Mesh Quality and conservative projection in Lagrangian compressible hydrodynamic

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Roma, December 2007

OUTLINE

1. A good alternative method to Lagrangian code: non direct ALE (Arbitrary Lagrangian Eulerian)
   - ALE (1) : Rezone = Smoothing mesh process
     - Escobar Optimization process extended to arbitrary connectivity
     - Control Of Quality: Nodal quality definition & consequences
   - ALE (2) : Remapping = Conservative interpolation
     - Approximations of the Exact problem
     - Maximum principle and second order
2. Cemracs Project 2007: Adding Adaptation between Lagrangian and ALE
   - Dynamic polygonal adaptation with "Welding" lines
   - A strategy

Lagrangian step 1

Conservations Laws :

$$\begin{cases} D_t\rho + \rho\nabla.u = 0, & \text{mesh is moving with speed flow} \\ \rho D_t u + \nabla P = 0, & \\ \rho D_t E + \nabla.(Pu) = 0. & \end{cases} \quad (1)$$

ρ density, u speed, E total energy, ϵ internal energy.
PROS: Pure Lagrangian formulation permits:

1. cell mass conservation.
2. if multi-materials then it keeps non diffused interfaces between each.

CONS: The counter parts, the mesh "quality" can become "very bad" very quickly (non convex quads, tangled mesh ...). The mesh quality may become very bad very quickly (non convex quads, tangled mesh ...)

Lagrangian Step 2

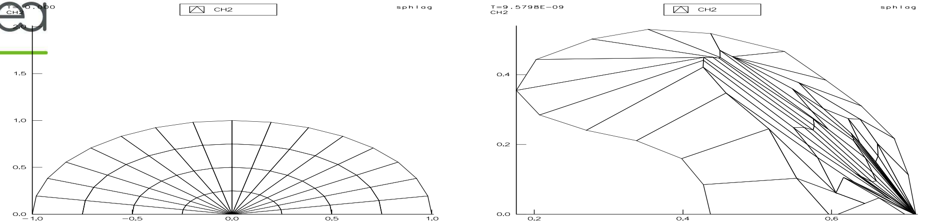
Mainly 3 different Lagrangian schemes:

1. Staggered (Wilkins type: 1964, and new ones Shashkov and al.)
    1. Mixed Q1/P0 (Speed/Thermo).
    2. Internal energy formulation $D_t\epsilon + PD_t\frac{1.}{\rho} = 0$.
    3. **hourglass** correction (non physical oscillation of quad. mesh).
    4. **Pseudo viscosity** (for shocks in speed/pressure).
2. Centered (Despres/Mazeran 2002 and Maire/Breil 2003)
    1. All variables are centered (finite volumes type).
    2. Nodal fluxes (compatiblity of mesh movement and continuity equation).

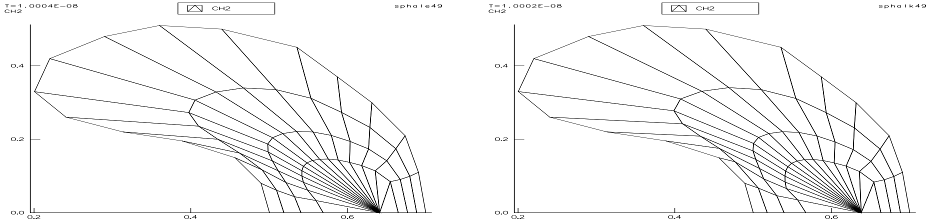
    Centered version are very simple to implement... still in improvement...

We principally use Lagrangian schemes for quadrangular types of meshes, but VERY interesting for problems involving layers, symetries ..

Gains with non direct ALE (Rezone+Remapping)



Lagrangian Computation of an half ball with external pressure (Initial/final Time)



ALE Computation without and with special care to non convex cells

Generality on numerical simulations

Lagrange scheme go far . . . BUT generic difficulties :

1. Interacting shocks can destroy mesh quality.
2. High curvature of interfaces and boundaries (with fast variations), especially for rarefaction waves from a solid into a light material (vaccum).

Consequences

1. **problem 1** thermal conduction (if coupling), diffusion scheme are very sensitive wrt mesh.
2. **problem 2** hydrodynamic (time step very small)

→*Mesh Smoothing : keep same mesh connectivity*

→*Need to define the unkonwn on this new mesh*

Rezoning process

Here, we want to use smoothing methods that keep the **same** connectivity of the Lagrangian mesh.

Two main ways:

1. Approximate regularizing PDE problem.
2. Approximate an optimization problem: $\min F_i(x)$ (cost function).

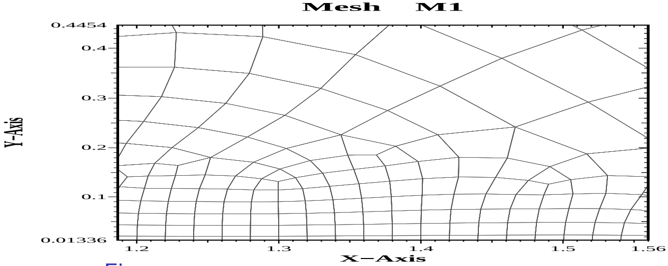
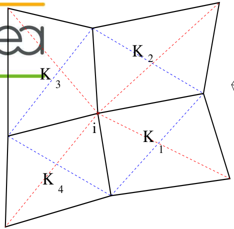
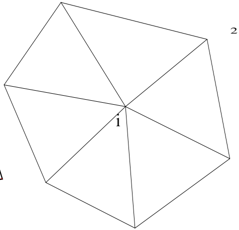


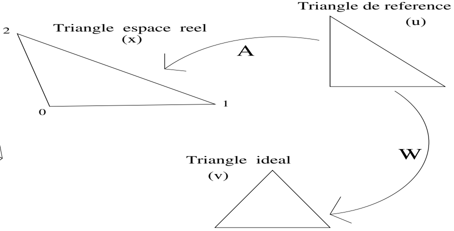
Figure: typical arbitrary mesh : node with 3,4 ou 5 connexion

We use an extension of Escobar smoothing (untangled tetrahedral mesh and smooth), the cost function is defined **everywhere**!!
Our modification is in the adaptation to arbitrary connectivity.

