Principes de construction des modèles mathématiques thermodynamiquement corrects des milieux continus hétérogènes

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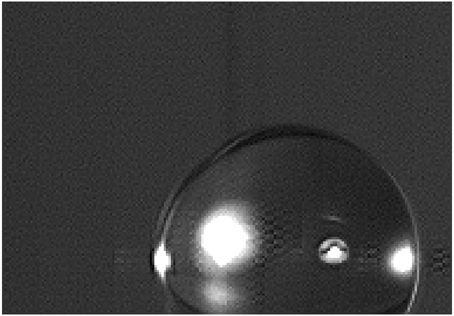
Interfaces between solids and fluids

- Diffuse interfaces

Interfaces between solids and fluids

- Sharp interfaces

Shock-droplet interaction (G. Jourdan and L. Houas)



Classical diffuse interfaces

- Cahn-Hilliard theory (no motion)
- Van der Waals-Korteweg theory of capillarity (P. Casal, M. Eglit, H. Gouin, M. Slemrod, L. Truskinovsky, Ph. Le Floch, D. Jamet, S. Benzoni-Gavage, R. Danchin, ...)

$$T = \int_{\mathcal{D}} \rho \frac{\|\mathbf{u}\|^2}{2} dD, \tag{1}$$

$$W = \int_{\mathcal{D}} \rho\varepsilon(\rho, \|\nabla\rho\|, \eta) dD. \tag{2}$$

Constraints :

$$\rho_t + \mathrm{div}(\rho\mathbf{u}) = 0, \quad \eta_t + \mathbf{u}\cdot\nabla\eta = 0.$$

Weakness of the diffuse interface approach

- How does the specific energy depend on the density gradient ?

Level set approach

$$T = \int_{\mathcal{D}} \rho \frac{\|\mathbf{u}\|^2}{2} dD, \tag{3}$$

$$W = \int_{\mathcal{D}} \rho \varepsilon(\rho, c, \|\nabla c\|, \eta) dD. \tag{4}$$

Constraints :

$$\rho_t + \mathrm{div}(\rho \mathbf{u}) = 0,$$

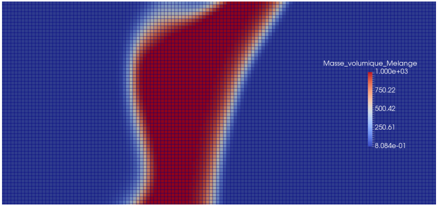
$$c_t + \mathbf{u} \cdot \boldsymbol{\nabla} c = 0, \quad \eta_t + \mathbf{u} \cdot \nabla \eta = 0.$$

Weakness of the level set approach

- The meaning of the order parameter is not always clear. Volume fraction ? Mass fraction ?
- How does the specific energy depend on the order parameter ?

Modelling of moving ‘sharp’ but a little bit ‘diffuse’ interfaces : multiphase approach

Fluid-fluid interfaces : interface as a heterogeneous mixture zone separating two pure fluids (Abgrall and Karni, Saurel and Abgrall). The corresponding interface is considered as a ‘diffuse’ interface. Dynamic and kinematic conditions at the interface are satisfied. Fluid-solid and solid-solid interaction (SG, Favrie and Ndanou).



We solve only Cauchy problem !

Multi-component flows

- *Classical variables* : velocities, deformation measures, densities, entropies.
- *Micro-structure variables* : volume fractions, sizes of inclusions, ...
- *Gradients and temporal derivatives of micro-structure variables*.

Simplified Lagrangian

$$L = \int_{\mathcal{D}} \rho \left(\frac{\|\mathbf{u}\|^2}{2} - \sum_{k=1}^{N} Y_k \varepsilon_k \right) dD,$$

$$\rho = \sum_{k=1}^{N} \alpha_k \rho_k, \ \varepsilon_k = \varepsilon_k(\rho_k, \eta_k).$$

A new variation with respect to α_i, $i = 1, ..., N-1$ is needed ! ! !

