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Thanks to
PhD:
Mazeran,
Kluth,
Franck,
CEA:
Delpino,
Labourasse,
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. . .,
and all
colleagues
along these
years.

Numerical methods for FCI
Part II: Hydrodynamics

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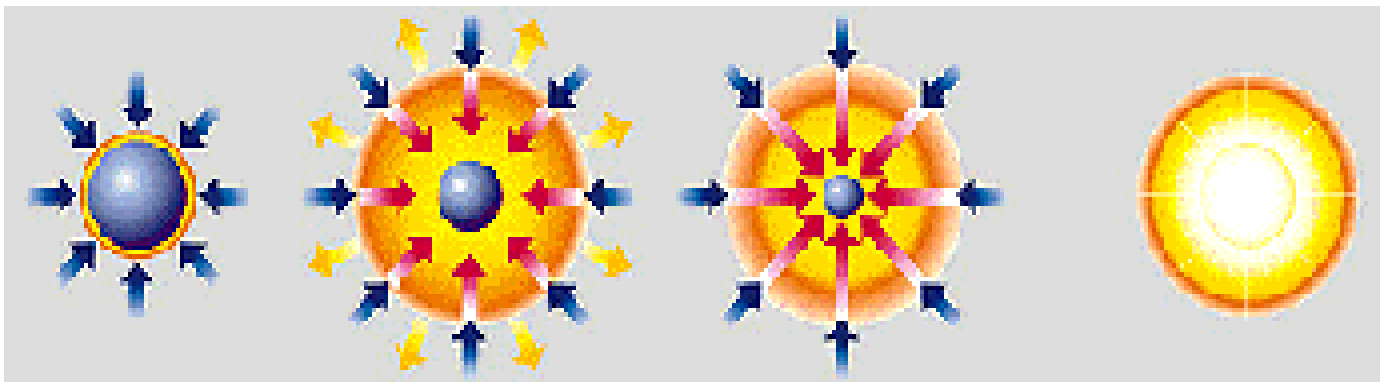
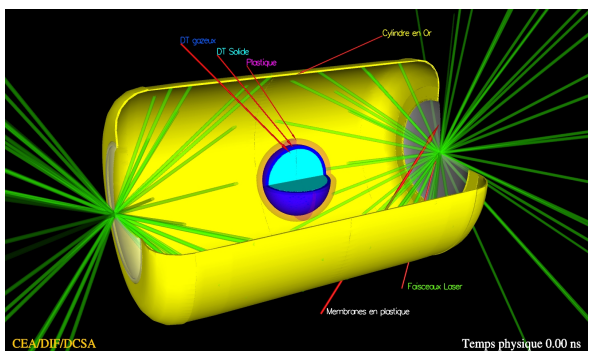
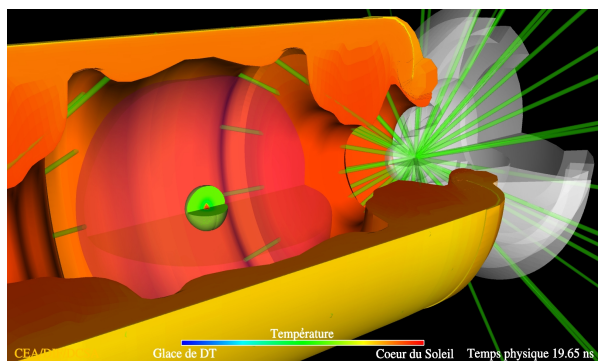
FCI scenario



Hydrodynamic is dominant in the implosion stage

DT capsule in a gold cylinder, heated by laser beams
Credit CEA/DAM/DIF

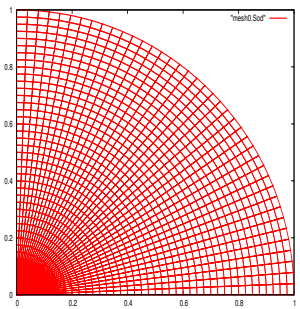


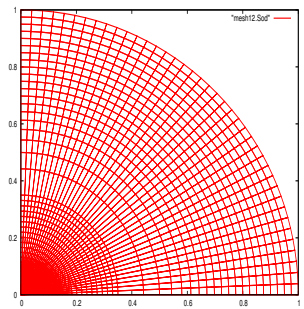


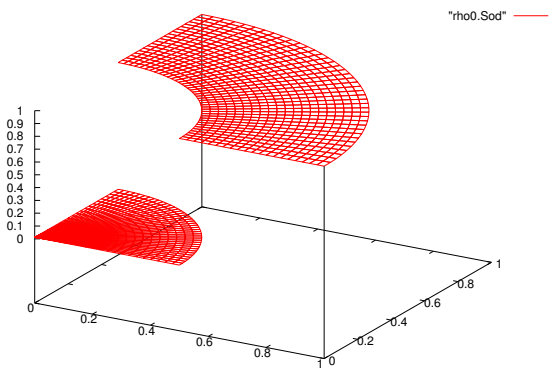
The radiation push is not perfectly symetric

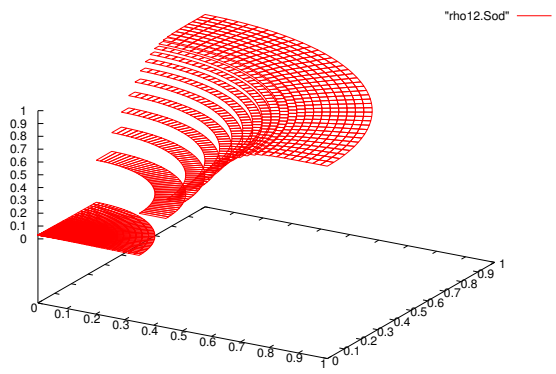
Why Lagrangian scheme for compressible flows ?

- Lagrangian methods are written in the fluid frame
- easy discretization of free boundaries (external and internal),
- naturally adapted for multimaterial flows,
- very good accuracy for transport dominated flows