Escobar : Detail in a simplex







Linear application from Ideal to real space : $x - x_i = Sv$ avec $S = AW^{-1}$.

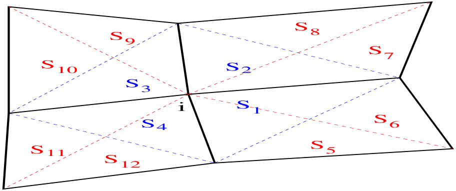
1. Cell quality: $q(S) = \frac{2}{|S||S^{-1}|}$, Frobenius Norm: $|S| = \sqrt{tr({}^tSS)}$, $\Sigma = \sigma S^{-1}$, with $\sigma = det(S)$, **ideal := equilateral**.

2. Objectif function associated to the m^{eme} simplex $f_m = 1/q(S)$, $f_m = \frac{|S_m||\Sigma_m|}{2\sigma_m}$ BUT $\sigma_m > 0$ . . . modification: $\tilde{f}_m = \frac{|S_m||\Sigma_m|}{\sigma_m + \sqrt{\sigma_m^2 + \epsilon}}$, is defined on the whole space!
   Escobar : local Functionnal : $F_i(x) = \sum_{m=1}^{NbSimplexe} \tilde{f}_m$.

Extension by adaptation w.r.t connectivity

For arbitrary meshes, we do not know about the ideal triangle : W ? ..
For each simplex, we will introduce a parameter (W_α), and we will adapt this to the non homogeneous local connectivity arround each node:

$$W_\alpha = \begin{pmatrix} 1 & cos(\alpha) \\ 0 & sin(\alpha) \end{pmatrix} \qquad S^\alpha = AW_\alpha^{-1}$$



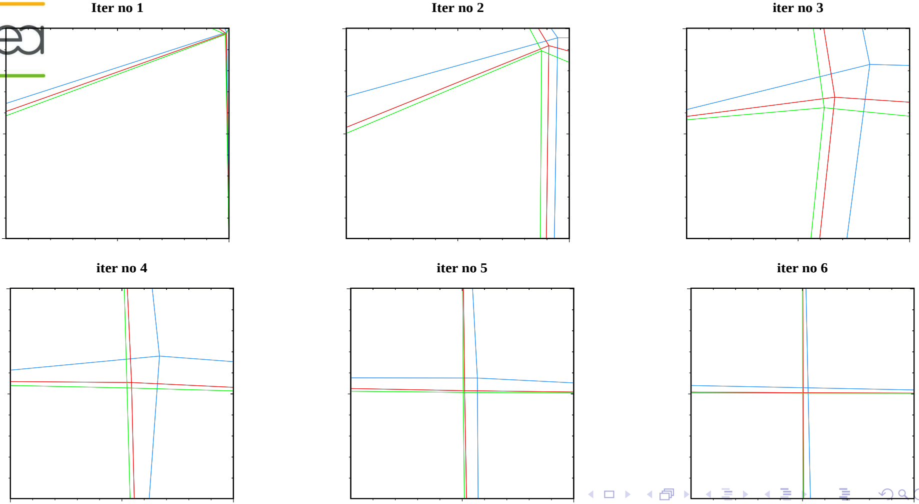
Adapatation of the parameter

1. For internal simplices : $\alpha = \frac{2\pi}{\mathbf{degree(i)}}$
2. For external simplices belonging to the m'th cell:

$$\alpha = \frac{\mathbf{2\pi}}{\mathbf{degree(i)(number\_of\_nodes(m)} - \mathbf{2)}}$$

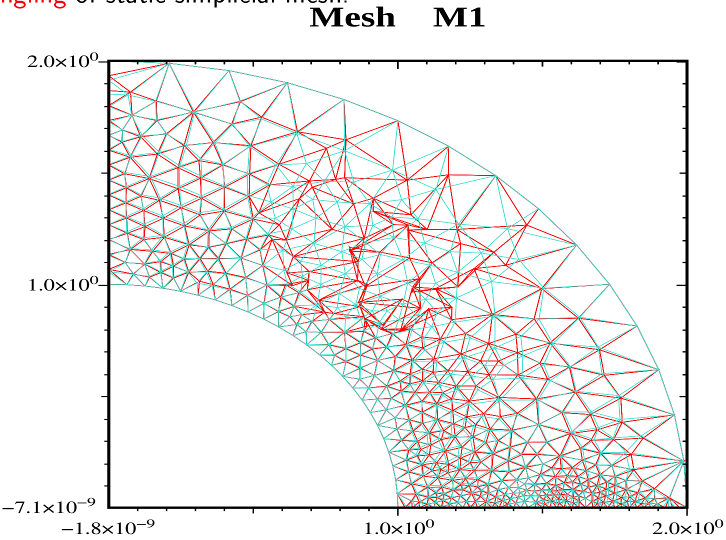
ESCOBAR_MULTI_CONNEXION : Analytic test case

Bad initial aspect ratio, Classical Escobar (red, $\alpha = \pi/3$), Escobar ortho (blue, $\alpha = 0$), and new Escobar (green, α connectivity adaptation) .