Fluid case : Kapila *et al.* model

$$\begin{cases} \frac{\partial \rho}{\partial t} + div\,(\rho \mathbf{u}) = 0, \\ (\rho \mathbf{u})_t + div(\rho \mathbf{u} \otimes \mathbf{u} + p\mathbf{I}) = 0,\ p = \sum_{k=1}^{N} \alpha_k p_k, \\ \frac{DY_k}{Dt} = 0,\ \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla, \\ \frac{D\eta_k}{Dt} = 0, \\ p_1 = ... = p_N, \end{cases}$$

Wood's sound speed :

$$\frac{1}{\rho c_W^2} = \sum_{k=1}^{N} \frac{\alpha_k}{\rho_k c_k^2} \tag{5}$$

Relaxation equation for α_k

To avoid the resolution of algebraic equations, one uses 'relaxation equations' for α_k :

$$\frac{D\alpha_k}{Dt} = \mu_k (p_k - p_I), \; p_I \text{ is an 'interface' pressure.}$$

'Frozen' sound speed :

$$c_f^2 = \sum_{k=1}^{N} Y_k c_k^2,$$

Important inequality (Whitham's sub-characteristic condition) :

$$c_f^2 > c_W^2.$$

Well-posedness of mathematical models with relaxation

- Hyperbolicity
- Whitham' sub-characteristic condition

Example

$$\rho_t + (\rho u)_x = 0, \quad (\rho u)_t + (\rho u^2 + p(\rho))_x = \lambda(U(\rho) - u).$$

Sub-characteristic condition

$$u - \sqrt{\frac{dp}{d\rho}} < \frac{d(\rho U(\rho))}{d\rho} < u + \sqrt{\frac{dp}{d\rho}}.$$

Linearized equation

$$\varepsilon^2(u_{tt} - c^2 u_{xx}) + u_t + a u_x = 0,$$

Wellposedness

$$-c < a < c.$$

Extended Lagrangian for two-velocity model

$$L = \int_{\mathcal{D}} \rho \left(\frac{Y_1 \|\mathbf{u}_1\|^2}{2} + \frac{Y_2 \|\mathbf{u}_2\|^2}{2} - \sum_{k=1}^{2} Y_k \varepsilon_k \right) dD,$$

$$\rho = \sum_{k=1}^{N} \alpha_k \rho_k, \ \varepsilon_k = \varepsilon_k(\rho_k, \eta_k).$$

Constraints :

$$(\alpha_k \rho_k)_t + div\,(\alpha_k \rho_k \mathbf{u}_k) = 0, \quad \frac{D_k \eta_k}{Dt} = 0,$$

Extended Lagrangian for two-velocity model : equal pressures

$$(\alpha_1\rho_1)_t + div\,(\alpha_1\rho_1\ \mathbf{u}_1) = 0, (\alpha_2\rho_2)_t + div\,(\alpha_2\rho_2\ \mathbf{u}_2) = 0,$$

$$(\alpha_1\rho_1\mathbf{u}_1)_t + div\,(\alpha_1\rho_1\mathbf{u}_1 \otimes \mathbf{u}_1 + \alpha_1 p_1 \mathbf{I}) = p\boldsymbol{\nabla}\alpha_1,$$

$$(\alpha_2\rho_2\mathbf{u}_2)_t + div\,(\alpha_2\rho_2\mathbf{u}_2 \otimes \mathbf{u}_2 + \alpha_2 p_2 \mathbf{I}) = p\boldsymbol{\nabla}\alpha_2,$$

$$\frac{D_k\eta_k}{Dt} = 0,\ \ k = 1, 2,$$

$$p = \alpha_1 p_1 + \alpha_2 p_2 = p_1 = p_2.$$

The system has two complex eigenvalues for small relative velocity !

Extended Lagrangian for two-velocity model : Baer-Nunziato model, 1986

$$(\alpha_1\rho_1)_t + div\left(\alpha_1\rho_1\ \mathbf{u}_1\right) = 0, (\alpha_2\rho_2)_t + div\left(\alpha_2\rho_2\ \mathbf{u}_2\right) = 0,$$

$$(\alpha_1\rho_1\mathbf{u}_1)_t + div\left(\alpha_1\rho_1\mathbf{u}_1\otimes\mathbf{u}_1 + \alpha_1 p_1\mathbf{I}\right) = p_I\boldsymbol{\nabla}\alpha_1 + \lambda\left(\mathbf{u}_2 - \mathbf{u}_1\right),$$

$$(\alpha_2\rho_2\mathbf{u}_2)_t + div\left(\alpha_2\rho_2\mathbf{u}_2\otimes\mathbf{u}_2 + \alpha_2 p_2\mathbf{I}\right) = p_I\boldsymbol{\nabla}\alpha_2 + \lambda\left(\mathbf{u}_1 - \mathbf{u}_2\right),$$

$$\frac{D_I\alpha_1}{Dt} = \mu_1(p_1 - p_I),$$

$$\alpha_k\rho_k\theta_k\frac{D_k\eta_k}{Dt} = f_k,\ k = 1, 2,\ \frac{f_1}{\theta_1} + \frac{f_2}{\theta_2} \geq 0.$$

BN choice : $p_I = p_1,\ \mathbf{u}_I = \mathbf{u}_2$. The system is almost hyperbolic : the eigenvalues are real and the eigenvectors form a basis excepting the 'resonance' surfaces !

