Adaptive multiresolution for the simulation of multi-species, compressible, viscous flows.

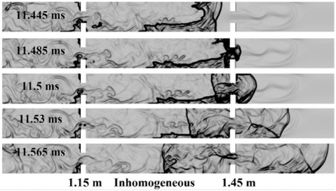
Christian TENAUD [1]

[1] Laboratoire EM2C - CNRS UPR 288, Gif-Sur-Yvette, France.

Evian-Le-Bains; 14th June 2022

Introduction

Multiple time and space scales: flame acceleration in H_2 / Air mixing.



From L. R. Boeck *et al.* (2016), Shock Waves 26: 181–192.

Simulations need **capturing time and space multiple scales**
from 1 m à 100μm and from 1 s à 10μs

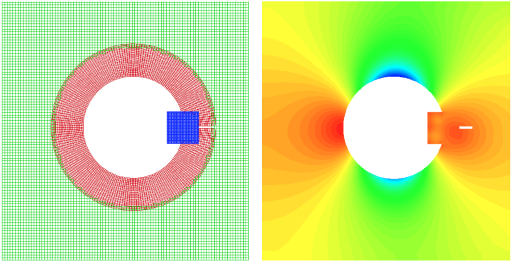
- Compressible effects: high gradients and discontinuities;
- Thermodiffusive instabilities and turbulence;
- Large Temperature variation, localised chemical reactions;
- Flame acceleration and transition to detonation structures.

High-order approximations coupled with dynamic grid adaption.

Multi-level techniques.

- Multi-level adaptive technique (MLAT) [Brandt (1977)]:
  Adaptive discretization and Multi-Grid methods
- Method of assembling overlapping grids - Chimera method
  [Volkov (1968), Steger *et al.* (1983), Peron & Benoît (2013)]

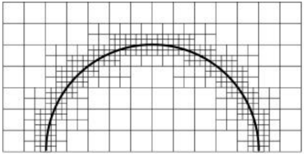
  – Manage overlapping with ghost cells
  – Well adapted for complex geometries (local geometrical details)
  – Well adapted for sliding mesh



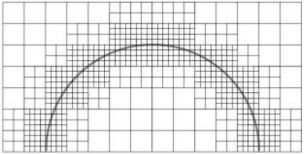
From Peron, PhD Thesis (2014).

Adaptive grid techniques.

- AMR [Berger, Oliger, Collela (1984–1989)]:
  - ▷ Cell- / Block-, and Patch-based AMR: [Dunning *et al.* (2020), Gunney *et al.* (2006–2017), Berger *et al.* (1984–1998)]

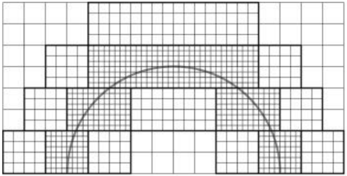


Cell-based AMR with 382 cells

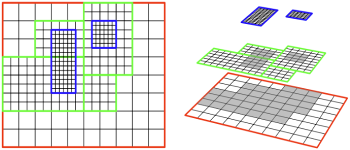


Block-based AMR with 596 cells

From Dunning et al. (2020)



Patch-based AMR with 836 cells



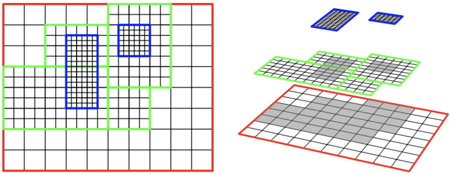
From Gunnet et al. (2013)

Adaptive grid techniques.

▷ Block-, and Patch-based AMR: [Berger *et al.* (1984–1998), Gunney *et al.* (2006–2017)]

- Advantage of regular grid;
- But refines large sub-sections;
- Manage boundary conditions / ghost cells;
- Manage Proxy / Mapping connectors;
- Allows divisions ≥ 2;

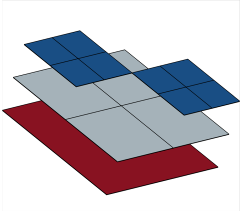
- Several softwares: SAMRAI, AMRClaw, AMROC, AMReX, PARAMESH, BoxLib, SAMURAI, ...

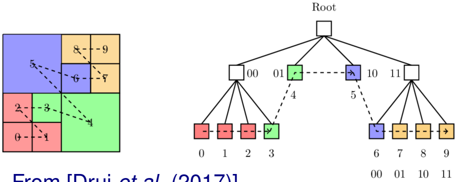


From [Gunney *et al.* (2013)]

Adaptive grid techniques.

- Cell-based AMR: [De Zeeuw & Powell (1993), Khokhlov (1998), Dunning *et al.* (2020)]
  - Generally based on binary trees (octree);
  - Limit cell number near gradient;
  - Manage boundary conditions / ghost cells;
  - Several softwares: P4est, PABLO, CLAMR, SAGE/RAGE, SAMURAI, ...