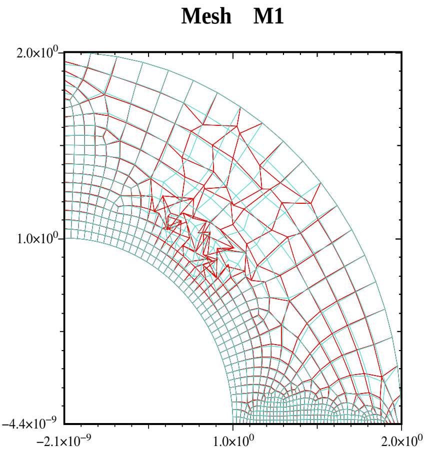
ESCOBAR_MULTI_CONNEXION : TEST CASE 1

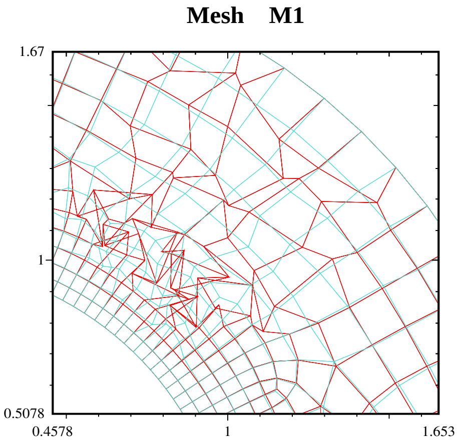
Untangling of static simplicial mesh.



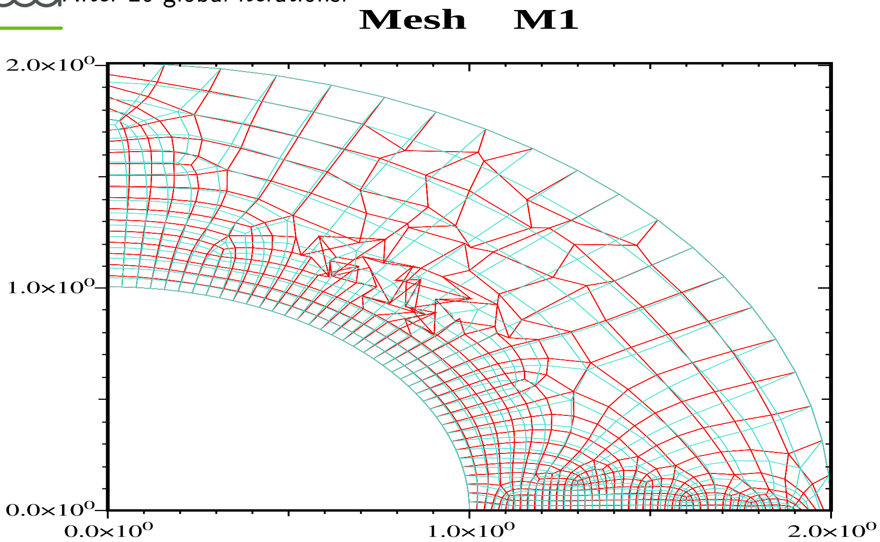
ESCOBAR_MULTI_CONNEXION : TEST CASE 2

Untangling quadr. mesh, 2 iterations





After 20 global iterations.



What to remind

Escobar with adaptation W^{α} :

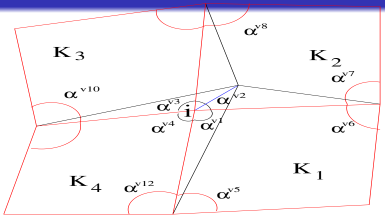
1. Extension of Escobar functionnal with arbitrary connectivity.
2. Speed to convergence is faster than original Escobar.
3. Warning : No preservation of aspect ratios.

Remarque

1. *Practically (coupling with hydrodynamic), we* **never go until convergence**.
2. *The smoothed mesh need to be* **as close as possible to the Lagrangian grid**.
3. *The optimization algorithms are much more time consuming than elliptic ones (Tipton/Jun).*

We need to control very closely the quality of the ALE mesh...

Control Of Quality: Nodal quality definition, consequences



Definition

Q_i *Nodal Quality of i, 3 ex.:*

1. $Q_i^{sin} = \min sin(\alpha^v)$ *(to keep symmetries/and or keep local orthogonality).*
2. $Q_i^{sin,rel} = \dfrac{\min sin(\alpha^v)}{\max(\max sin(\alpha^v), |\min sin(\alpha^v)|)}$
3. $Q_i^{aire,rel} = \dfrac{\min Aire^v}{\max(\max Aire(\alpha^v), |\min Aire(\alpha^v)|)}$ *(to keep good aspect-ratio).*

Properties: $-1 \leq Q_i \leq 1$

$Q_i \simeq 1$: locally optimal

$Q_i \leq 0$: local degeneracy (non convex cell, tangling, ...)

Definiton of the Quality of a mesh M

$\mathbf{Q_i^M}$: Nodal Quality for node i in mesh M.

Definition

Q^M : Quality of M, **2 choices***:*

- $Q_\infty^M = \min_i \mathbf{Q_i^M}$
- $Q_1^M = \frac{1}{N_v} \sum_i^{N_v} \mathbf{Q_i^M}$ *(N_v : Number of vertices)*

Q_{ref} : global reference quality.

$Nb^M(Q_{ref})$: Number of nodes such that $\mathbf{Q_i^M} < Q_{ref}$.

Q_∞^M is for the vertex having the lesser nodal quality.
If $Q_\infty^M >= Qmin$, then stay automatically Lagrangian (good for shocks arrival times).