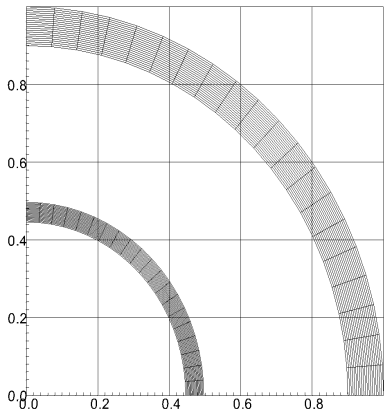


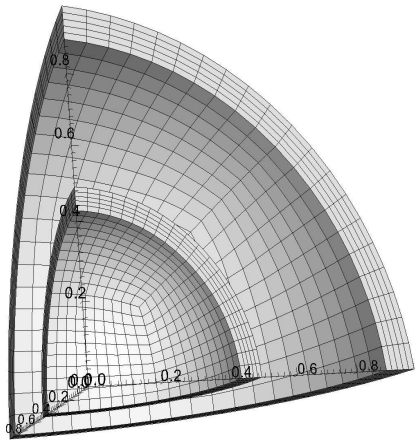


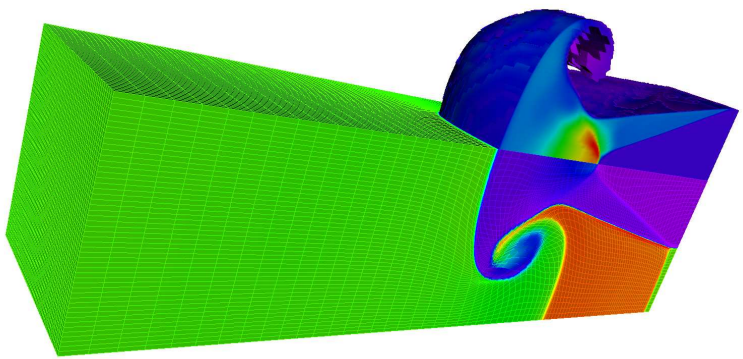


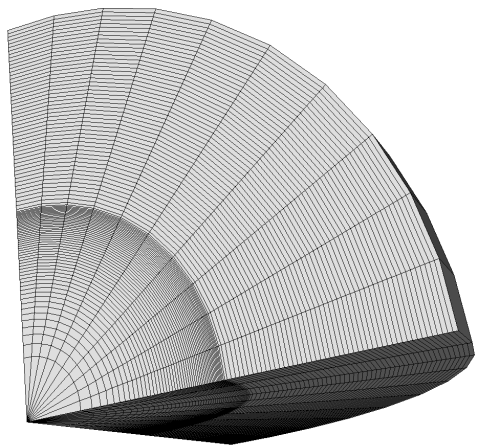


3D examples



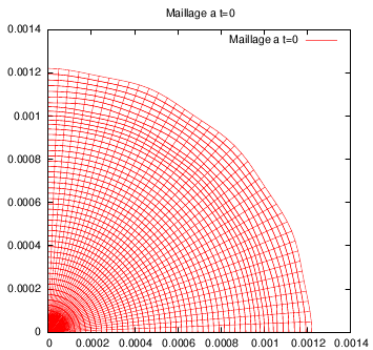


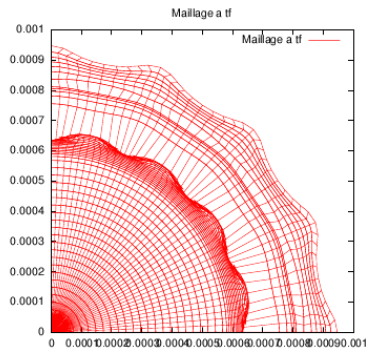




Perturbation of a basic flow

ICF flows are very sensitive to hydrodynamic perturbation. That is a even very small initial pertubation may have a dramatic influence on the solution. The reason is that ICF flows are quite close to instability, so that the growth rate of the perturbations may be large. Numerical methods are very useful to quantify the influence these perturbations. Here we illustrate with the result of a very simple numerical simulation done by E. Franck during his Master 2.





The mesh at $t = 0$ is displayed on the left. The perturbation is a $n = 16$ mode. On the right the result at time $t_f = 10^{-9}s$. On this simulation the growth rate of the perturbation is reasonnable.

Lagrangian methods are essential for such simulations.

Eulerian methods on Cartesian meshes are less efficient.

Plan

- Partial Differential Equations
- Meshes and schemes
- Numerical analysis : stability, CFL, convergence (new)
- $T_i - T_e$ discretization
- Extension to radiation.
- Development of Hele-Shaw models (for stability of ICF flows, with H. Egly and R. Sentis).

Euler equations

The Euler equation for compressible gas dynamics are

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = 0, \\ \partial_t (\rho e) + \nabla \cdot (\rho \mathbf{u} e + p \mathbf{u}) = 0, \\ \partial_t (\rho S) + \nabla \cdot (\rho \mathbf{u} S) \geq 0. \end{cases}$$

The density is $\rho > 0$. The velocity is $\mathbf{u} \in \mathbb{R}^d$. The density of total energy is $e = \varepsilon + \frac{1}{2} |\mathbf{u}|^2$.

Possible EOS

$$p = (\gamma - 1)\rho\varepsilon, \quad p = (\gamma - 1)\rho\varepsilon - \gamma p_0, \quad p = \text{tabulated}, \quad p = \text{analytic}.$$

Assumption : there exists a temperature $T > 0$ such that

$$T dS = d\varepsilon + p d\tau, \quad \tau = \frac{1}{\rho}.$$

The pressure $p = p(\tau, \varepsilon)$ is provided by the equation of state.

The entropy inequality selects the entropy solutions of the Euler system.

For a perfect gas EOS, $\varepsilon = C_v T$ and $S = \log(\varepsilon \tau^{\gamma - 1})$.

Quasi-Lagrange in 2D

It writes

$$\begin{cases} \rho D_t \tau - \nabla \cdot \mathbf{u} = 0, \\ \rho D_t \mathbf{u} + \nabla p = 0, \\ \rho D_t e + \nabla \cdot (p\mathbf{u}) = 0, \end{cases}$$

where the material derivative is $D_t = \partial_t + \mathbf{u} \cdot \nabla$.
Or also with an artificial viscosity q

$$\begin{cases} \rho D_t \tau - \nabla \cdot \mathbf{u} = 0, \\ \rho D_t \mathbf{u} + \nabla (p + q) = 0, \\ \rho D_t \varepsilon + (p + q) \nabla \cdot \mathbf{u} = 0. \end{cases}$$

By construction

$$\rho T d_t S = \rho D_t \varepsilon + p \rho D_t \tau = -q \nabla \cdot \mathbf{u} \geq 0$$

A possible artificial viscosity is $q = C \Delta x \max(0, -\nabla \cdot \mathbf{u}) \geq 0$.
I will not discuss these methods which are non conservative. The seminal idea's comes from Von Neumann.

- A non linear system of conservation laws with an entropy writes

$$\partial_t U + \partial_x f(U) + \partial_y g(U) = 0.$$

- Assume the system is endowed with a strictly convex entropy $\widehat{S}(U) \in \mathbb{R}$: smooth solutions satisfy $\partial_t \widehat{S}(U) + \partial_x F(U) + \partial_y G(U) = 0$.
- Then the system is hyperbolic, which implies stability around constant, and well posedness of the Cauchy problem for smooth initial data in finite time $0 < t < T$.
- Discontinuous solutions satisfy the Rankine Hugoniot relation

$$-\sigma (U_R - U_L) + n_x (f(U_R) - f(U_L)) n_y (g(U_R) - g(U_L)) = 0$$

and the entropy inequality

$$-\sigma \left(\widehat{S}(U_R) - \widehat{S}(U_L)\right) + n_x (F(U_R) - F(U_L)) n_y (G(U_R) - G(U_L)) \geq 0.$$

Problem : the Quasi-Lagrange formulations are not conservative.

Question : how to write pure conservative Lagrange PDE's ? cf Godlewski-Raviart, Serre, ...

Question : how about hyperbolicity for Lagrangian systems ?

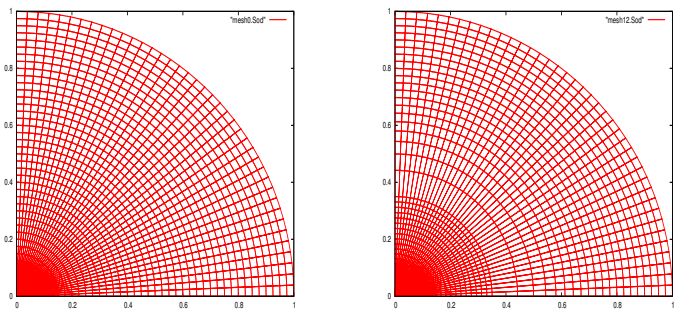
From Euler to Lagrange

To shorten the notations we set

$$\mathbf{x} = (x, y) \text{ and } \mathbf{X} = (X, Y).$$

Let us consider the Euler-to-Lagrange change of frame defined by

$$\partial_t \mathbf{x}(\mathbf{X}, t) = u(\mathbf{x}(\mathbf{X}, t), t) \text{ with initialization } \mathbf{x}(\mathbf{X}, 0) = \mathbf{X}.$$



Principle : A Lagrange formulation is written in the reference frame coordinate X.

We need a tool to rewrite the equations in the **X** frame.

Piola's transformations

Rule 1 A smooth change of variable $\mathbf{x} \mapsto \mathbf{X}(\mathbf{x})$ is such that $\mathbf{n} d\sigma = \mathrm{cof}\,(\nabla_{\mathbf{X}} \mathbf{x})\, \mathbf{n}_X d\sigma_X$. where $\mathrm{cof}\,(M) \in \mathbb{R}^{d \times d}$ is the comatrix of M.

Rule 2 A system of conservation laws $\nabla_{\mathbf{x}} F(U) = 0$ written in the eulerian variable is transformed in a lagrangian system written with the $\mathbf{X}$ variable

$$\nabla_X . \left[F(U) \mathrm{cof}\,(\nabla_{\mathbf{X}} \mathbf{x}) \right] = 0.$$

This is a consequence of rule 1.

Rule 3 One must not forget the Piola's identity

$$\nabla_X . \mathrm{cof}\,(\nabla_{\mathbf{X}} \mathbf{x}) = 0.$$

A reason is that the system contains a new unknown $\mathrm{cof}\,(\nabla_{\mathbf{X}} \mathbf{x})$. Therefore we need a new equation to close the system..

