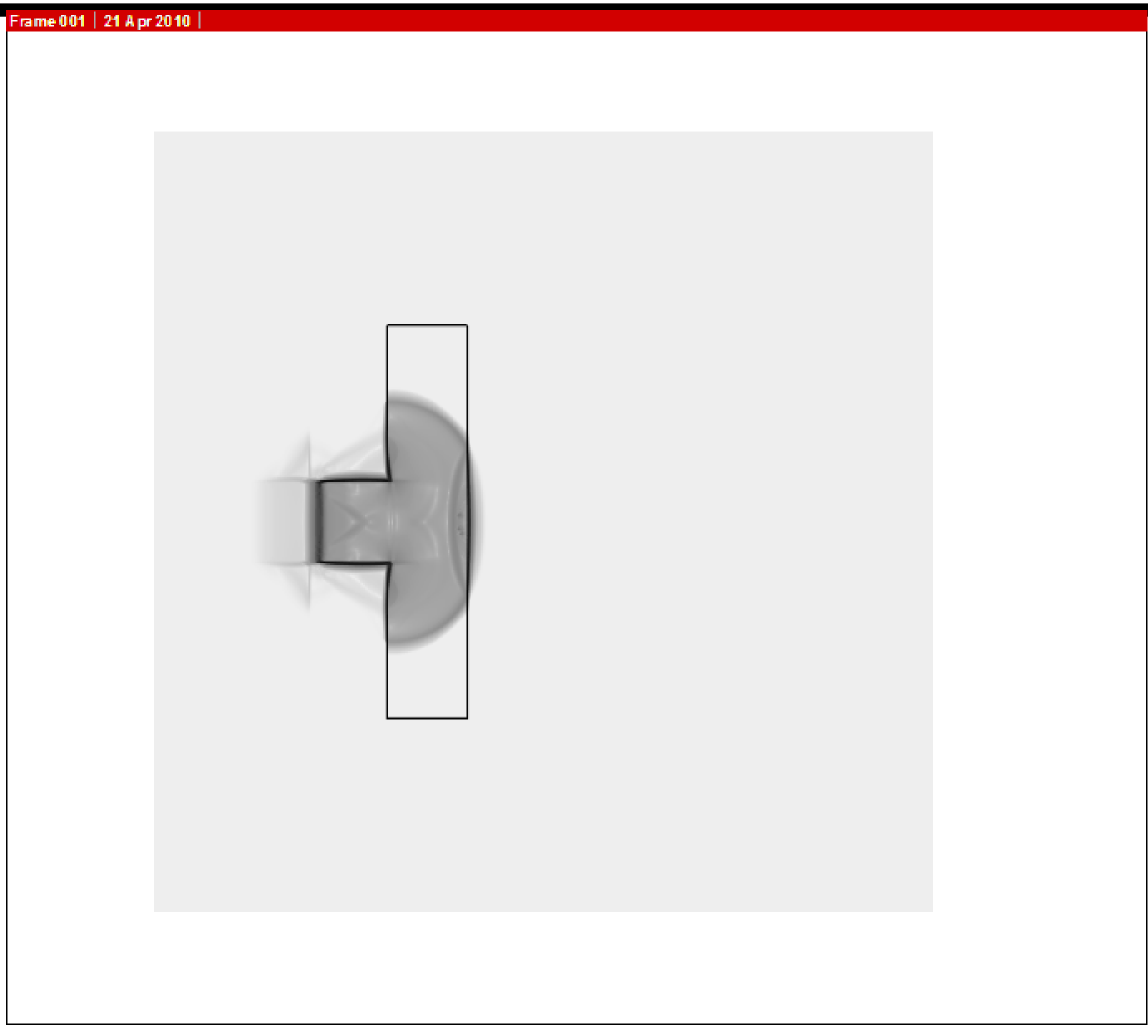
$\rho_s = 8900\ \text{kg}/\text{m}^3$

$\mu_s = 92\ \text{GPa}$

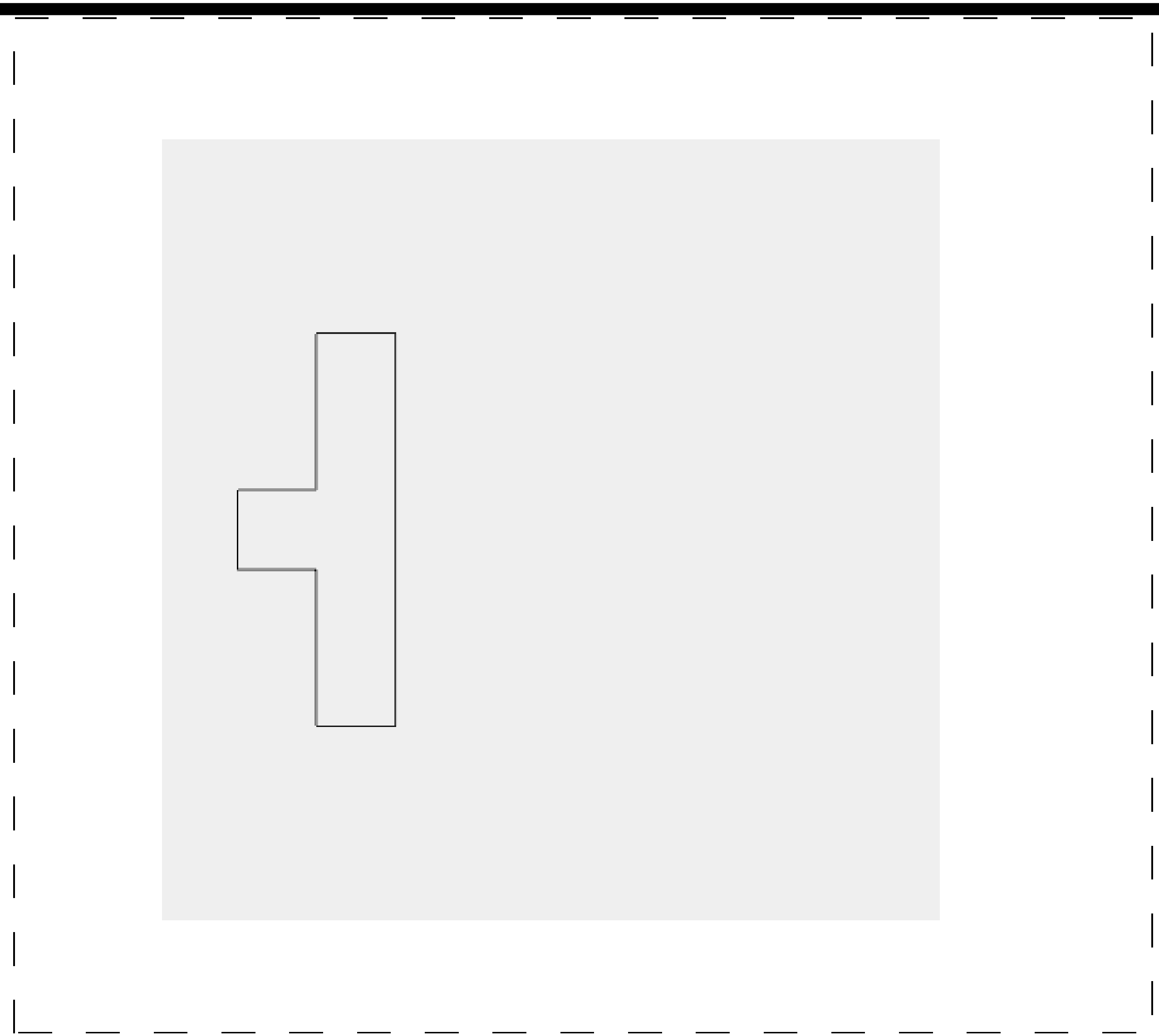
$Y_s = 2.49\ \text{GPa}$