Consequence 1: We can compare 2 meshes M_1 et M_2

If we want to hunt the non convex cells ($Q_i < 0$),

Definition

M_1 is better than M_2 iff:

1. If $Q_\infty^{M_1} > 0$ and $Q_\infty^{M_2} > 0$
   - $Q_\infty^{M_1} > Q_\infty^{M_2}$ **and** $Nb^{M_1}(Q_{ref}) \leq Nb^{M_2}(Q_{ref})$, *OR*
   - $Q_\infty^{M_1} \geq Q_\infty^{M_2}$ **and** $Nb^{M_1}(Q_{ref}) < Nb^{M_2}(Q_{ref})$, *OR*
   - $Q_\infty^{M_1} = Q_\infty^{M_2}$ **and** $Nb^{M_1}(Q_{ref}) = Nb^{M_2}(Q_{ref})$ **and** $Q_1^{M_1} > Q_1^{M_2}$
2. $Q_\infty^{M_1} > 0$ *and* $Q_\infty^{M_2} < 0$
3. If $Q_\infty^{M_1} < 0$ and $Q_\infty^{M_2} < 0$
   - $Q_1^{M_1} > Q_1^{M_2}$ **and** $Nb^{M_1}(Q_{ref}) \leq Nb^{M_2}(Q_{ref})$
   - $Q_1^{M_1} \geq Q_1^{M_2}$ **and** $Nb^{M_1}(Q_{ref}) < Nb^{M_2}(Q_{ref})$

Consequence 2 : Non-linear nodal mesh Relaxation

Definition

*Let M^1 and M^2 (**close enough**) with the **same connectivity**, and Q_i^M a nodal quality function, we define a third M^3 by :*

$$\forall i,\ \ i^{th} \text{ vertex of } M^3 : \qquad M_i^3 = M_i^1 + w(Q_i^{M^1}, Q_i^{M^2})(M_i^2 - M_i^1)$$

$w(Q_i^{M^1}, Q_i^{M^2})$ *is a weight function with values in [0,1].*

Exemples

1. $w(Q_i^{M^1}, Q_i^{M^2}) = \frac{1+Q_i^{M^1}}{2+Q_i^{M^1}+Q_i^{M^2}}$ ($Q_i^{M^1}$ and $Q_i^{M^2} \neq -1$)
2. Heaviside kind process:
$$w(Q_i^{M^1}, Q_i^{M^2}) = \begin{cases} 0, & si\ \ Q_i^{M^1} > Q_i^{M^2}, \\ 1, & sinon. \end{cases}$$
The last (the bounds are always reached for every node) is called the **"intersected " mesh**.

Properties

Properties

1. Independent of the numbering, the build is very fast (only positions differs)
2. M^3 is close to M^1 and M^2.
3. CONS: No order preservation of the qualities : $Q_i^{M^1} > Q_i^{M^2}$ do not implies $Q_i^{M^3} \geq Q_i^{M^1} > Q_i^{M^2}$!!!!

Practically, we need to test the quality of the third mesh (see. Oxford 2005).

Consequence 3 : Nodal Priority order for Mixing between algorithms

Let a nodal quality mesh function be given, we can define a priority order of the nodes.

Exemple:

1. $(Q_i^M \geq Q^*)$: then elliptic algorithm with Jacobi update (Titpon or Jun).
2. $(Q_i^M \leq Q^*)$: then optimization algorithm with Gauss-Seidel update (Escobar type).

Remarque

1. *Speed Gain is between 5 and 10 (wrt to full optimization).*
2. *We can conserve symmetries, orthogonality and aspect ratio with the two first nodal quality function (sin based).*

In practice : How to deal with all this new features

1. Independent of the smoothing algorithm.
2. Compatibility with any kind of nodal statute (depending on criteria such as angles, area, etc) definition of degrees of freedom set.
3. Adaptative (in time) nodal quality function between Q_i^{sin} and Q_i^{area} with some sensor for symmetries and orthogonality.
4. Choice of the "best mesh" among all of global iteration, stop if satisfactory, if not we use non linear relaxation (sometimes you may need to remove the proximity of the smoothed mesh).
5. Candidates for meshes M1 and M2 in the choice of "better mesh" are: Lagrangian, Euler, Smoothed, or any intermediate (Lagrange/Smoothed or Euler/Smoothed) etc ...

In summary, this approach can be viewed as an **over layer** with previous versions of ALE smoothing, and at the end, we can check Q_∞^M, Q_1^M and $Nb^M(Q_{ref})$ for both Lagrangian and final smoothed mesh.

Exact problem of Conservative interpolation

Discrete balance [Margolin,Shashkov]: $K_i^N = K_i^A \cup \left(\cup_{j \in V(K_i^A)} K_i^N \cap K_j^A\right) / \left(\cup_{j \in V(K_i^A)} K_i^A \cap K_j^N\right)$

$$\int_{K_i^N} QdV = \int_{K_i^A} QdV + \sum_{j \in V(K_i^A)} F_{ij}^Q \tag{2}$$

Quantity $F_{ij}^Q \stackrel{def}{=} \left[\int_{K_i^N \cap K_j^A} QdV - \int_{K_i^A \cap K_j^N} QdV\right]$ is the exact flux (but we have to compute intersection between 2 meshes).

$$F_{ij}^Q = -F_{ji}^Q, \tag{3}$$

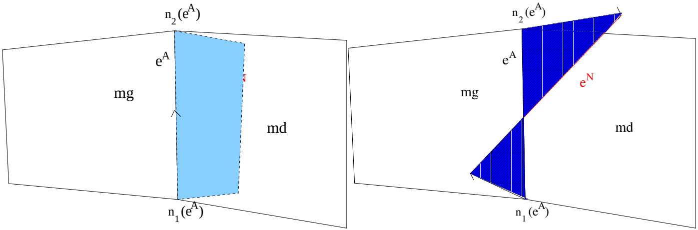
First order scheme:

$$|K_i^N|\bar{Q}_i^N = |K_i^A|\bar{Q}_i^A + \sum_{j \in V(K_i^A)} \left(|K_i^N \cap K_j^A|\bar{Q}_j^A - |K_i^A \cap K_j^N|\bar{Q}_i^A\right) \tag{4}$$

Positivity condition : $|K_i^A| > \sum_{j \in V(K_i^A)} |K_i^A \cap K_j^N|$, gives a local maximum principle (wrt Edge and Corner neighborood).