PDEs in 1D

We consider the change of coordinates $(x, t) \mapsto X, t)$ in $\mathbf{R}^2$. The gradient of the space-time transformation is $\begin{pmatrix} 1 & 0 \\ u & J \end{pmatrix}$ with the Jacobian $J = \frac{\partial x}{\partial X}$. The comatrix is cof $= \begin{pmatrix} J & -u \\ 0 & 1 \end{pmatrix}$.
The Lagrangian system is

$$\nabla_{X,t} \cdot \left[\begin{pmatrix} \rho & \rho u \\ \rho u & \rho u^2 + p \\ \rho e & \rho u e + p u \end{pmatrix} \begin{pmatrix} J & -u \\ 0 & 1 \end{pmatrix} \right] = \partial_t \begin{pmatrix} \rho J \\ \rho J u \\ \rho J e \end{pmatrix} + \partial_X \begin{pmatrix} 0 \\ p \\ p u \end{pmatrix} = 0.$$

The Piola identity writes

$$\partial_t J - \partial_X u = 0.$$

It is usual to define the mass variable

$$dm = \rho(x, t)dx = \rho(X, 0)dX$$

which is independent of the time, to eliminate the density

$$\rho J = \rho(X, 0)$$

and to get the system of conservation laws in the mass variable

$$\begin{cases} \partial_t \tau - \partial_m u = 0, \\ \partial_t u + \partial_m p = 0, \\ \partial_t e + \partial_m (p u) = 0. \end{cases}$$

Notice that $\rho > 0$ is necessary for the validity of the transformation.

Let us define for convenience the components of the deformation gradient $\mathbf{F} = \nabla_{\mathbf{X}}\mathbf{x}$ as $A = \partial_X x$, $B = \partial_X y$, $L = \partial_Y x$ and $M = \partial_Y y$.
The algebra of the Euler-Lagrange transformation is as follows. The space-time deformation gradient is $\begin{pmatrix} 1 & 0 & 0 \\ u & A & L \\ v & B & M \end{pmatrix}$. The comatrix is $\text{cof} = \begin{pmatrix} J & -uM + vL & uB - vA \\ 0 & M & -B \\ 0 & -L & A \end{pmatrix}$ where the space Jacobian is $J = AM - BL$. The product of matrices is

$$\begin{pmatrix} \rho & \rho u & \rho v \\ \rho u & \rho u^2 + p & \rho uv \\ \rho v & \rho uv & \rho v^2 + p \\ \rho e & \rho ue + pu & \rho ve + pv \end{pmatrix} \text{cof} = \begin{pmatrix} \rho J & 0 & 0 \\ \rho uJ & pM & -pB \\ \rho vJ & -pL & pA \\ \rho eJ & puM - pvL & -puB + pvA \end{pmatrix}.$$

So the Eulerian system is transformed into the Lagrangian system

$$\begin{cases} \partial_t(\rho J) = 0, \\ \partial_t(\rho Ju) + \partial_X(pM) + \partial_Y(-pB) = 0, \\ \partial_t(\rho Jv) + \partial_X(-pL) + \partial_Y(pA) = 0, \\ \partial_t(\rho Je) + \partial_X(puM - pvL) + \partial_Y(pvA - puB) = 0. \end{cases}$$

The Piola's identities writes

$$\begin{cases} \partial_t J - \partial_X(uM - vL) - \partial_Y(vA - uB) = 0, \\ \partial_X M - \partial_Y B = 0, \\ -\partial_X L + \partial_Y A = 0. \end{cases}$$

It is not a closed system of conservation laws.

Hui's system

- The Hui's system is closed

$$\begin{cases} \partial_t(\rho J) = 0, \\ \partial_t(\rho J u) + \partial_X(pM) + \partial_Y(-pB) = 0, \\ \partial_t(\rho J v) + \partial_X(-pL) + \partial_Y(pA) = 0, \\ \partial_t(\rho J e) + \partial_X(puM - pvL) + \partial_Y(pvA - puB) = 0, \\ \partial_t A = \partial_X u, \\ \partial_t B = \partial_X v, \\ \partial_t L = \partial_Y u, \\ \partial_t M = \partial_Y v, \\ J = AM - BL. \end{cases}$$

- A second system is more concerned with the formal symetry of the fluxes

$$\begin{cases} \rho_0 \partial_t \tau - \partial_X(uM - vL) - \partial_Y(vA - uB) = 0, \\ \rho_0 \partial_t u + \partial_X(pM) + \partial_Y(-pB) = 0, \\ \rho_0 \partial_t v + \partial_X(-pL) + \partial_Y(pA) = 0, \\ \rho_0 \partial_t e + \partial_X(puM - pvL) + \partial_Y(pvA - puB) = 0. \end{cases} \qquad \rho_0 = \rho J, \quad \tau = \frac{1}{\rho},$$

The symetry is related to the fact that (M, L) appears only in the X derivative, and (A, B) is the Y derivative.

A potential closed formulation

The third formulation makes use of the Piola-Kirkhoff tensor (with G. Kluth). Since $\rho J = \rho_0$ then $\tau = \frac{AM-BL}{\rho_0}$ and therefore

$$\sigma^{PK} = \rho_0 \nabla_{\mathbf{F}|S} \varepsilon = \left(\rho_0 \frac{\partial \varepsilon}{\partial \tau |S} \right) \nabla_{\mathbf{F}} \tau = -p \begin{pmatrix} M & -B \\ -L & A \end{pmatrix}.$$

It writes in a compact form

$$\begin{cases} \partial_t \mathbf{F} = \nabla_{\mathbf{X}} \mathbf{u}, \\ \rho_0 \partial_t \mathbf{u} = \nabla_{\mathbf{X}} \cdot \sigma^{PK}, \\ \rho_0 \partial_t e = \nabla_{\mathbf{X}} \cdot (\mathbf{u}^t \sigma^{PK}). \end{cases}$$

Entropy : One has from the fundamental principle of thermodynamics $\rho_0 \partial_t \varepsilon = \rho_0 \left(T \partial_t S + \nabla_{\mathbf{F}|S} \varepsilon : \partial_t \mathbf{F} \right)$. Therefore

$$\rho_0 T \partial_t S = -\sigma^{PK} : \partial_t \mathbf{F} + \rho_0 \partial_t e - \mathbf{u}.\rho_0 \partial_t \mathbf{u}$$

$$= -\sigma^{PK} : \nabla_{\mathbf{X}} \mathbf{u} - \mathbf{u}.\nabla_{\mathbf{X}} \cdot \sigma^{PK} + \nabla_{\mathbf{X}} \cdot (\mathbf{u}^t \sigma^{PK}) = 0.$$

For shock solutions

$$\partial_t S \geq 0$$

in the sense of distributions.

Mass variables in 2D

Assumption : there exists two independent variables (α, β) such that

$$d\alpha = \rho_0 dX \text{ and } d\beta = \rho_0 dY.$$

The chain rule implies

$$\partial_\alpha = \frac{\partial X}{\partial \alpha}\partial_X + \frac{\partial Y}{\partial \alpha}\partial_Y = \frac{1}{\rho_0}\partial_X \Longrightarrow \frac{1}{\rho_0} = \frac{\partial X}{\partial \alpha} \text{ and } 0 = \frac{\partial Y}{\partial \alpha}$$

and

$$\partial_\beta = \frac{\partial X}{\partial \beta}\partial_X + \frac{\partial Y}{\partial \beta}\partial_Y = \frac{1}{\rho_0}\partial_Y \Longrightarrow \frac{1}{\rho_0} = \frac{\partial Y}{\partial \beta} \text{ and } 0 = \frac{\partial X}{\partial \beta}.$$

In this case $\frac{\partial \rho^{-1}}{\partial_\beta} = \frac{\partial^2 X}{\partial \alpha \partial \beta} = 0$ and $\frac{\partial \rho^{-1}}{\partial_\alpha} = \frac{\partial^2 Y}{\partial \alpha \partial \beta} = 0$. So the density ρ is a constant.

It is not possible to define simple mass variables as in dimension one.

Hyperbolicity

• In dimension one, the size of the lagrangian system is $s = 3$. One checks easily that $-S = -\log(\varepsilon\tau^{\gamma-1})$ is strictly convex with respect to τ, u, e. Therefore the lagrangian system is hyperbolic in 1D.