A copper projectile impacts a copper plate at 800m/s

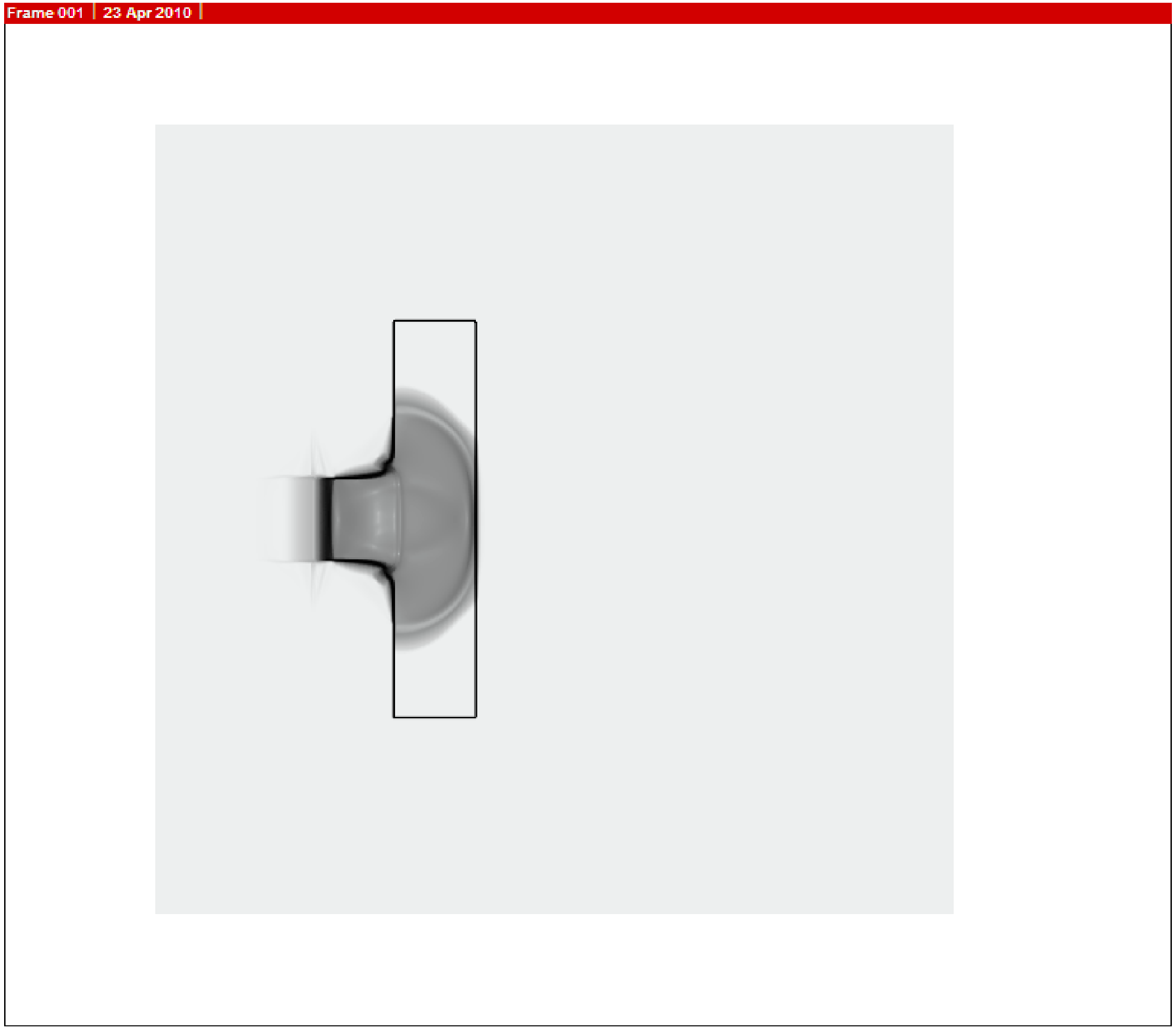
A copper projectile impacts a copper plate surrounded with air (the impact velocity is 800 m/s) : elastic model



A “fluid” projectile impacts a “fluid” plate surrounded with air (the impact velocity is 800 m/s)