Approximation 1: No intersection computing

Approximated flux are computed by swept **regions** δF_{ik}.: Algebraic volumes swept by the edges displacement.



First order Flux δF_{ik} : donor cell interpretation

First Order [Margolin,Shashkov]

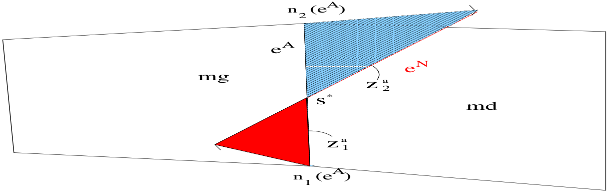
$$F_{ik}^{sda,1} = max(0, V(\delta F_{ik}))\bar{Q}^A_{mv(i,k)} + min(0, V(\delta F_{ik}))\bar{Q}^A_i$$

Positive scheme: $|K_i^A| > |\sum_{V(\delta F_{ik})<0} V(\delta F_{ik})|$, gives a local maximum principle (wrt Edge neighboorood).

Approximation 2: self-intersection scheme (more accurate)

Definition

Self-intersection flux, *is a flux that eventually compute a "self-tangled" patch created by edge displacement :* $e^A \cap e^N = \{S^*\}$ *and* $S^* \neq \{\emptyset\}$



Self-intersection flux

The first order self intersection flux:

$$G_e^Q = \sum_{k=1}^{nblmt(e)} sign(m, e, k) V(Z_k^a) Q_k^e$$

Positivity: $|K_i^A| > |\sum_{V(Z_i^A)<0} V(Z_k^a)|$ gives a local maximum principle

Specific energie, and speed

Projection $\rho^A \to \rho^N$ and $(\rho e)^A \to (\rho e)^N$ and $e^N := \frac{(\rho e)^{\boldsymbol{N}}}{\rho^{\boldsymbol{N}}}$.

For second order, two approach:

1. Linear representation (ρe):

$$(\rho e)^{1,h} = (\rho e)_j + \nabla(\rho e)_j(x - x_j) \tag{5}$$

   BUT no maximum principle in e even if true for ρ AND ρe.

2. Indeed (5) rewrite cf ([W.B. VanderHeyden, B.A. Kashiwa]) $(\rho e)^{1,h} = \rho_j e_j + e_j \nabla \rho_j (x - x_j) + \rho_j \nabla e_j (x - x_j)$ and then:

$$e^{1,h} = e_j + \frac{\rho_j(x - x_j)}{\rho_j + \nabla\rho_j(x - x_j)} \nabla e_j \tag{6}$$

   Non-linear representation of e, Dukowicz/Kodis limitor (maximum principle).

We do the same with the speed (on the dual mesh if staggered hydro).

Numerical study of the projection for specific energy and speed

We consider 3 options:

I Volumes Fluxing computation (2 options) :

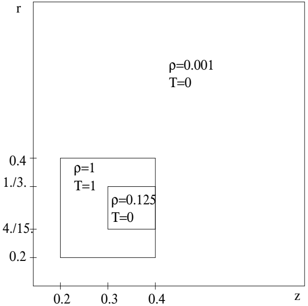
- (0) Without self-intersection.
- (1) With self-intersection.

II The gradient are computed by Green formula and the limitation is based on a maximum principle (Dukowicz-Kodis).

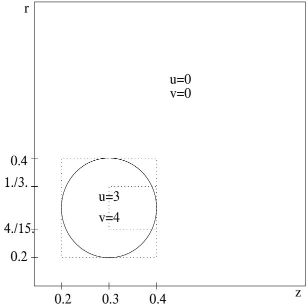
1. The limitation for **specific quantities** : s_j (projection of ρs_j)
   - (0) Non linear limitation (first ρ and on s_j)
   - (1) Linear limitation (on ρs_j)
2. and **the speed**
   - (-1) First Order
   - (0) Non linear limitation (idem specific quantity)
   - (1) Linear limitation (idem specific quantity)

Initial Data

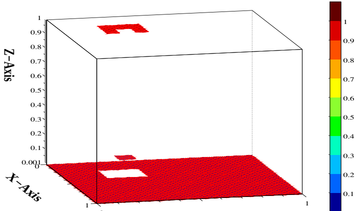
Initial conditions (density/temperature) and speed:

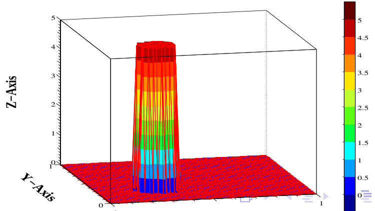


Densite ini



Norme vitesse ini





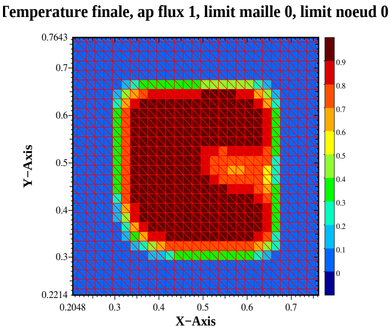
Influence on specific quantity : I

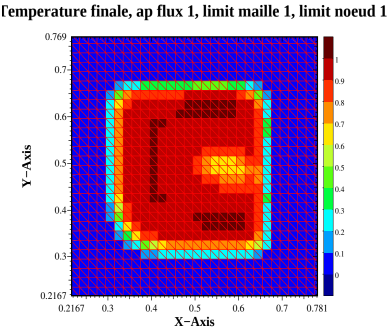
Test Case : Advection (diagonale direction (.005,0.005))

Recall : density min/max initial :0.001/1, temperature min/max initial : 0/1.

nx	Flux	Limit. maille	density min/max	Temperature min/max
50	0/1	0	0.001/0.953157874	0/0.999775443
50	0/1	1	0.001/0.953157874	0/1.023732158

Non respect of global maximum principle on temperature for linear limiteur.