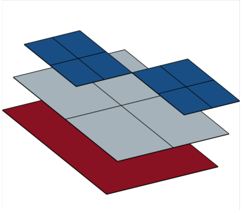


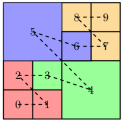


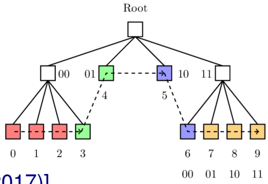
From [Drui *et al.* (2017)]

Adaptive grid techniques.

- ▷ Cell-based AMR: [De Zeeuw & Powell (1993), Khokhlov (1998), Dunning *et al.* (2020)]
  - – Generally based on binary trees (octree);
  - – Limit cell number near gradient;
  - – Manage boundary conditions / ghost cells;
  - Several softwares: P4est, PABLO, CLAMR, SAGE/RAGE, SAMURAI, ...







From [Drui *et al.* (2017)]

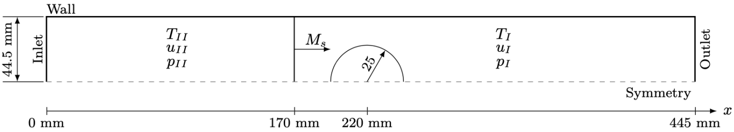
- based on ad hoc heuristic criteria ;
- difficult to control refinement error $||Q^{(AMR)} - Q^{(UFG)}||$

⇒ Adjoint-based error estimate for AMR [Narechania *et al.* (2017)]: mainly for steady or slowly evolving flows. Cart3D.

Multiresolution techniques.

- MRA : Multi-Resolution Analysis
  - ▷ Harten (1994-1995): multirésolution & syst. hyperbolique;
  - ▷ Cohen *et al.* (2003): formalisme base d'ondelettes, multirésoltion complètement adaptative;
  - ▷ Brix *et al.* (2011): Data structures, implementation and parallelization;
  - ▷ Duarte *et al.* (2013): MRA coupled with time adaptive method;
  - ▷ Deiterding *et al.* (2020): MRA into AMROC, comparisons.

Shock wave ($M_s = 1.22$) interacting with R_{22} bubble [Haas & Sturtevant (1987)]



Nested grids

Dyadic grids: Grid level : $l \in [0, L]$

Cell referenced by position and grid-level:(j, l)

$$(j, l) \to (2j, l+1)\ ,\ (2j+1, l+1)$$

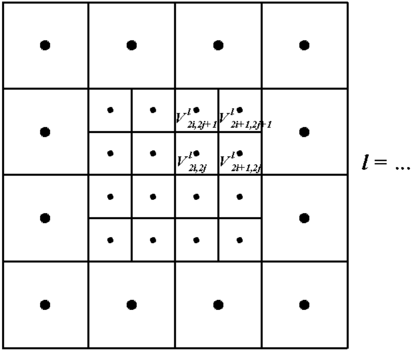
$$\Omega = \bigcup_{j \in I_l} V_j^l \quad \text{with} \quad \left| V_j^l \bigcap V_k^l \right| = 0,$$

for $j \neq k$; $j, k \in I_l$.

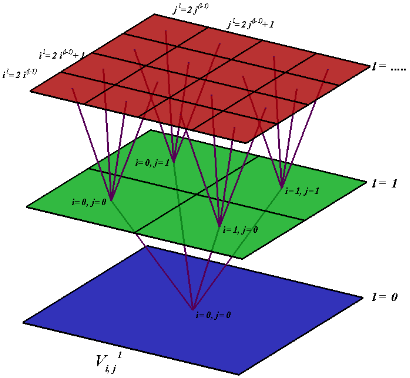
Refinement process:

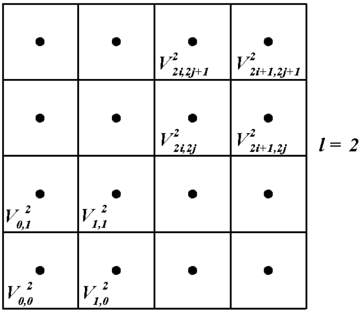
$$V_j^l = \bigcup_{p \in \mathcal{C}_j^l} V_p^{l+1},$$

$\mathcal{C}_j^l$ set of *chidren* indexes of V_j^l.



