DE LA RECHERCHE À L'INDUSTRIE

Local convex-Hull preserving second-order extension for cell-centered ALE schemes

2013 MultiMat - San Francisco | Hoch P., Labourasse E.

03 September 2013

www.cea.fr

Outline

Summary/Objectives

1) Second-order or higher centered scheme using local reconstruction (gradient or higher-order terms) are made local bound preserving [HAL]* [MOOD]# for scalar quantities (or component wise) with a post-process on arbitrary mesh connectivity

   *[HAL] P. Hoch,"An arbitrary Lagrangian-Eulerian strategy to solve compressible flows", Technical Report, CEA. HAL :hal-00366858.Available at :<http ://hal.archives-ouvertes.fr/docs/00/36/68/58/PDF/ale2d.pdf>,2009.

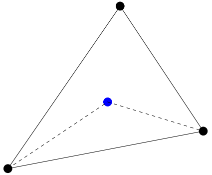
   #[MOOD] S.Clain, S. Diot, R Loubère, "A high-order finite volume method for systems of conservation laws-Multi-Dimensional Optimal Order Detection (MOOD)", J. of Comput. Physics, 230, pp 4028-4050,2011

2) On other hand, [VIP]% uses an intrinsic definition of vector limitation using a convex-Hull of neighboor values giving admissibility criteria for the linear reconstruction.

   %[VIP] G. Luttwak, F. Falkovitz,"Slope Limiting for vectors : a novel limiting algorithm", Numerical Methods in Fluids, 65, 2011.

We essentially want to couple 1) and 2).

Convex-Hull characterization of data $\{\mathbf{v_j}\}_{\mathbf{j=1}}^{\mathbf{M}}$



initial-hull — convex-hull

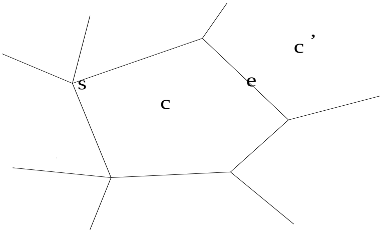
convex-hull construction : smallest convex set containing data

Characterization

$$\mathbf{v}_j \in \mathbb{R}^d, \quad CvxH(\{\mathbf{v}_j\}) = \left\{ \sum_j \lambda_j \mathbf{v}_j, \ \lambda_j \in \mathbb{R}^+ \ \sum_j \lambda_j = 1 \right\}.$$

1. Definition is invariant wrt uniform rotation/translation.
2. Useful convex-Hull relationship :
   (a) $CvxH(\{v^* + \{v_j\}\}) \subset CvxH(\{v^* + CvxH(\{v_j\})\})$.
   (b) If dimension d=1, $CvxH(\{v_j\}) = [min_j(v_j), max_j(v_j)]$.
   (c) If d=2, but one dimensional symmetry, same as (b) for non-constant component.

Connectivity Neighborhood definition



For cell data, there are many choices :

1. cell/edge : Neigh_e(c)
2. cell/node : Neigh_s(c), cell/face in three dimension.

Neigh(c) is a generic cell neighborhood of cell c (in practice Neigh_s(c)).

Local Convex-Hull Preservation : LCHP (stability)

Let us consider a generic scheme S discretizing the evolution of a vector field $\mathbf{u}$, acting on a mesh $\mathcal{M}^n$, eventually depending on Δt^n. $S(\mathcal{M}^n, \mathcal{M}^{n+1}, R^{\mathbf{u}}(x))$ is defined by it's (cell) reconstruction $R^{\mathbf{u}}(x)$.

Definition

For a given neighborhood of cell c, $Neigh(c)$, we say that if

$$\mathbf{u}_C^{n+1} \in CvxH(\{\mathbf{u}_c^n, \{\mathbf{u}_{c'}^n\}_{c' \subset Neigh(c)}\})$$

S verifies Local Convex-Hull Preservation (LCHP).

In the same spirit of Luttwak and Falkovitz for spatial reconstruction (not sufficient to obtain time stability LCHP ..), **LCHP is a natural extension for vector to scalar local bound preservation**.