• In dimension two, the situation is less evident because the algebra is tricky and the interpretation of the results may depend on particular version of the lagrangian chosen for the analysis. In all cases the result is that lagrangian systems in dimension greater or equal to two are weakly hyperbolic. Perhaps more important is to understand what are the consequences of weak hyperbolicity on the one hand for the solution of the Cauchy problem in dimension two and more, and on the other hand for numerical simulations.

• The Cauchy problem of a system of conservation which is only weakly hyperbolic suffers of a loss of derivatives. That is one is able to show stability inequalities in ad-hoc functional spaces like

$$\|U(t)\|_{H^m} \leq C \|U(0)\|_{H^{m+p}}, \qquad 0 < t < T.$$

The integer $p > 0$ measures the number of derivatives which are loosed by the solution of Cauchy problem. Such a phenomenon is characteristic of a weakly hyperbolic system.

• Let us study a particular Cauchy problem for any lagrangian systems in dimension two. The initial data are

$$p(X, Y, 0) \text{ is a constant, and } u(X, Y, 0) = w(Y), \ v(X, Y, 0) = 0.$$

The physical solution is of course a pure shear flow

$$x(X, Y, t) = X + tw(Y) \text{ and } y(X, Y, t) = Y.$$

Therefore

$$\mathbf{F}(t) = \begin{pmatrix} 1 & tw'(Y) \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & t\partial_Y u(0) \\ 0 & 1 \end{pmatrix}$$

So the deformation gradient is a function of the Y derivative of the velocity at time $t = 0$. In consequence the Cauchy problem suffers for the loss of at least one derivative.

Context

- Historical topic : Von Neumann-Richtmyer VNR scheme, Godunov Gaia scheme (Godunov-Lagrange)
- Other active researchers on Lagrangian numerical methods : R. Loubere, G. Scovazzi (Sandia), M. Shaskov (T7), ..., C.W. Shu, ...

- CELIA group : Multi-scale Godunov-type method for bf cell-centered discrete Lagrangian hydrodynamics JCP 2009, Maire-Nkonga
- CEA group : A **cell-centered** Lagrangian hydrodynamics scheme on general unstructured meshes in arbitrary dimension JCP 2009, Carré, Del Pino, D. et Labourasse

In 1D

In dimension one, it is sufficient to rely on the theory of the solutions to the Riemann problem in order to establish a rigorous and efficient basis for the development of numerical schemes.
The basic scheme that one obtains with this method writes

$$\left\{\begin{array}{l} \frac{M_j}{\Delta t}(\tau_j^{n+1}-\tau_j^n)-u^*_{j+\frac{1}{2}}+u^*_{j-\frac{1}{2}}=0,\\ \frac{M_j}{\Delta t}(u_j^{n+1}-u_j^n)+p^*_{j+\frac{1}{2}}-p^*_{j-\frac{1}{2}}=0,\\ \frac{M_j}{\Delta t}(e_j^{n+1}-e_j^n)+p^*_{j+\frac{1}{2}}u^*_{j+\frac{1}{2}}-p^*_{j-\frac{1}{2}}u^*_{j-\frac{1}{2}}=0. \end{array}\right.$$

where the fluxes are defined by an approximation of the Riemann problem. For example

$$\left\{\begin{array}{l} u^*_{j+\frac{1}{2}}=\frac{1}{2}(u_j^n+u_{j+1}^n)+\frac{1}{2\rho c}(p_j^n-p_{j+1}^n)\\ p^*_{j+\frac{1}{2}}=\frac{1}{2}(p_j^n+p_{j+1}^n)+\frac{\rho c}{2}(u_j^n-u_{j+1}^n). \end{array}\right.$$

The local acoustic ρc impedance is povided by an approximated formula : for example by $(\rho c)_{j+\frac{1}{2}}=\frac{1}{2}\left[(\rho c)_j^n+(\rho c)_{j+1}^n\right]$. More robust and accurate formulas for the local impedance are possible.
The mass of cell number j is

$$M_j=\rho_j^0\Delta x_j^0=\rho_j^n\Delta x_j^n.$$

The displacement of the cell is defined by

$$x^{n+1}_{j+\frac{1}{2}}=x^n_{j+\frac{1}{2}}+\Delta t u^*_{j+\frac{1}{2}}.$$

It is a enlightening classroom exercise to show that all these formulas are compatible.

Exercize + correction

We want by induction on n to show the compatibility of the discrete equations

$$\begin{cases} \frac{M_j}{\Delta t}(\tau_j^{n+1} - \tau_j^n) - u^*_{j+\frac{1}{2}} + u^*_{j-\frac{1}{2}} = 0, \\ M_j = \rho_j^n \Delta x_j^n, \\ x^{n+1}_{j+\frac{1}{2}} = x^n_{j+\frac{1}{2}} + \Delta t u^*_{j+\frac{1}{2}}. \end{cases}$$

The starting point is $M_j^n = \rho_j^n \Delta x_j^n = \rho_j^n \left(x^n_{j+\frac{1}{2}} - x^n_{j-\frac{1}{2}} \right)$. So

$$\frac{\rho_j^n \Delta x_j^n}{\rho_j^{n+1}} = \Delta x_j^n + \Delta t \left(u^*_{j+\frac{1}{2}} - u^*_{j-\frac{1}{2}} \right) = \Delta x_j^{n+1}.$$

CQFD.

Implementation

$$\begin{cases} \frac{M_j}{\Delta t}(u_j^{n+1} - u_j^n) + p^*_{j+\frac{1}{2}} - p^*_{j-\frac{1}{2}} = 0, \\ \frac{M_j}{\Delta t}(e_j^{n+1} - e_j^n) + p^*_{j+\frac{1}{2}} u^*_{j+\frac{1}{2}} - p^*_{j-\frac{1}{2}} u^*_{j-\frac{1}{2}} = 0. \end{cases}$$

At the same time move the mesh

$$x^{n+1}_{j+\frac{1}{2}} = x^n_{j+\frac{1}{2}} + \Delta t u^*_{j+\frac{1}{2}},$$

and recompue the density

$$\rho_j^{n+1} = \frac{M_j}{\Delta x_j^{n+1}}.$$

Entropy : $S_j'(t) \geq 0$

For simplicity consider the semi-discrete scheme

$$u^*_{j+\frac{1}{2}} + u^*_{j-\frac{1}{2}} \begin{cases} M_j \tau_j'(t) - u^*_{j+\frac{1}{2}} + u^*_{j-\frac{1}{2}} = 0, \\ M_j u_j'(t) + p^*_{j+\frac{1}{2}} - p^*_{j-\frac{1}{2}} = 0, \\ M_j e_j'(t) + p^*_{j+\frac{1}{2}} u^*_{j+\frac{1}{2}} - p^*_{j-\frac{1}{2}} u^*_{j-\frac{1}{2}} = 0. \end{cases}$$

The fundamental principle of thermodynamics $TdS = d\varepsilon + pd\tau$ implies

$$M_j T_j(t) S_j'(t) = M_j \left(\varepsilon_j'(t) + p_j \tau_j'(t)\right) = M_j e_j'(t) - M_j u_j u_j'(t) + M_j p_j \tau_j'(t)$$

$$= -\left(p^*_{j+\frac{1}{2}} u^*_{j+\frac{1}{2}} - p^*_{j-\frac{1}{2}} u^*_{j-\frac{1}{2}}\right) + u_j \left(p^*_{j+\frac{1}{2}} - p^*_{j-\frac{1}{2}}\right) + p_j \left(u^*_{j+\frac{1}{2}} - u^*_{j-\frac{1}{2}}\right) - (0 = (p_j u_j - p_j u_j))$$

$$= -\left(p^*_{j+\frac{1}{2}} - p_j\right)\left(u^*_{j+\frac{1}{2}} - u_j\right) + \left(p^*_{j-\frac{1}{2}} - p_j\right)\left(u^*_{j-\frac{1}{2}} - u_j\right)$$