Solid-fluid interaction model : multiphase approach

Simplified Lagrangian

$$L = \int_{\mathcal{D}} \rho \left(\frac{\|\mathbf{u}\|^2}{2} - \sum_{k=1}^{N} Y_k \varepsilon_k \right) dD,$$

$$\rho = \sum_{k=1}^{N} \alpha_k \rho_k, \ \varepsilon_k = \varepsilon_k^h(\rho_k, \eta_k) + \varepsilon_k^e(j_{1k}, j_{2k}).$$

A new variation with respect to α_i, $i = 1, ..., N-1$ is needed ! ! !

EL equations for the simplified Lagrangian

$$
\begin{cases}
\frac{\partial \rho}{\partial t} + div\left(\rho \mathbf{u}\right) = 0, \\[2ex]
\frac{D\mathbf{e}_k^\beta}{Dt} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)^T \mathbf{e}_k^\beta = 0, \\[2ex]
\left(\rho \mathbf{u}\right)_t + div(\rho \mathbf{u} \otimes \mathbf{u} - \boldsymbol{\sigma}) = 0,\ \boldsymbol{\sigma} = \sum_{k=1}^{N} \alpha_k \boldsymbol{\sigma}_k, \\[2ex]
\frac{DY_k}{Dt} = 0,\ \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla, \\[2ex]
\frac{D\eta_k}{Dt} = 0, \\[2ex]
p_1 = ... = p_N,
\end{cases}
$$

The model is hyperbolic, if the energy of each phase is rank-one convex.

$N \geq 2$ interacting solids undergoing large deformations

Ndanou, Favrie and SG, *JCP*, 2015.

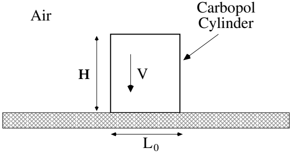
Properties of the governing equations

1. The volume fractions of components are new microstructure variables ($N > 2$).
2. The system contains $12xN + 3 + 1$ (or $12xN + 3N + 1$ for different velocities) differential equations.
3. The model looks as a Russian wood doll ('matreshka') (easy to add or remove any number of solids, the equations are similar).
4. The model is hyperbolic if each solid possesses a 'hyperbolic' equation of state.
5. The entropy inequality is satisfied.
6. Whitham's sub-characteristic condition is satisfied.

Impact of a jelly-like substance (carbopol), S. Hank, SG, N. Favrie, J. Massoni, 2017

- The maximal droplet spreading area as a function of the velocity impact ?
- Influence of the parameter a on the spreading area ?

Material	γ	P_∞ (Pa)	μ (Pa)	ρ_0 (kg/m^3)
Carbopol	4.4	10^6	85	1020
Air	1.4	-	-	1.2



$$H = 8mm,\ L_0 = 12mm,\ V = -3m/s$$

Case $a = 0$

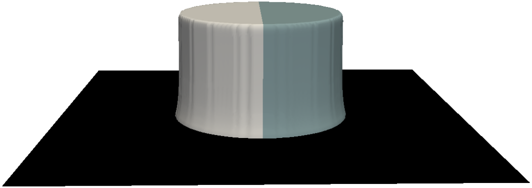
$$e^e(\mathbf{g}) = \frac{\mu}{4\rho}\left(\frac{j_1^2}{3} - 3\right)$$

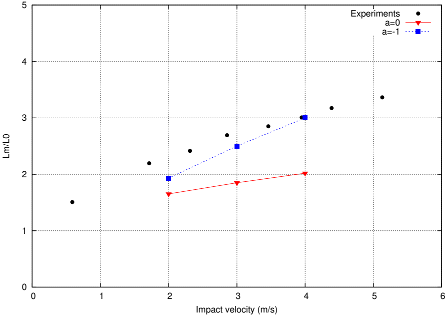
Case $a = -1$

$$e^e(\mathbf{g}) = \frac{\mu}{4\rho}\left(j_1^2 - j_2 - 6\right)$$

-Mesh size : 0.15 mm
-Physical time : 16 ms
-At the right : a=-1
-At the left : a=0

L.-H.Luu, Y.Forterre (2009)

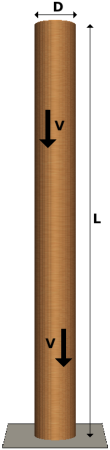




The parameter *a* essentially modifies the spreading area !