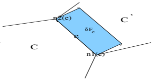
First-order remapping scheme

Remap with grid velocity $\mathbf{u^g}$: for Q $= 1,\ \rho,\ \rho\mathbf{u},\ \rho E$

$$\frac{d}{dt}\int_c Q dx = \int_{\partial c} Q(\mathbf{u^g}.\mathbf{n}) ds.$$

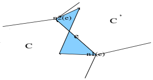
The flux on edges between cells c and c' is denoted $F_{cc'}$ and is given by any of the three schemes :

1. Swept :



$$F^{swept}_{cc'} = \delta V^{cc'} Q^{cc'} = \max(0, \delta V^{cc'}) Q_{c'} + \min(0, \delta V^{cc'}) Q_c.$$

2. Self-intersection :



$$F^{self}_{cc'} = \sum_{k=1}^{nblmt(cc')} \delta V_k^{cc'} Q_k^{cc'}, \quad \delta V_k^{cc'} Q_k^{cc'} = \max(0, \delta V_k^{cc'}) Q_{c'} + \min(0, \delta V_k^{cc'}) Q_c.$$

3. Exact Intersection.

Properties : First order remapping scheme

$c^+ = \{c' \subset Neigh(c), \delta V_{cc'} > 0\}$, $c^- = \{c' \subset Neigh(c), \delta V_{cc'} < 0\}$, $\nu_c = \frac{\sum_{c' \in c^-} |\delta V_{cc'}|}{|c|^n}$.

1. DGCL :

$$|c|^{n+1} = |c|^n + \sum_{c' \in c^+} |\delta V_{cc'}| - \sum_{c' \in c^-} |\delta V_{cc'}|, \;\; with \;\; \nu_c \leq 1 \tag{1}$$

2. Density : ρ

$$|c|^{n+1} \rho_c^{n+1} = |c|^n \rho_c^n + \sum_{c' \in c^+} |\delta V_{cc'}| \rho_{c'}^n - \sum_{c' \in c^-} |\delta V_{cc'}| \rho_c^n \tag{2}$$

   is ConVex ComBination (CVCB) due to (1)

3. Momentum : $\rho \mathbf{u}$

$$|c|^{n+1} (\rho \mathbf{u})_c^{n+1} = |c|^n (\rho \mathbf{u})_c^n + \sum_{c' \in c^+} |\delta V_{cc'}| (\rho \mathbf{u})_{c'}^n - \sum_{c' \in c^-} |\delta V_{cc'}| (\rho \mathbf{u})_c^n \tag{3}$$

   also (CVCB) and $\mathbf{u}_c^{n+1} \in CvxH(\{u_c^n, \{u_{c'}^n\}; c' \in c^+\})$ due to (1)(2).

4. Total Energy : ρE same stability as (3) for (massic) scalar quantity.

(INtrinsic) a Posteriori ITerAtive LImitation : (IN)-APITALI

Let a "second-order" scheme for a **volumic** quantity $\mathbf{f^v} \in \mathbb{R}^{d \geq 1}$:

$$\mathbf{f^v}_c^{n+1} = S(\mathcal{M}^n, \mathcal{M}^{n+1}, R^{\mathbf{f^v}}(x)_c = \mathbf{f^v}_c + \alpha_c^{(i)} (\nabla \mathbf{f^v})_c (x - x_c)) \qquad (4)$$

$\forall c$, the sequence $\alpha_c^{(i)}$, $i \in Nn \subset \mathbb{N}$ is such that :

1. $\alpha_c^{(0)} = 1$.
2. $0 \leq \alpha_c^{(i+1)} \leq \alpha_c^{(i)}$.
3. Nn is a finite set.

LCHP enforcement : if cell c does not verify (LCHP) criteria for (4)

(a) In cell c : $\alpha_c^{(i)}$ is multiplied by $\kappa_1^{(i)} < 1$.

(b) In the neighborhood $c' \in Neigh(c)$: $\alpha_{c'}^{(i)}$ is multiplied by $\kappa_2^{(i)} \leq 1$.

(c) $i \rightarrow i + 1$ and re-evaluate (4).

Remarks

1. Existence : $\exists$ at least a sequence verifying (LCHP).
   For instance $\alpha_c^{(1)} = 0, \ \forall c$.
2. Aim/Goal : Construct a sequence "as close to 1 as possible" to obtain better accuracy (APITALI sequence contains a distance measure to unlimited gradient) ... Challenging.
3. Interpretation : Iterative projector onto CvxH.
4. For scalar value, APITALI "reduces" to MOOD with card{Nn}=2.
   In this case, if cell does not verify (LCHP), $\alpha_c^{(1)} = 0$, $\alpha_{c'}^{(1)} = 0$: it acts like an instant diminution of the polynomial degree's.
5. In practice $(\nabla \mathbf{f^v})_c$ is preliminarily limited with a VIP procedure, in order to reduce the number of APITALI iterations, but it is not theoretically mandatory.