The Riemann solver is the solution of the system

$$\begin{cases} p^*_{j+\frac{1}{2}} - p_j + (\rho c)_{j+\frac{1}{2}} \left(u^*_{j+\frac{1}{2}} - u_j\right) = 0, \\ p^*_{j+\frac{1}{2}} - p_{j+1} - (\rho c)_{j+\frac{1}{2}} \left(u^*_{j+\frac{1}{2}} - u_j\right) = 0 \end{cases}$$

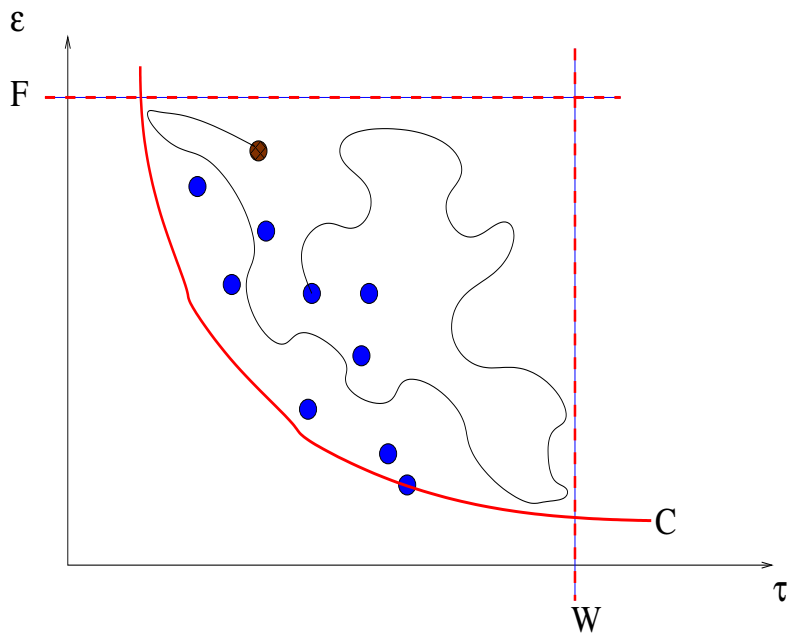
Therefore $S_j'(t) \geq 0$.

For design and justification, the equations for the Riemann solver are more important than its solution

Why the mesh is stable

For simplicity we consider the semi-discrete case (continuous in time scheme) and a perfect gas equation of state with $\gamma = 2$

$$S = \log(\varepsilon\tau).$$



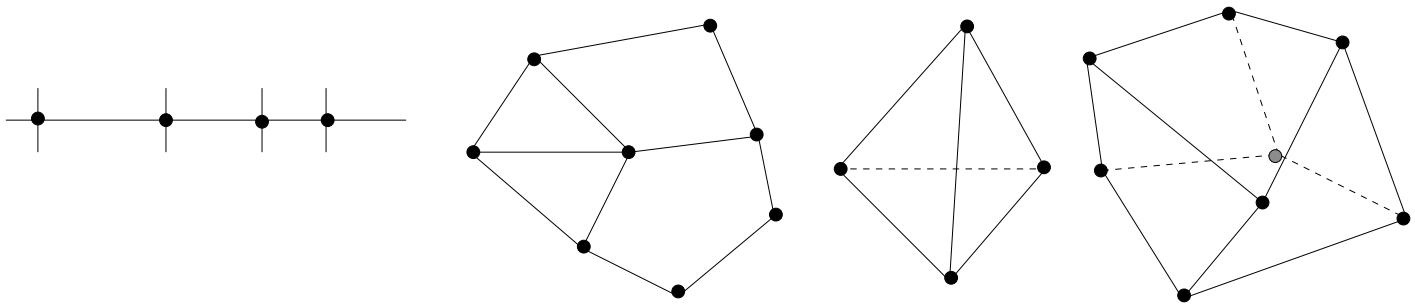
$$C = \min_j \left(\varepsilon_j^0 \tau_j^0\right), \quad F \leq \frac{\sum_p M_p e_p}{M_j} \leq \frac{E^0}{\min_j M_j}, \quad W \leq \frac{\sum_p M_p \tau_p^0}{M_j} = \frac{V^0}{\min M_j}$$

Therefore

$$\tau_j(t) > 0 \Longrightarrow \Delta x_j(t) = \frac{M_j}{\tau_j(t)} > 0.$$

It shows a very strong coupling of thermodynamics and mesh stability.

Moving meshes in ND



j is the index of the cell, k denotes the time step. V_j^k is the volume at time step k.

We assume that a formula holds that gives the volume in function of the vertices

$$(\mathbf{x}_1, \cdots, \mathbf{x}_r, \cdots) \mapsto V_j(\mathbf{x}_1, \cdots, \mathbf{x}_r, \cdots).$$

This is the key assumption.

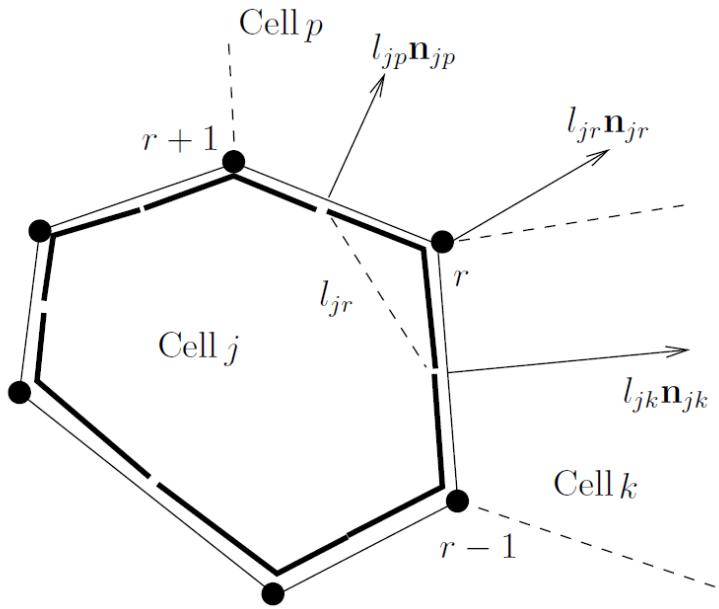
For example such a formula holds for the isoparametric element ($=Q^1$) even if the faces are **warped**.
Let us denote $\mathbf{x}^k = \left(\mathbf{x}_1^k, \cdots, \mathbf{x}_r^k, \cdots\right)$ the collection of all vertices of the mesh.
A fundamental discrete object defined even for cells with warped faces is

$$\mathbf{C}_{jr} = \nabla_{\mathbf{x}_r} V_j = \begin{pmatrix} \frac{\partial}{\partial \mathbf{x}_{r,1}} V_j \\ \cdots \\ \frac{\partial}{\partial \mathbf{x}_{r,d}} V_j \end{pmatrix} \in \mathbb{R}^d.$$

What is $\mathbf{C}_{jr}$?

• **1D** : $r = j + \frac{1}{2}$ is the vertex between j and $j+1$. Then $V_j = x_{j+\frac{1}{2}} - x_{j-\frac{1}{2}}$.
So $\mathbf{C}_{j,j+\frac{1}{2}} = 1$ and $\mathbf{C}_{j,j-\frac{1}{2}} = -1$.

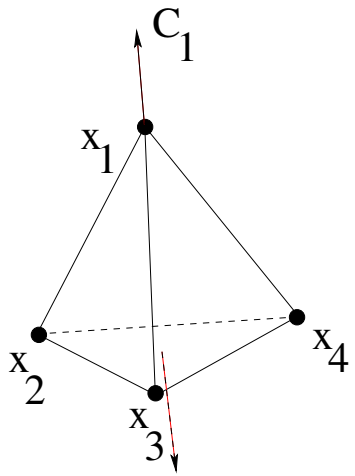
• **2D** : $V_j = \sum_r \frac{1}{2}\left(x_r y_{r+1} - y_r x_{r+1}\right) \Longrightarrow \mathbf{C}_{jr} = \frac{1}{2}\begin{pmatrix} -y_{r-1} + y_{r+1} \\ x_{r-1} - x_{r+1} \end{pmatrix}$



Answer : $\mathbf{C}_{jr} = l_{jr}\mathbf{n}_{jr}$ is a **corner generalization** of the face quantity $l_j\mathbf{n}_f$.