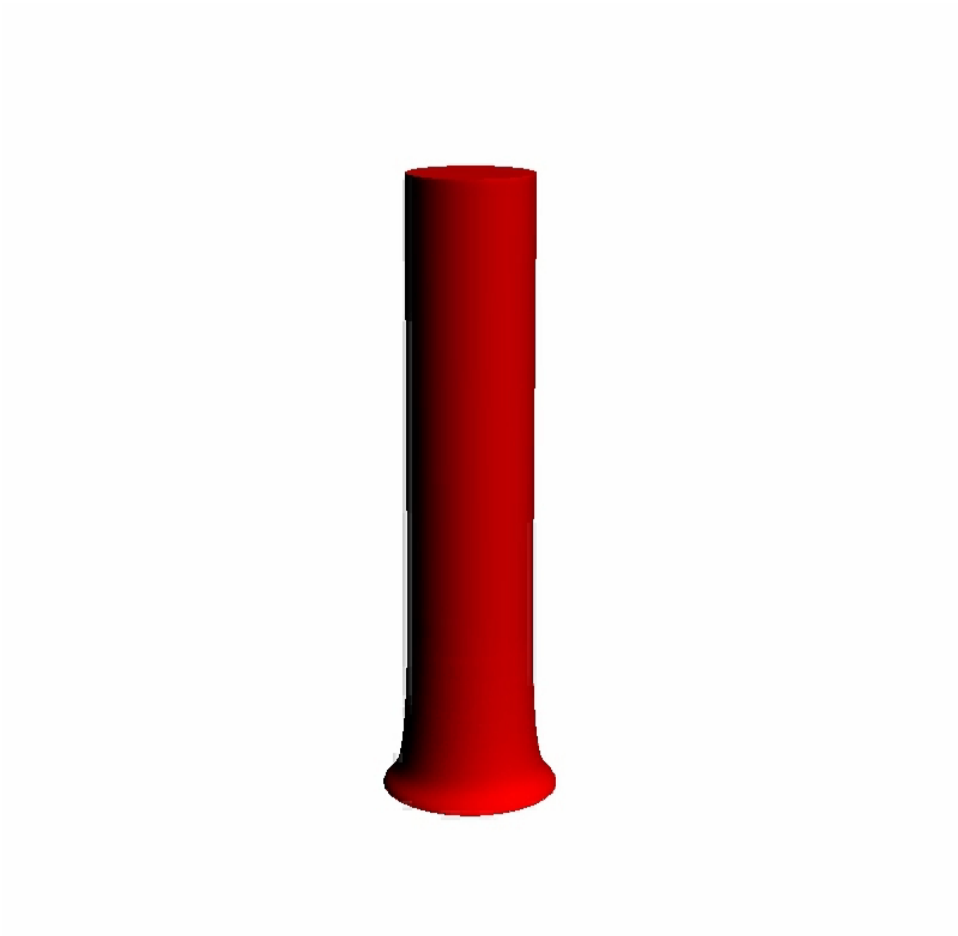
A copper projectile impacts a copper plate surrounded with air (the impact velocity is 800 m/s) : visco-plastic model



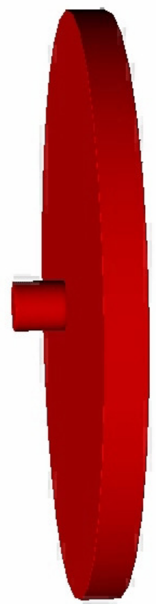
The Taylor impact problem

The rode made of copper has a length 32,4 mm and a diameter 6,4 mm.

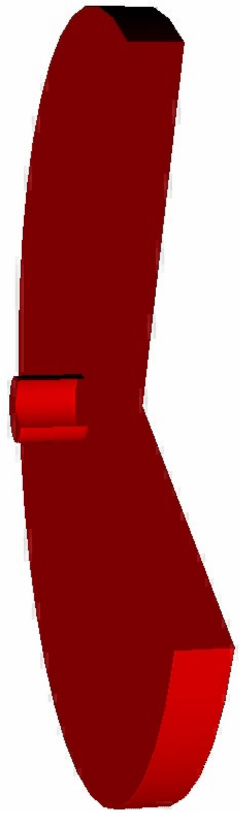
The impact velocity is 400 m/s : visco-plastic model



A copper bullet (having a length 10cm, a diameter 10 cm and velocity 800 m/s) impacting and perforating a copper target (of width 10 cm and diameter 120 cm) : visco-plastic model



A copper bullet (having a length 1cm, a diameter 10 cm and velocity 800 m/s) impacting and perforating a copper target (of width 10 cm and diameter 120 cm) : visco-plastic model



Experiments

Conclusion

- A new hyperbolic model describing large deformations of solid-fluid interfaces has been built.
- A broad range of applications has been presented.

The results obtained are published in JCP, 2008, 2009, 2012, Phil. Tr. Royal Soc. 2011, Book "Variational Models and Methods in Solid and Fluid Mechanics", Springer, 2011.

End