Massic (scalar/vector) quantity

For the remapping of a weighted quantity of type (ρf), $f = E$ or $f = \mathbf{u}$, LCHP must be applied to f :

1. Use previous APITALI principle on $f^v = \rho$, let $\nabla^\infty \rho$ be the final gradient such that ρ_c^{n+1} is LCHP.
2. Construct an APITALI sequence $\beta_c^{(i)}$ on the following scheme :

$$\begin{cases} \mathbf{f}_c^{n+1} := \frac{(\rho \mathbf{f})_c^{n+1}}{\rho_c^{n+1}}. \\ \mathbf{f}_c^{n+1} = S(\mathcal{M}^n, \mathcal{M}^{n+1}, R^\rho(x)_c, R^{\mathbf{f}}(x)_c = \mathbf{f}_c + \frac{\rho_c}{\rho_c + \nabla^\infty \rho_c (x - x_c)} \beta_c^{(i)} \nabla \mathbf{f}_c (x - x_c)) \end{cases} \quad (5)$$

Remarks

1. (5) comes from $\nabla(ab) = b\nabla a + a\nabla b$ and $R^f(x) = \frac{R^{\rho f}(x)}{R^\rho(x)}$ .. non linear reconstruction (see VanderHeyden and Kashiwa (JCP 1998)).
2. $\exists$ at least a sequence verifying (LCHP). For instance $\beta_c^{(1)} = 0, \ \forall c$.
3. Aim/Goal : (same f^v) Construct a sequence "as close to 1 as possible".
4. Mood cannot maintain high-order due to linear reconstruction.

Practical issues

1. Due to DGCL error ($\varepsilon^{machinery}$), the test of being inside CvxH must be true up to this $\varepsilon^{machinery}$.
2. In the sequel, the sequence $\alpha_c^{(i)}$ (also $\beta_c^{(i)}$) are constructed by : $\alpha_c^{(i+1)}(\nabla\mathbf{Q})_c := \nabla\mathbf{Q}_c^{(i+1)}(= \alpha_c^{(i)}\nabla\mathbf{Q}_c^{(i)}..)$

$$\begin{cases} \dfrac{\alpha_c^{(i+1)}}{\alpha_c^{(i)}} & = \quad \kappa_1 = 0.5, \qquad \textit{if} \;\; i < I^*, \\ \\ \alpha_c^{(i+1)} & = \quad 0, \qquad \textit{else}. \end{cases}$$

(same for c' : $\kappa_2 = \kappa_1$.)
3. card(Nn) $= 20$ (Maximum Number of Iteration after what $\alpha_c^{(i)} = 0$ for c not LCHP (and c').)
4. I^* is user defined. In practice we use $I^* = card(Nn) - 1$.

How it works..

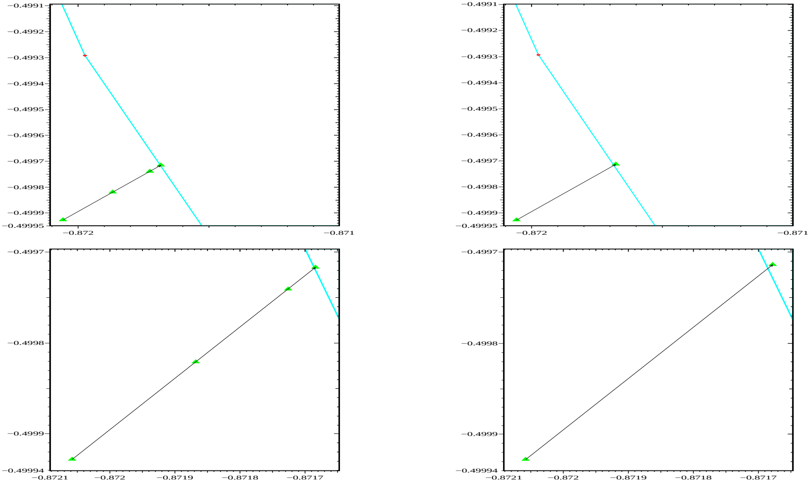


FIGURE : Comparison between APITALI (convergence to LHCP in 4 iter) and vanishing gradient after first iteration ($I^* = 1$), card(Nn)=20 for both