$\mathbf{C}_{jr}$ in 3D

- Tetrahedrons



$$\mathbf{C}_{j1} = \frac{1}{6}\left(\begin{vmatrix} y_2 & y_3 & y_4 \\ z_2 & z_3 & z_4 \\ 1 & 1 & 1 \end{vmatrix}, - \begin{vmatrix} x_2 & x_3 & x_4 \\ z_2 & z_3 & z_4 \\ 1 & 1 & 1 \end{vmatrix}, \begin{vmatrix} x_2 & x_3 & x_4 \\ y_2 & y_3 & y_4 \\ 1 & 1 & 1 \end{vmatrix} \right)^t = -\frac{1}{3} |f_{234}| \, \mathbf{n}_{234}.$$

- Hexahedrons

$$\mathbf{C}_1 = \nabla_{\mathbf{x}_1} V = \frac{1}{12} \sum_{r=2}^{8} \sum_{s=r+1}^{8} \mathbf{x}_r \wedge \mathbf{x}_s, \qquad \mathbf{x}_1, \mathbf{x}_r, \mathbf{x}_s \in \text{same face}.$$

Warped faces are allowed.

Properties

- One has

$$\frac{d}{dt} V_j = \left(\nabla_{\mathbf{x}} V_j, \mathbf{x}' \right) = \sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r \right) .$$

- By homogeneity :

$$V_j = \frac{1}{d} \left(\nabla_{\mathbf{x}} V_j, \mathbf{x} \right) = \frac{1}{d} \sum_r \left(\mathbf{C}_{jr}, \mathbf{x}_r \right) .$$

- For all cell j one has

$$\sum_r \mathbf{C}_{jr} = \mathbf{0}.$$

- For all interior vertices $\mathbf{x}_r$

$$\sum_j \mathbf{C}_{jr} = \mathbf{0}.$$

.

The mass of a Lagrangian cell is constant in time : $V_j(\mathbf{x}(t))\rho_j(t) = M_j$ is independent of the time t. So

$$M_j \tau_j'(t) = \frac{d}{dt} V_j(\mathbf{x}(t)) = \sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r \right) , \quad \tau_j = \frac{1}{\rho_j} .$$

The hydrodynamics equations imply $\rho \frac{d}{dt} \tau = \nabla \cdot \mathbf{u}$. It means that $\sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r \right)$ is an approximation in the **Finite Volume sense** of $\nabla \cdot \mathbf{u}$ over the moving cell j

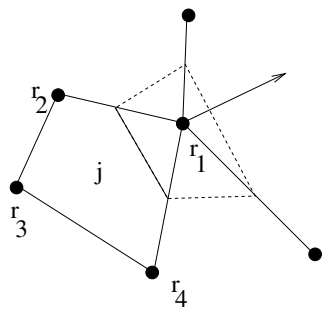
$$\int_{V_j} \nabla \cdot \mathbf{u} \, dx = \int_{\partial V_j} (\mathbf{u}, \mathbf{n}) \, d\sigma \approx \sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r \right) .$$

In some the Finite Volume scheme is **corner based**.

The nodal solver for cell centered data $(\rho_j, \mathbf{u}_j, \cdots)$

- The first formula expresses that the sum of all forces around the vertex $\mathbf{x}_r$ is zero

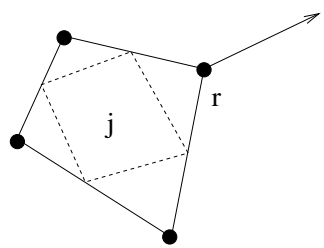
$$\sum_j \mathbf{C}_{jr} p_{jr} = 0.$$



This natural formula, also used for staggered schemes, enforces the conservation of momentum.

- The second formula is a multidimensional generalization of a first-order Riemann solver

$$p_{jr} - p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr}\right) = 0, \qquad \mathbf{n}_{jr} = \frac{\mathbf{C}_{jr}}{|\mathbf{C}_{jr}|}, \quad |\mathbf{n}_{jr}| = 1.$$



This **the magic formula** for those not acquainted wit acoustic Riemann solvers.

Solution

One can eliminate the pressures and gets a linear system : $\mathbf{A}_r \mathbf{u}_r = \mathbf{b}_r$.
The unknown vector is the node velocity $\mathbf{u}_r \in \mathbb{R}^d$. The matrix is

$$\mathbf{A}_r = \sum_j \rho_j c_j \frac{\mathbf{C}_{jr} \otimes \mathbf{C}_{jr}}{|\mathbf{C}_{jr}|} \in \mathbb{R}^{d \times d} = \mathbf{A}_r^t > 0.$$

The right hand side is

$$\mathbf{b}_r = \sum_j \mathbf{C}_{jr} p_j + \sum_j \rho_j c_j \frac{\mathbf{C}_{jr} \otimes \mathbf{C}_{jr}}{|\mathbf{C}_{jr}|} \mathbf{u}_j \in \mathbb{R}^d.$$

The solution of the linear system is $\mathbf{u}_r = \mathbf{A}_r^{-1} \mathbf{b}_r$. Once the nodal velocities $\mathbf{u}_r$ have been calculated, one computes the nodal pressures p_{jr} $p_{jr} = p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr} \right)$.

1) Compute the geometrical vectors $\mathbf{C}_{jr}^k$ for all j, r.
2) Determine the nodal velocities $\mathbf{u}_r^k$ and the nodal pressures p_{jr}^k using the nodal solver.
3) Update the momentum

$$M_j \frac{\mathbf{u}_j^{k+1} - \mathbf{u}_j^k}{\Delta t} = - \sum_r \mathbf{C}_{jr}^k p_{jr}^k.$$

The total energy is updated with

$$M_j \frac{e_j^{k+1} - e_j^k}{\Delta t} = - \sum_r \left(\mathbf{C}_{jr}^k, \mathbf{u}_r^k \right) p_{jr}^k.$$

4) Then the vertices are moved $\mathbf{x}_r^{k+1} = \mathbf{x}_r^k + \Delta t \, \mathbf{u}_r^k$.
5) Update the new density in the cell $\rho_j^{k+1} = \frac{M_j}{V_j^{k+1}}$.

Finite Volume Lagrangian cell-centered schemes are possible, but at the price of changing the notion of what is a Finite Volume flux.

Consequence : The structure of the code is slightly different.

The Kidder test problem

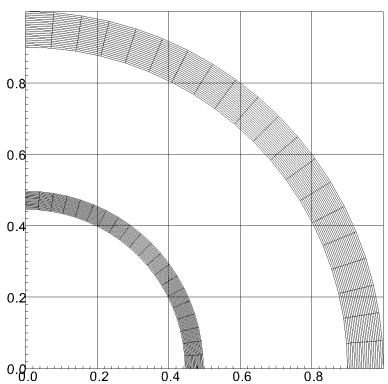
A portion of a shell $r_i = 0.9 \leq r \leq 1 = r_e$ is filled with a perfect gas. The adiabatic constant of the gas is $\gamma = 2$ in 2D and $\gamma = \frac{5}{3}$ in 3D. At at $t = 0$

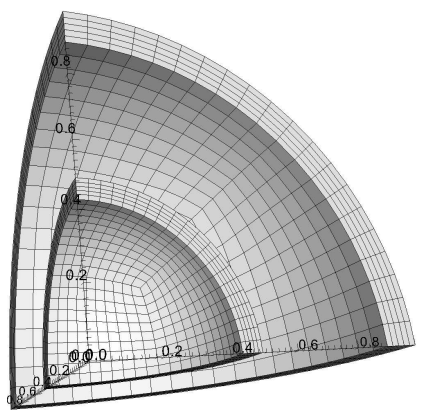
$$\rho_0(r) = \left(\frac{r_e^2 - r^2}{r_e^2 - r_i^2} \rho_i^{\gamma-1} + \frac{r^2 - r_i^2}{r_e^2 - r_i^2} \rho_e^{\gamma-1} \right)^{\frac{1}{\gamma-1}},$$

with $\rho_i = 1$ and $\rho_e = 2$. The initial the pressure is $p_0(r) = \rho_0(r)^\gamma$. The initial entropy is uniform $s_0 = \frac{p_0}{\rho_0^\gamma} = 1$. The velocity is $\mathbf{u}_0 = 0$ at $t = 0$.