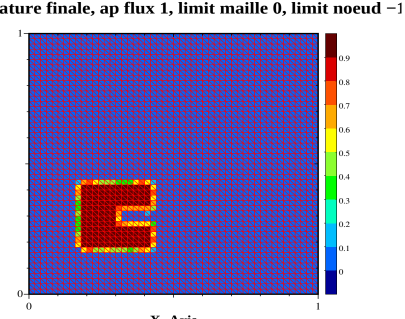
Influence on specific quantities : II

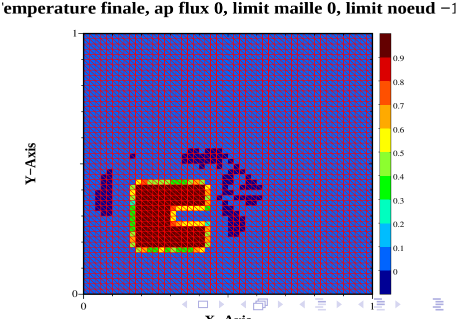
Test Case : Random Cyclique Rezoning

Recall : density min/max initial : 0.001/1, temperature min/max initial : 0/1.

nx	Flux	Limit. cell	density min/max	Temperature min/max
50	1	0	0.001/0.999994937	0/0.999999724
50	1	1	0.001/0.999994937	0/1.000276494
50	0	0	0.000999984/0.999997086	-0.000008013/0.999999854
50	0	1	0.000999984/0.999997086	-0.000015653/1.000144011

Non respect of global maximum principle on density and temperature if no self-intersection.

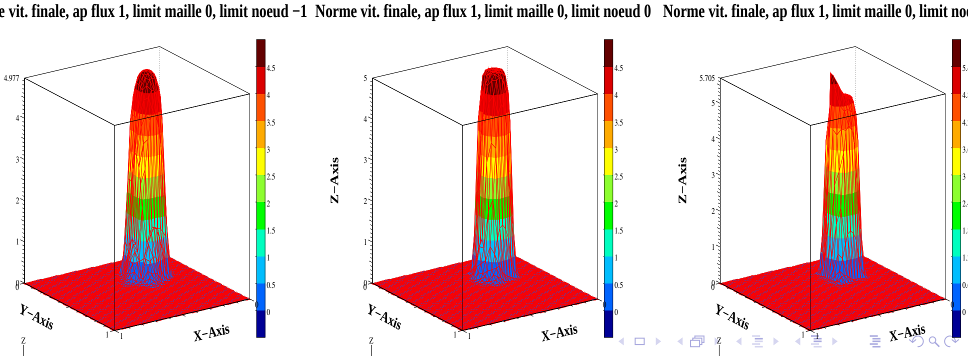




Influence on speeds: cyclique Rezonning

Recall : Norm of the speed min/max initial : 0/5

nx	Flux	Node Limit	norm vit min/max
50	1	-1	0/4.976664317
50	1	0	0/4.999652095
50	1	1	0/5.705191088
50	0	-1	0/4.977538773
50	0	0	0/4.999712297
50	0	1	0/5.704911304



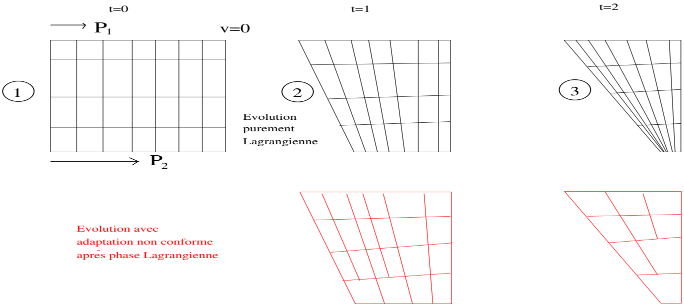
Conclusion on projection

The projection with the following options gives the best results:

1. self-intersection
2. Linear limitation on ρ primal and non-linear on specific quantities (e ...)
3. Linear limitation on ρ dual and non-linear on speed.

Cemracs project : Improving ALE results ....

Collaboration : Sandrine Marchal (Institut Elie-Cartan Nancy), Yana Vasilenko (University of West Bohemia in Pilsen), Amir Ali Feiz (Université de Marne La Vallée Champs sur Marne).



In some situations, we need to clear and/or add some elements.... the smoothing process is quiet robust, and we do so that we want this step to be as few as possible (in time and space).

Project (cont)

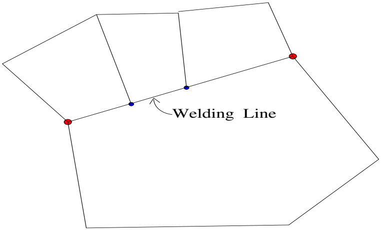
1. We want to essentially keep quadrangles after this process (because of layers and symmetries), but we can admit some triangles.
2. We have an ALE code : Lagrangian + Rezone + Remapping **(first order)**, with swapping adaptation if triangles.

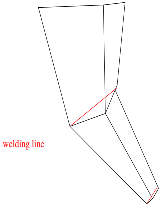
At the end, we want to obtain such a general scheme:

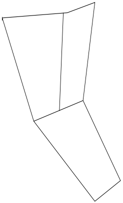
1. **Lagrangian** step,
2. refinement/unrafinement study and **Adaptation**,
3. **Rezone** and **Remapping**.