Rezone+Remap : Recipes of case tests

Initial cartesian grid, smooth data, smooth cyclic rezone :

$$\mathbf{u^g} = c(t) \begin{pmatrix} \sin(5\pi x)\cos(5\pi y) \\ \cos(5\pi x)\sin(5\pi y) \end{pmatrix} \qquad \begin{pmatrix} \rho \\ u_x \\ u_y \\ E \end{pmatrix} = \begin{pmatrix} 4 + c1\sin(4\pi x)^2 \\ c1\sin(4\pi x)\cos(4\pi y) \\ c1\sin(4\pi y)\cos(4\pi x) \\ 5 + \exp(\pi x) \end{pmatrix}$$

L1 error :

nx	density (ρ)	x-velocity (u_x)	y-velocity (u_y)	massic energy (E)
51	0.2752	0.3951	0.4071	0.0872
101	0.1104	0.1075	0.1160	0.0259
201	0.0281	0.0269	0.0292	0.0066
401	0.0070	0.0067	0.0073	0.0016

Second order for all quantities (APITALI sequence acts on very few cells and converge in at most two iterations).

Second-order extension for the Lagrangian hydrodynamics

Lagrange step of the Lagrange+Remap algorithm :

- Cell-centered schemes (Glace[‡] or Eucclhyd[¶]).
- Second order Runge-Kutta time integration.
- Least-squares procedure for the gradients of the spatial MUSCL reconstruction.
- Barth-Jespersen[♭] limiter for pressure 2nd-order extension.
- VIP[%,*] limiter for velocity 2nd-order extension (cf next slide).

‡ B. Després and C. Mazeran, Arch. Rational Mech. Anal., 2005.

¶ P.-H. Maire, R. Abgrall, J. Breil and J. Ovadia, SIAM J. Sci. Comput., 2007.

♭ T. J. Barth and D. C. Jespersen, AIAA Paper 89-0366, 1989.

% G. Luttwak and J. Falkovitz, Int. J. Numer. Meth. Fluids, 2010.

* M. Kucharik, M. Shashkov, ECCOMAS, 2012.

Focus on VIP for Cell-Centered schemes : outline

The Goal is to compute $\mathbf{u}_{cs}^{\mathcal{R}}$ the reconstruction at the vertex s of the cell c velocity $\mathbf{u}_c$, to "feed" the Rieman invariant :

$$\forall c, \forall n, p_{cs}^* - p_{cs}^{\mathcal{R}} + \alpha_c(\mathbf{u}_s^* - \mathbf{u}_{cs}^{\mathcal{R}}) \cdot \mathbf{n}_{cs} = 0.$$

$\mathbf{u}_{cs}^{\mathcal{R}}$ is computed as

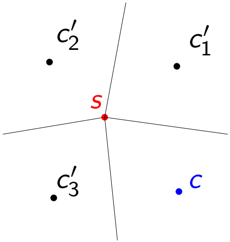
$$\mathbf{u}_{cs}^{\mathcal{R}} = \mathbf{u}_c + \mathbf{w}_{cs},$$

where $\mathbf{w}_{cs} = \mathcal{P}_{CvxH(cs)}(\nabla \mathbf{u}_c \cdot (\mathbf{x}_s - \mathbf{x}_c))$ is the reconstructed and limited gap from $\mathbf{u}_c$ to $\mathbf{u}_{cs}^{\mathcal{R}}$.

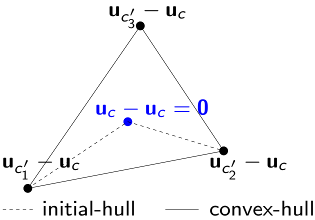
$\mathcal{P}_{CvxH(cs)}(\mathbf{v})$ operates a "limitation" of $\mathbf{v}$ with respect to the convex-Hull $CvxH(cs)$.

if $\mathcal{P}_{CvxH(cs)}(\mathbf{v}) = \mathbf{0}, \forall \mathbf{v}, \forall c, \forall s$, the scheme is first-order in space.