Let us denote the sound speed as c. The solution is an isentropic compression ($s = \frac{p}{\rho^\gamma} = 1$) such that the position at time $t > 0$ is $R(r, t) = h(t)r$, where the compression rate is $h(t) = \sqrt{1 - \frac{t^2}{\tau_{\text{foc}}^2}}$ and the focalisation time is

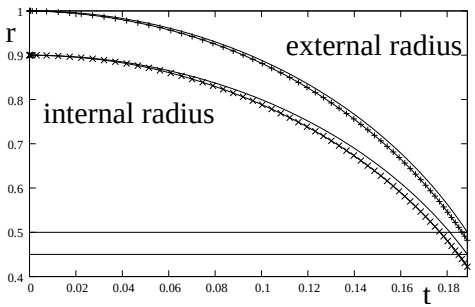
$$\tau_{\text{foc}} = \sqrt{\frac{(\gamma - 1)(r_e^2 - r_i^2)}{2(c_i^2 - c_e^2)}}.$$



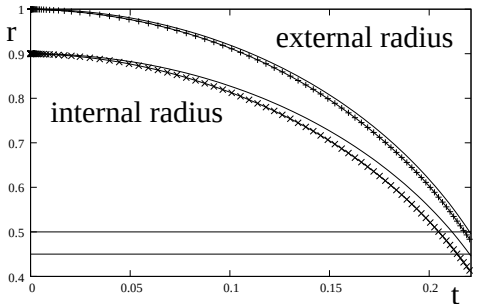


Order of convergence

The analytical solution is the continuous line, the discrete solution is plotted with symbols.



2D



3D

In 2D we used four meshes : M_1 is a $10 \times 10 = 100$ cells mesh, that is 10 sectors and and 10 layers ; M_2 is $20 \times 20 = 400$ cells ; M_3 is $40 \times 40 = 1600$ cells ; and finally M_4 is $80 \times 80 = 6400$ cells.
In 3D we use three meshes : the first mesh N_1 has 10 sectors per facets and 5 layers, since the exterior and interior boundary are designed with 3 square meshes, then the total number of cells is $3 \times 5 \times 10 \times 10 = 1500$ cells ; then we double the number of cells in each direction, that N_2 is a 12000 cells mesh ; and finally N_3 is a 96000 cells mesh. The order is one (O_1) or two (O_2).

d.	m.	o.	$r_i(t_f)$	$r_e(t_f)$	o.	$r_i(t_f)$	$r_e(t_f)$
2	M_1	O_1	0.4223	0.4820	O_2	0.4343	0.4880
2	M_2	O_1	0.4392	0.4937	O_2	0.4458	0.4966
2	M_3	O_1	0.4453	0.4975	O_2	0.4487	0.4991
2	M_4	O_1	0.4478	0.4989	O_2	0.4495	0.4997
conv. o.			≈ 1.09	≈ 1.18		≈ 1.37	≈ 1.58
3	N_1	O_1	0.4133	0.4833	O_2	0.4269	0.4885
3	N_2	O_1	0.4339	0.4929	O_2	0.4422	0.4963
3	N_3	O_1	0.4424	0.4967	O_2	0.4472	0.4987
conv. o.			≈ 1.08	≈ 1.10		≈ 1.47	≈ 1.50

Numerical analysis

We distinguish 4 properties

- Conservation : mass, momentun, total energy
- Stability : entropy

$$S_j^{k+1} \geq S_j^k \qquad \forall j$$

under ad-hoc CFL

$$\max_j \left(\frac{c_j^k}{\Delta x_j^k} \right) \Delta t^k \leq 1$$

and

$$\frac{\left| V_j^{k+1} - V_j^k \right|}{V_j^k} \leq \frac{1}{10}.$$

- Stability : mesh.
  Can we garantee that $V_j^k > 0$ for all cells j and all time step k ?
  This is completely open.
- Convergence to the Euler equations in the Lax sense.

Conservation

The nodal solver writes

$$\begin{cases} \sum_j \mathbf{C}_{jr} p_{jr} = 0, \\ p_{jr} - p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr}\right) = 0, \qquad \mathbf{n}_{jr} = \dfrac{\mathbf{C}_{jr}}{\left|\mathbf{C}_{jr}\right|}, \end{cases}$$

The momentum equation

$$M_j \frac{\mathbf{u}_j^{new} - \mathbf{u}_j}{\Delta t} = -\sum_r \mathbf{C}_{jr} p_{jr}$$

Therefore

$$\sum_j M_j \frac{\mathbf{u}_j^{new} - \mathbf{u}_j}{\Delta t} = -\sum_j \sum_r \mathbf{C}_{jr} p_{jr} = -\sum_r \sum_j \mathbf{C}_{jr} p_{jr} = 0.$$

That is by induction

$$\sum_j M_j \mathbf{u}_j^{new} = \sum_j M_j \mathbf{u}_j = \sum_j M_j \mathbf{u}_j^{ini}.$$

Similarily

$$\sum_j M_j \frac{e_j^{new} - e_j}{\Delta t} = -\sum_j \sum_r \left(\mathbf{C}_{jr} \cdot \mathbf{u}_r\right) p_{jr} = -\sum_r \left(\sum_j \mathbf{C}_{jr} p_{jr} \cdot \mathbf{u}_r \right) = 0.$$

Conservation is insuder at corners, and not at faces as in standard Finite Volume methods.

What is the method ?

Answer Use the semi-discrete scheme

$$\begin{cases} M_j \tau_j'(t) = +\sum_r \left(\mathbf{C}_{jr} \cdot \mathbf{u}_r\right) & \Longleftrightarrow \mathbf{x}_r'(t) = \mathbf{u}_r, \\ M_j \mathbf{u}_j'(t) = -\sum_r \mathbf{C}_{jr} p_{jr}, \\ M_j e_j'(t) = -\sum_r \left(\mathbf{C}_{jr} \cdot \mathbf{u}_r\right) p_{jr} \end{cases}$$

the corner flux equation

$$p_{jr} - p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \frac{\mathbf{C}_{jr}}{|\mathbf{C}_{jr}|}\right),$$

and the close contour relation

$$\sum_r \mathbf{C}_{jr} = 0.$$

The **algebra** is

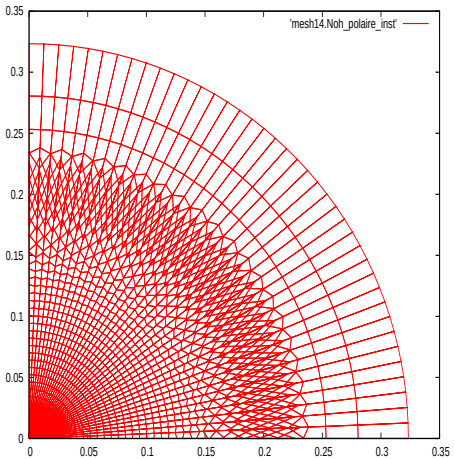
$$T_j M_j \frac{d}{dt} S_j = M_j e_j'(t) - \left(\mathbf{u}_j, M_j \mathbf{u}_j'(t)\right) + p_j M_j \tau_j'(t)$$

$$= -\sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r\right) p_{jr} + \left(\mathbf{u}_j, \sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r\right) p_{jr}\right) + p_j \sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r\right)$$

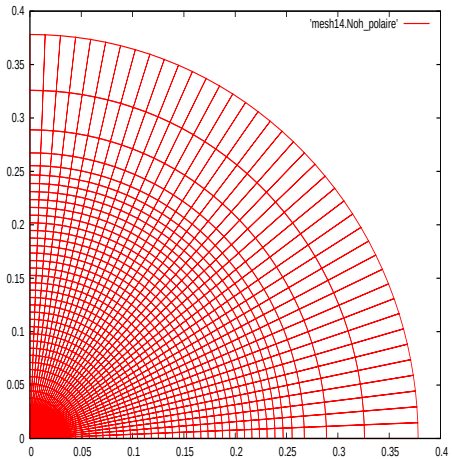
$$= \sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r - \mathbf{u}_j\right) \left(p_{jr} - p_j\right) \geq 0.$$

CQFD

Mesh stability in 2D (and nD)



spurious modes



with stabilization

Solution 1 Use only simplices (triangles, tets in 3D) : *Theorem* (with C. Mazeran). The semi-discrete scheme with simplicies is mesh-stable.