Taylor impact experiments (copper rod-on-rod impact)

(L.C.Forde et al. 2009)



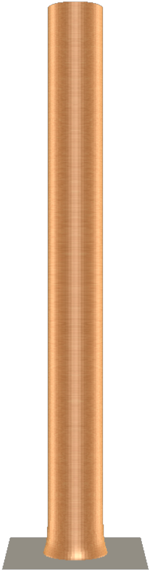
Material parameters were calculated by using ‘Shock wave database’www.ficp.ac.ru/rusbank/ (A.V. Bushman, I.V. Lomonosov, K.V. Khishchenko) .

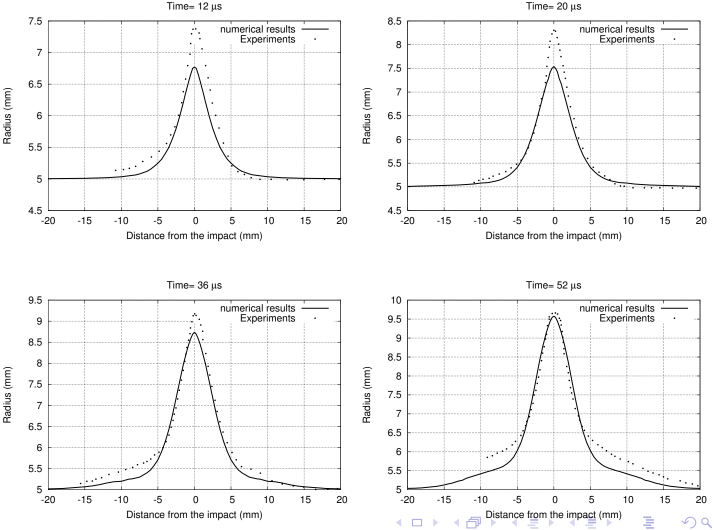
Materials	γ	P_∞ (Pa)	μ (Pa)	ρ_0 (kg/m^3)	σ_Y (Mpa)
Copper	4.54	29.9 10^9	48.5 10^9	8924	400
Air	1.4	-	-	1.2	-

L=100 mm , D= 10 mm, $\mathbf{V}=(0,0,-197.5)^T$ m/s
Final time : 368 μs

$2D$ axisymmetric code, 725760 mesh cells, 4h on 48 processors.

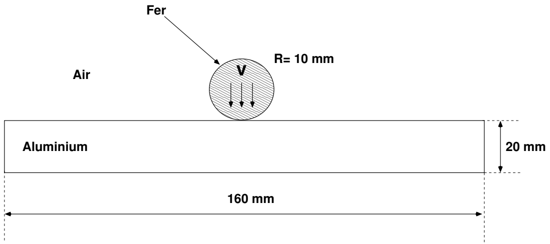
Taylor impact experiments





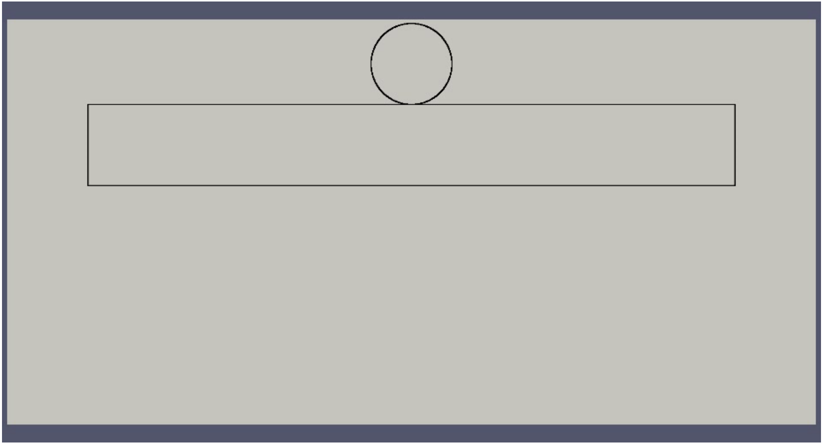
Impact Fer/Aluminium, (S.Ndanou, N.Favrie and SG (2015))

An iron cylinder impacts an aluminium plate at 800 m/s.