Focus on VIP for Cell-Centered schemes : definition of convex-Hull



Stencil for $CvxH(cs)$



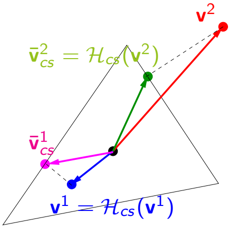
Example of $CvxH(cs)$

For each zone c and each vertex s, we define $CvxH(cs)$ as follow :

$$CvxH(cs) = CvxH(\{\mathbf{u}_{c'} - \mathbf{u}_c ; c' \in Neigh_s(c)\}).$$

This way the convex-Hull is "centered" in $\mathbf{u}_c$, and $\mathcal{P}_{CvxH(cs)}(\mathbf{v}) = \mathbf{0}$ gives the first-order scheme.

Focus on VIP for Cell-Centered schemes : limitation procedure



examples of projection

We call $\bar{\mathbf{v}}_{cs}$ the projection of $\mathbf{v}$ on $\partial CvxH(cs)$.

Let define : $\mathcal{H}_{cs}(\mathbf{v}) = \begin{cases} \mathbf{v} \text{ if } \mathbf{v} \in CvxH(cs), \\ \bar{\mathbf{v}}_{cs} \text{ else.} \end{cases}$

We take

$$\mathcal{P}_{CvxH(cs)}(\mathbf{v}) = \varphi(r)\mathcal{H}_{cs}(\mathbf{v}),$$

with $r = \frac{|\bar{\mathbf{v}}_{cs}|}{|\mathbf{v}|}$.

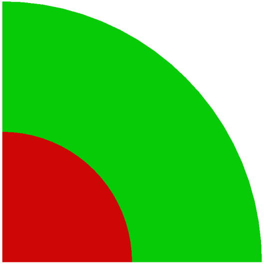
In general we simply use $\varphi(r) = 1$, recovering the classical Barth-Jespersen limiter for scalar. Any usual fonction φ can also be used to recover the corresponding limiter for scalar quantities.

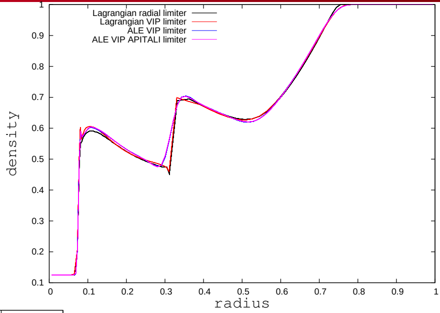
The whole reconstruction procedure is rotationally invariant.

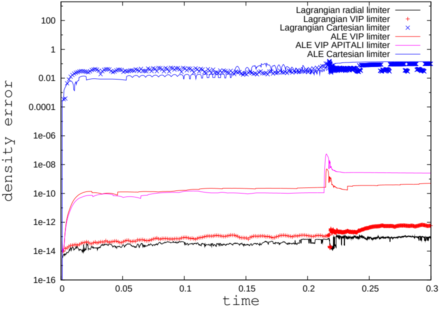
Numerical test problems

1. 2D Sod on polar grid
2. 2D Noh problem on a Cartesian grid.
3. 2D-axysimetric instability problem.

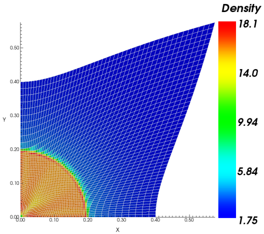
Sod on polar mesh



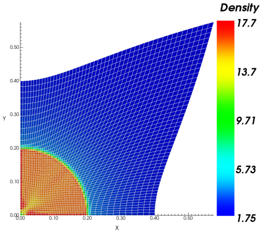




Cylindrical Noh problem on a 50×50 Cartesian grid



Lagrangian

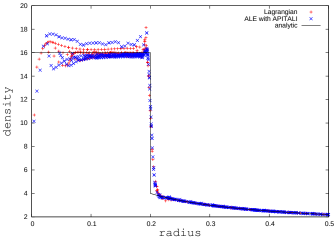


ALE with APITALI

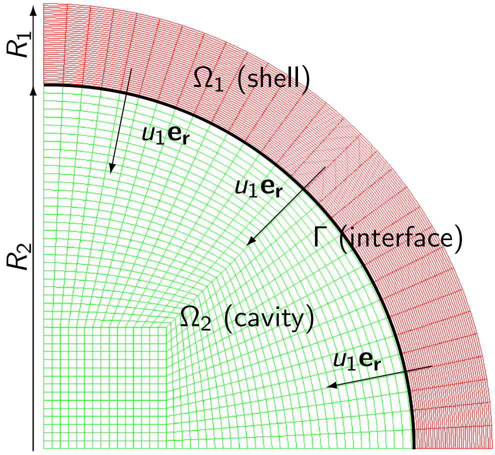
- Lagrange step with Eucclhyd and VIP
- Remap step with VIP and APITALI

Because of nearly zero initial internal energy, this case is challenging for ALE.