Solution 2 Use a cell-centered scheme with less (no ?) spurious modes : the CHIC scheme.

Solution 3 Use ALE (Arbitrary Lagrange Euler). This is **easy** with cell-centered schemes.

This is still a an open problem. More research is needed.

Convergence *à la Lax*

Consider a given numerical scheme for the discretization of the compressible gas dynamics system. Assume that the numerical solution is bounded in L^∞ and converges in $L^1_{\rm loc}$ to some limit. Assume that we can prove that the limit is a weak solution to

$$\left\{\begin{array}{ll} \int_{t\in\mathbb{R}}\int_{\mathbf{x}\in\mathbb{R}^d}\left(\rho\partial_t\varphi+\rho\mathbf{u}\cdot\nabla\varphi\right)dtdx=0, & \forall\varphi\in\mathcal{D}_0, \\ \int_{t\in\mathbb{R}}\int_{\mathbf{x}\in\mathbb{R}^d}\left(\rho\mathbf{u}\cdot\partial_t\varphi+\rho\mathbf{u}\otimes\mathbf{u}+p\mathbf{l}\cdot\nabla\varphi\right)dtdx=0, & \forall\varphi\in\mathcal{D}_0^d, \\ \int_{t\in\mathbb{R}}\int_{\mathbf{x}\in\mathbb{R}^d}\left(\rho e\partial_t\varphi+\rho e\mathbf{u}\cdot\nabla\varphi\right)dtdx=0, & \forall\varphi\in\mathcal{D}_0, \\ \int_{t\in\mathbb{R}}\int_{\mathbf{x}\in\mathbb{R}^d}\left(\rho S\partial_t\varphi+\rho S\mathbf{u}\cdot\nabla\varphi\right)dtdx\leq 0, & \forall\varphi\in\mathcal{D}_0^+, \end{array}\right. \tag{1}$$

where $\mathcal{D}_0$ is the set of smooth test functions with compact support, and $\mathcal{D}_0\subset\mathcal{D}_0$ is the set of smooth non negative test functions with compact support.

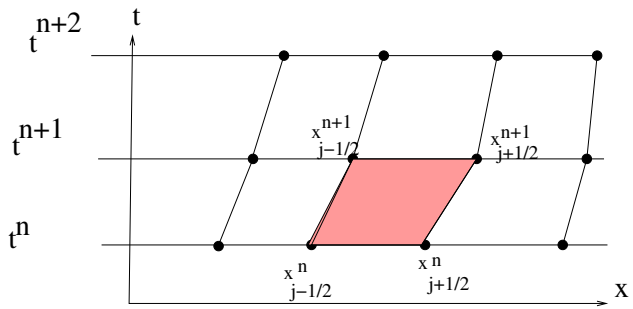
We will say that the scheme is weakly consistent.

In that game, we are allowed to add as many stability hypothesis as needed.

Theorem (2010) : Cell-centered Lagrangian schees are weakly consistent with the Euler equations of compressible gas dynamics.

Idea of the proof in 1D

Interpolate the mesh : $x_{j+\frac{1}{2}}(t) = x^n_{j+\frac{1}{2}} + (t - t^n)u^n_{j+\frac{1}{2}}$ for $t^n \leq t \leq t^{n+1}$; $\Delta x_j(t) = x_{j+\frac{1}{2}}(t) - x_{j-\frac{1}{2}}(t)$.



The red domain is $\Theta_j^{n+\frac{1}{2}} = \left\{ t^n < t < t^{n+1}, \quad x_{j-\frac{1}{2}}(t) < x < x_{j+\frac{1}{2}}(t) \right\}$.
Interpolate the numerical solution

$$\text{for } (x,t) \in \Theta_j^{n+\frac{1}{2}}, \text{ set } \begin{cases} \rho(x,t) = \dfrac{M_j}{\Delta x_j(t)}, \\ u(x,t) = u_j^n + \dfrac{t-t^n}{\Delta t}(u_j^{n+1} - u_j^n), \\ e(x,t) = e_j^n + \dfrac{t-t^n}{\Delta t}(e_j^{n+1} - e_j^n), \\ \\ \overline{u}(x,t) = \dfrac{x - x_{j-\frac{1}{2}}(t)}{\Delta x_j(t)} u_{j-\frac{1}{2}}(t) + \dfrac{x_{j+\frac{1}{2}}(t) - x}{\Delta x_j(t)} u_{j+\frac{1}{2}}(t) \neq u(x,t). \end{cases}$$

Property One has the identity

$$\partial_t \rho + \partial_x(\rho \overline{u}) = 0 \text{ in } \mathcal{D}'_{x,t}.$$

Results in multiD

One has the formula in the weak sense

$$\partial_t \rho_h + \nabla \cdot (\rho_h \bar{\mathbf{u}}_h) = A^1, \qquad \text{with } A^1 = \sum_j \left[\rho_j \left(\nabla . \bar{\mathbf{u}}_j - \frac{1}{V_j(t)} \int_{\Omega_j(t)} \nabla . \bar{\mathbf{u}}_j dx \right) \right] \mathbf{1}_{\mathbf{x} \in \Omega_j(t)}.$$

One has the formula

$$\partial_t (\rho_h \mathbf{u}_h) + \nabla \cdot (\rho_h \mathbf{u}_h \otimes \bar{\mathbf{u}}_h) = B^1 + B^2 + B^3$$

in the weak sense, where the interpolation error in space is

$$B^1 = \sum_j \left[\rho_j \mathbf{u}_j \left(\nabla . \bar{\mathbf{u}}_j - \frac{1}{V_j(t)} \int_{\Omega_j(t)} \nabla . \bar{\mathbf{u}}_j dx \right) \right] \mathbf{1}_{\mathbf{x} \in \Omega_j(t)},$$

the interpolation error in time is

$$B^2 = - \sum_j \left[\left(\frac{\mathbf{1}_{\mathbf{x} \in \Omega_j(t)}}{V_j(t)} - \frac{\mathbf{1}_{\mathbf{x} \in \Omega_j^k}}{V_j^k} \right) \sum_j \mathbf{C}_{jr}^k p_{jr}^k \right],$$

and the approximation of $-\nabla p$ is

$$B^3 = - \sum_j \left[\sum_r \mathbf{C}_{jr}^k p_{jr}^k \right] \frac{\mathbf{1}_{\mathbf{x} \in \Omega_j^k}}{V_j^k}.$$

Fundamental property

Theorem
Assume that the speed of sound is within the bounds $0 < \alpha_1 \leq \rho_j c_j < \alpha_2$ everywhere. Assume that the mesh is regular in the sense $\alpha_3 h^d \leq V_j$ and diam $(\Omega_j) \leq \alpha_4 h$ for all cells, with uniform constants $\alpha_3, \alpha_4 > 0$. Assume that (p_j) and $(\mathbf{u}_j)$ are bounded in L^∞ and are bounded in BV in the sense

$$\sum_j \sum_{k \in V(j)} h^{d-1} \left| p_j - p_k \right| \leq \alpha_5 \text{ and } \sum_j \sum_{k \in V(j)} h^{d-1} \left| \mathbf{u}_j - \mathbf{u}_k \right| \leq \alpha_6 .$$

Then $B = -\nabla p + O(h)$ in the weak sense. The residual $O(h)$ depends on the smooth test function $\varphi \in \mathcal{C}_0^2$.

The key property is the identity

$$\sum_r \mathbf{C}_{jr} \otimes \mathbf{x}_r = V_j \, \mathbf{I}_d$$

where $\mathbf{I}_d \in \mathbf{R}^{d \times d}$ stands for the identity matrix in dimension d.

The same identity seems essential in the recent works Droniou, Eymard, Herbin,Gallouet about the consistency of the diffusion equation.

Conclusion of the day

- Lagrangian methods are central for the simulation of ICF flows.
- Ongoing research show good potential of cell-centered schemes. The CHIC scheme is now routinely used for Direct Drive at CELIA.
- GLACE is less viscous (more accurate) than CHIC, but needs more stabilization.
- In 3D, GLACE is more natural than CHIC.
- Weak consistency is proved. It validates the use of such methods for ICF compressible flows with shocks.
- Coupling with radiation is an issue.