Adding dynamically simplified non conformal cells

The aim is to study a non-conformal strategy with “welding” line (a line with End Point called Masters Nodes and arbitrary number of Slaves Nodes distributed on it) see Fig.



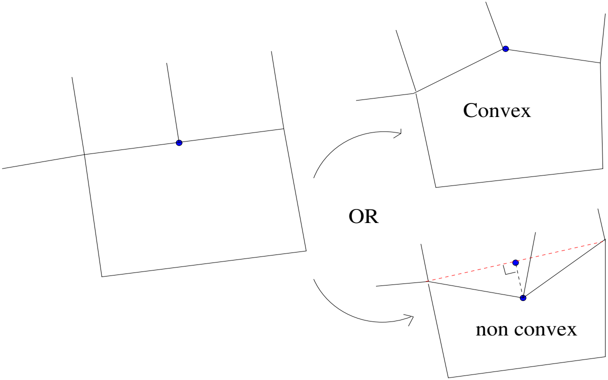




This straight line will take place of edges for which the aspect ratio is under some tol.
A way to obtain a conservative step, is the computation of the intersection between this line and some (very few) elements.

Strategy

(1) **Lagrange Step**: A Centered Lagrangian scheme is used to march in time with ALL the nodes considered as degree of freedom (meaning that slaves nodes of a welding line are moved without any constrained to slip along the two master end points).



Strategy (Cont)

(2) **Adaptation Step**:

(a) See Previous Fig. Orthogonal projection of slaves nodes on the line defined by master endpoints in the case of non convex cells around any of slaves (or we can do it each times). Computation of new conservative quantities over the new moved cells by self intersection flux (=exact problem).

(b) Refinement study with some criteria (geometrical/physic), see details after. Computation of new conservative quantities is straigthforward for first order scheme. To obtain convex sub-cells there are 3 ways:

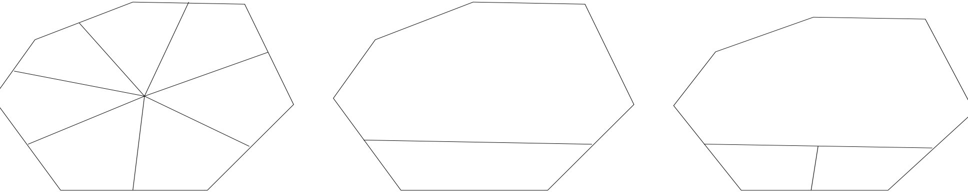


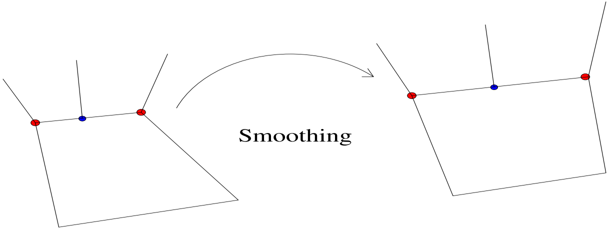
Figure: Isotropic 1D Quasi 1D

(c) Unrefinement study with some criteria (geometrical/physic), see details ... Computation of new conservative quantities is done by clipping (or self intersection...).

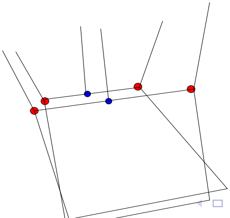
Strategy (Cont)

(3) **ALE Step**:

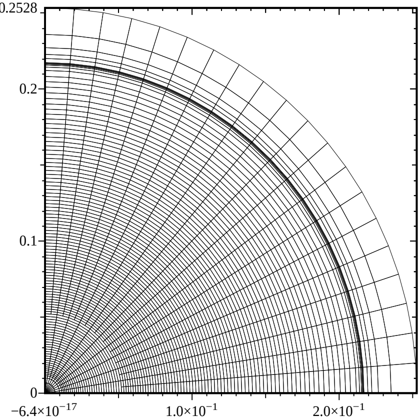
(a) Slaves nodes are moved after the movement of Masters endpoints.

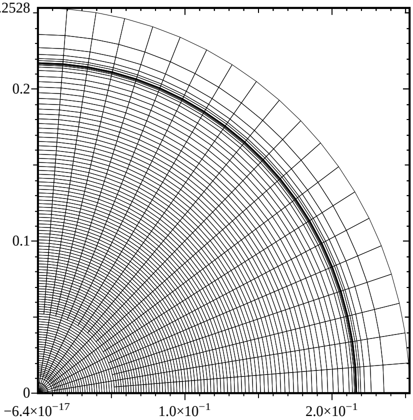


(b) Self intersection (or clipping) is used.

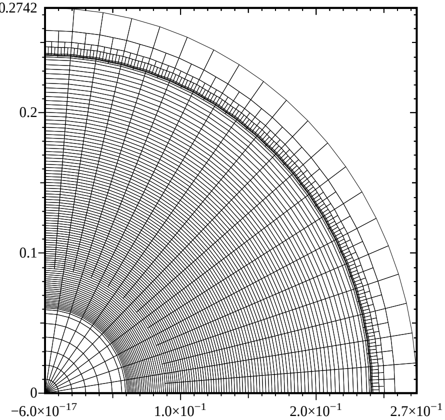


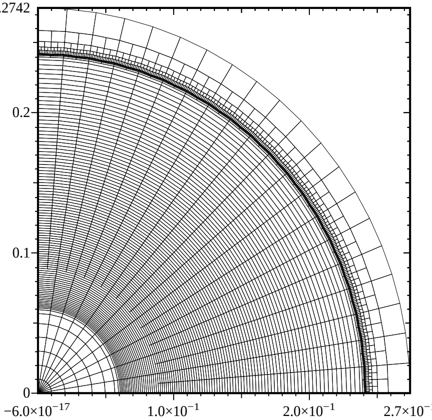
Refinement strategies I: dynamical refinement by Layer