Without APITALI, ALE simulation quickly crashes due to overestimation of the velocity, causing negative internal energy after projection.



2D-axysimetric instability problem : configuration



Initial conditions :

- For Ω_1 :
$\rho_1 = 1,\ p_1 = 1,\ u_1 = -10,\ R_1 = 0.55.$
- For Ω_2 : $\rho_2 = 0.125,\ p_2 = 1,\ u_2 = 0,\ R_2 = 0.45.$
- For Γ (perturbed interface) :
mode 6 (Legendre), amplitude $a_0 = 10^{-3}$.

Boundary Conditions :

Symmetry on the axis, $p = 1$ on the surface of the sphere.

Meshing :

- For Ω_1 :
(M1) 30 slices, automatic refinement criteria (ARC) for layers (2.5×10^{-3}).
- For Ω_2 :
(M1) 15×15 square box, then 30 layers.
- (M2) : (M1) refined by a factor of 2.
- (M3) : (M2) refined by a factor of 2.
- (M4) : (M3) refined by a factor of 2.

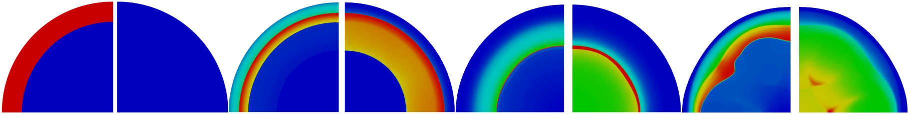
Parameters :

- Stopping time $t_{sale} = 0.08$ (ALE),
$t_{slag} = 0.04$ (Lagrangian).
- ARC disabled at $t = 0.05$ when mixing between Ω_1 and Ω_2 allowed.
- Free ALE (no Lagrangian constraints - no criteria).
- Small amount of subzonal entropy† on the external boundary.

† B. Després, E. Labourasse, J. Comput. Phys., 2012

2D-axysimetric instability problem : maps

$t = 0$	$t = 0.019$	$t = 0.038$	$t = 0.057$
density pressure	density pressure	density pressure	density pressure

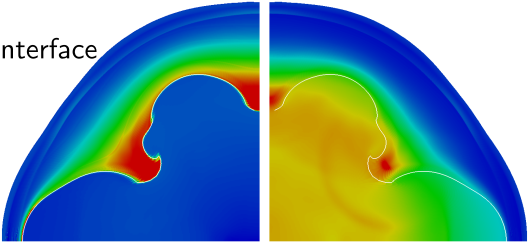


initial state	converging shock (until ~ 0.028)	diverging shock/ interface crossing	expansion phase

$t = t_{sale}$

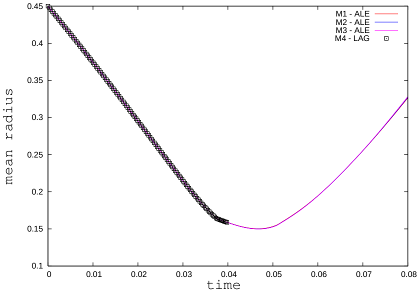
density pressure

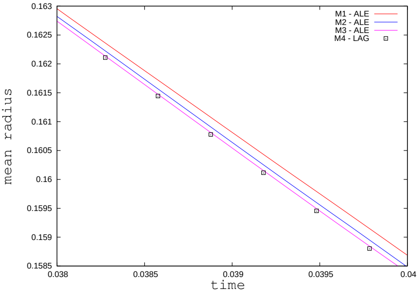
White line $\equiv$ interface



2D-axysimetric instability problem : mean flow

Radius of the interface versus time :
(LAG $\equiv$ Lagrangian with VIP limitation - ALE $\equiv$ this method)