Materials	γ	P_∞ (Pa)	μ (Pa)	ρ_0 (kg/m^3)	σ_Y (Mpa)
Aluminium	3.5	32 10^9	26 10^9	2712	60
Iron	3.9	43.6 10^9	82 10^9	7860	200
Air	1.4	-	-	1.2	-

Iron/Aluminium Impact

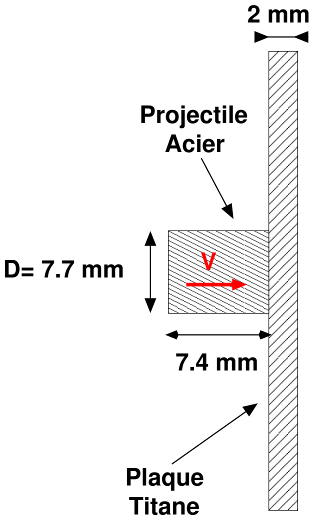


Steel/Titanium Impact

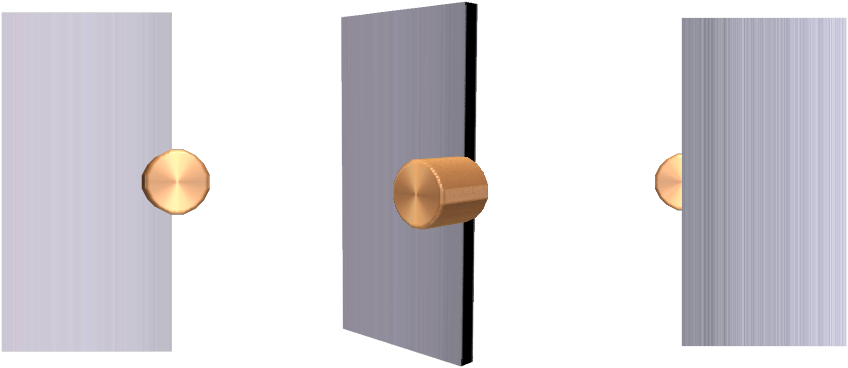
- A perforation of a titanium plate by a cylindrical steel projectile at striking velocity 5000 m/s

Materials	μ (GPa)	ρ_0 (kg/m^3)	σ_Y (Mpa)
Steel	81	7850	700
Titanium	44	4527	1030
Air	-	1.19	-

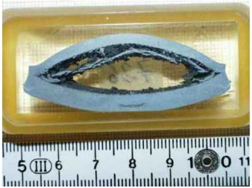
3D computation is performed on a Cartesian mesh with 10^6 cells, 96 processors, computation time 24h.



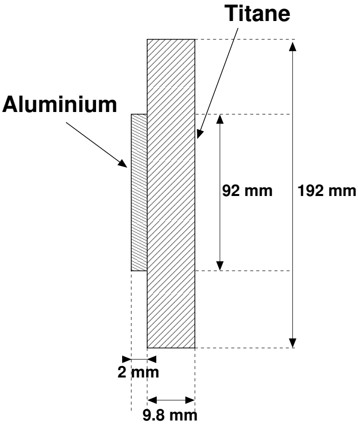
Physical time : 2.4μs



Spalling : aluminium plate-on-titanium plate impact at 700 m/s (S. Ndanou, N. Favrie and SG (2015))



Spalling of an iron plate (Ernstson *et al.*)

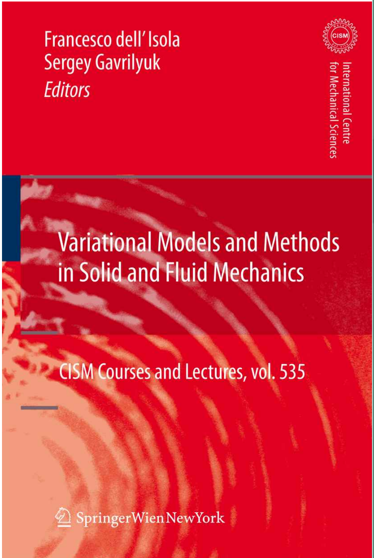


Spalling : aluminium plate-on-titanium plate impact at 700 m/s (S.Ndanou, N.Favrie and SG (2015))

Conclusion

- Always use Hamilton's principle of stationary action !
- Don't forget about the hyperbolicity and thermodynamics !

BOOKS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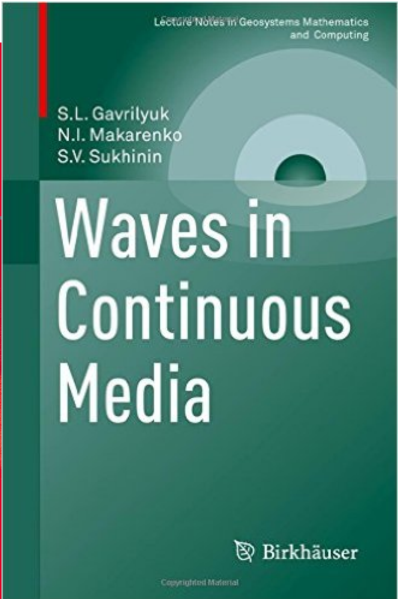
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