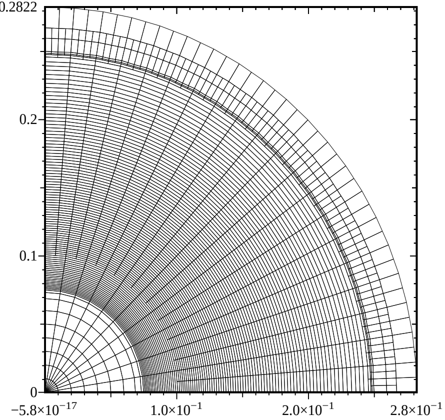


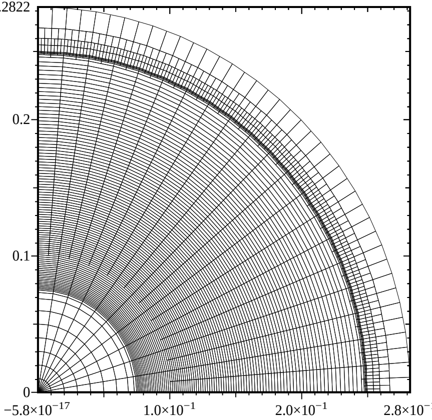
Refinement strategies II: dynamical refinement Quasi 1D



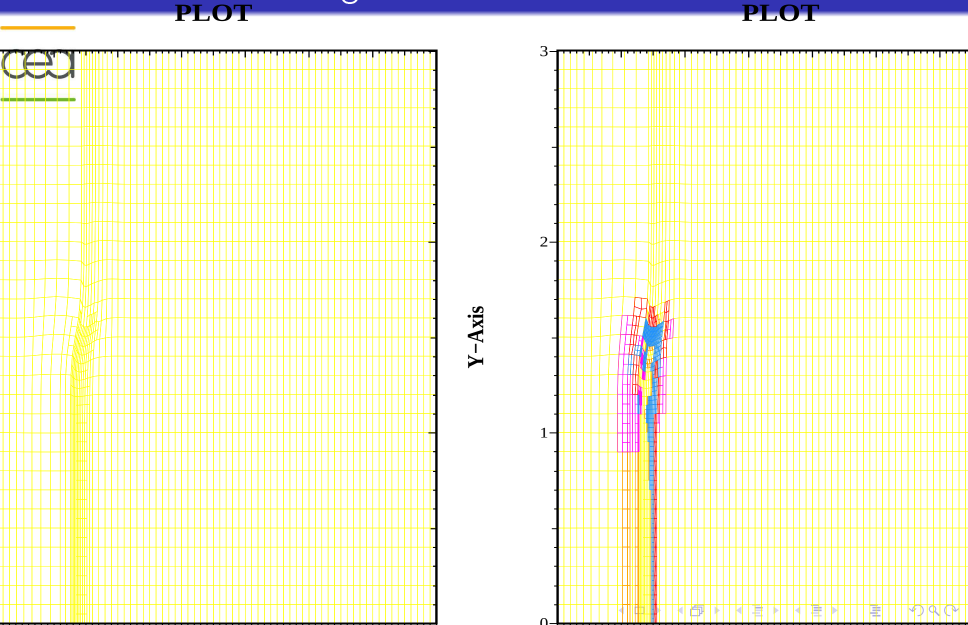


Refinement strategies III: dynamical refinement isotropic (AMR like)

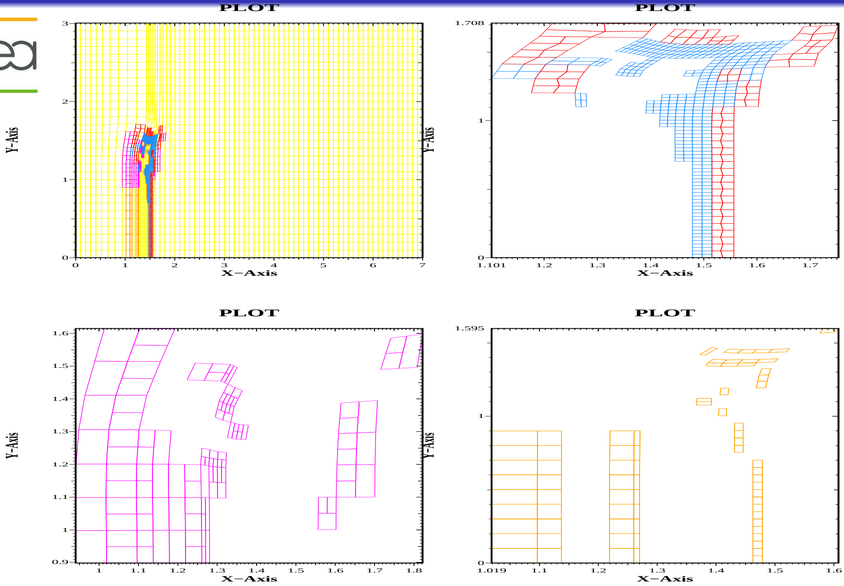




Refinement strategies IV: mixted refinement



Cont. ZOOM of each Refinement Situation



Prospects

(0) Strategy more or less generic wrt Lagrangian hydro (at least centered scheme of Despres/Mazeran and Ph Maire/Breil).

(1) For refinement, the AMR-ALE is recover as a special case among the 3 generic cases that we propose here (genericity for any convex polygonal cells).

(2) Test and implement a simplified computation of a generic building of welding line for unrefinement step.

(3) Improving tests for adaptation... Help us for good error estimators (anisotropic) !!