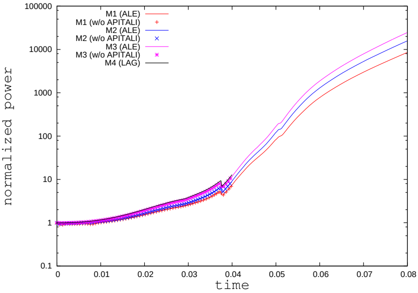


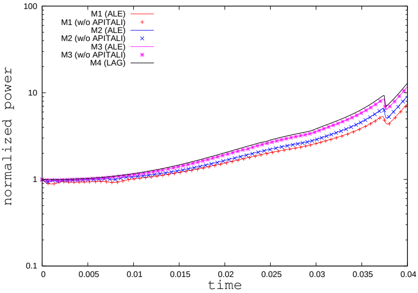


The mean flow is almost converged on the coarsest M1 mesh.

2D-axysimetric instability problem : convergence study on the 6^{th} mode

Normalized power (a^2/a_0^2) of the 6^{th} mode versus time :
(w/o APITALI $\equiv$ this method without the maximum principle enforcement)



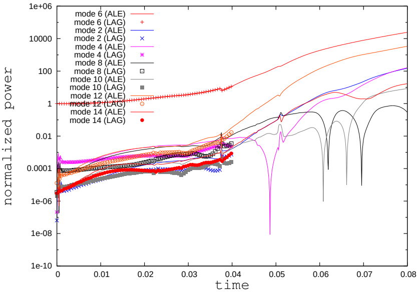


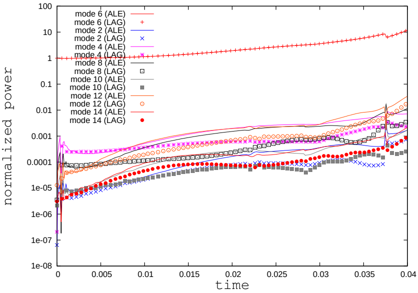
Convergence is almost achieved on the (M3) mesh until the interaction of the interface with the diverging shock.

The iterative enforcement of the maximum principle has almost no impact on the result, except on the robustness.

2D-axysimetric instability problem : modal analysis

Normalized power (a^2/a_0^2) of the modes 2, 4, 6, 8, 10, 12 and 14 : (on the (M3) mesh)



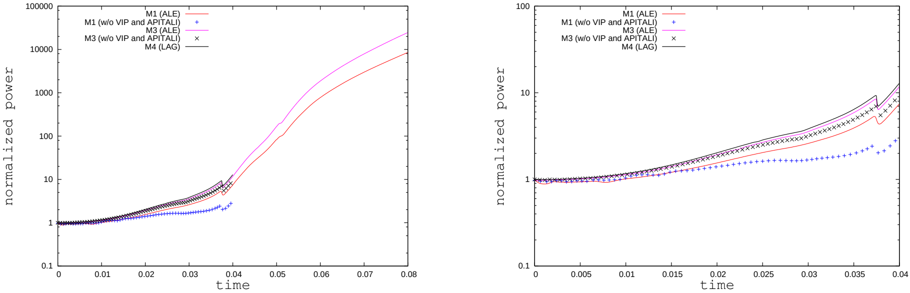


All the amplitudes (except for mode 6) remain negligible until t_{slag}. The first harmonic (mode 12) is then by far the most amplified.

Until t_{slag}, growth of mode 6 is very similar for LAG and ALE.

2D-axysimetric instability problem : effect of the rotational invariance

Normalized power (a^2/a_0^2) of the 6^{th} mode versus time :
(w/o VIP $\equiv$ component by component limiter)



As expected, component by component limiter fails to predict the correct growth rate on the (M1) coarsest mesh...

...but do converge.

Conclusion and prospects

- Conclusion
  - Design of an algorithm enforcing maximum principle on velocity, while remapping momentum.
  - Algorithm takes benefit of convex-Hull concept and iterative a posteriori procedure (APITALI), time stability for each variable is obtained in an intrinsic way (scalar or vector data).
  - Properly coupled with a rotational invariant Lagrange solver for Euler equations (using VIP limitation for vectors), the whole ALE algorithm is rotational invariant.
  - The whole limitation procedure (Lagrange + Remap) extends naturally to higher-order fluxes.
  - Relevant test problems show the benefit of the procedure.
- Prospects
  - Application to higher-order ALE schemes.
  - Extension to tensor limitation and 3D.