Tree data Structure





Terminology: *father* $(j/2, l-1)$; *children* $(2j, l+1)$, $(2j+1, l+1)$; *cousin* $(j+1, l)$, $(j-1, l)$

leaves are upper elements (with no *child*)

Projection operator:

$\mathbf{P}_{l+1 \to l}$: compute $\mathbf{v}_j^l$ knowing *children*-cells $\mathbf{v}_{2j}^{l+1}, \mathbf{v}_{2j+1}^{l+1}, \dots$

Nested grid: operator is *exact* **and** *unique* **[A. Cohen *et al.* (2000)]:**

Assuming cell average as: $\left(\mathbf{v}_j^l\right)^n = \frac{1}{|V_j^l|} \int_{V_j^l} \mathbf{w}(\mathbf{x}, n\,\delta t)\, d\mathbf{x}$

Projection operator:

$$\mathbf{P}_{l+1 \to l} : \quad \mathbf{v}_j^l = \frac{1}{|V_j^l|} \sum_{p \in \mathcal{C}_j^l} |V_p^{l+1}|\; v_p^{l+1};$$

$\mathcal{C}_j^l$ index set of the $2^{N_{dim}}$ *children*-cells at grid-level $l+1$, for current cell V_j^l.

Prediction operator:

$\mathbf{P}_{l\rightarrow l+1}$: maps $\mathbf{v}^l$ to an approximate value $\hat{\mathbf{v}}^{l+1}$ of $\mathbf{v}^{l+1}$.

$\mathbf{P}_{l\rightarrow l+1}$ is not unique and **prediction** needs to be:

- *local*; interpolation stencil must contain the *parent*-cell and its nearest neighbors in each direction [A. Cohen *et al.* (2000), M. Postel (2001)].
- *consistent with the projection* operator, *i.e.* $\mathbf{P}_{l+1\rightarrow l} \circ \mathbf{P}_{l\rightarrow l+1} = Id$.
  Conservativity:
  $$|V_j^l|\ v_j^l = \sum_{p\in\mathcal{C}_j^l} |V_p^{l+1}|\ \hat{v}_p^{l+1}$$
- *linear* (not mandatory...) $\rightarrow$ simplicity of the numerical analysis.
  Information on non-linear operator found in [F. Anràndiga *et al.* (1999)]

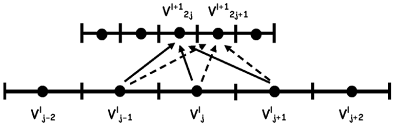
Prediction operator: interpolation

Prediction interpolation: centered linear polynomial

$$\mathbf{P}_{l\rightarrow l+1} : \begin{cases} \hat{v}_{2j}^{l+1} = v_j^l + \sum_{q=1}^{s} \xi_q \left(v_{j+q}^l - v_{j-q}^l \right), \\ \hat{v}_{2j+1}^{l+1} = v_j^l - \sum_{q=1}^{s} \xi_q \left(v_{j+q}^l - v_{j-q}^l \right), \end{cases}$$

Coefficients of centered linear polynomial:

order (o)	s	ξ_1	ξ_2
1	0	0	0
3	1	$\frac{-1}{8}$	0
5	2	$\frac{-22}{128}$	$\frac{3}{128}$



for $s = 1$

Prediction operator: multi-D interpolations

Extension to multidimensional Cartesian grids:

Tensorial product of 1-D operator [B.L. Bihari & A. Harten (1997), O. Roussel *et al.* (2003)].

2D-interpolation

$$\hat{v}^{l+1}_{2j+p,2k+q} = v^l_{j,k} + (-1)^p \; Q^s(j;\mathbf{v}^l_{\cdot,k}) + (-1)^q \; Q^s(k;\mathbf{v}^l_{j,\cdot}) - (-1)^{(p+q)} \; Q^s_2(j,k;\mathbf{v}^l),$$

with $p, q \in [0, 1]$ and:

$$Q^s\left(j; v^l\right) = \sum_{q=1}^{s} \xi_q \left(v^l_{j+q} - v^l_{j-q}\right),$$

$$Q^s_2\left(j,k;\mathbf{v}^l\right) = \sum_{a=1}^{s} \xi_a \sum_{b=1}^{s} \xi_b \left(v^l_{j+a,k+b} - v^l_{j-a,k+b} - v^l_{j-a,k+b} + v^l_{j-a,k-b}\right).$$

Prediction operator: *details*

prediction error: *details* (d_j^l)

details

$$\mathbf{d}_j^l = \mathbf{v}_j^l - \hat{\mathbf{v}}_j^l.$$

Consistency assumption [A. Harten (1995)]: $\sum_{p \in \mathcal{C}_j^l} |V_p^l| \; d_p^l = 0.$

Knowing $2^{N_{dim}}$ cell-averages $\mathbf{v}_\cdot^{l+1} \Leftrightarrow$ knowing $\mathbf{v}_j^l$ and $(2^{N_{dim}} - 1)$ $\mathbf{d}_\cdot^l$:

$$v_{2k}^{l+1} = \hat{v}_{2k}^{l+1} + d_{2k}^{l+1};$$

$$v_{2k+1}^{l+1} = \frac{|V_j^l|}{|V_{2k+1}^{l+1}|} \; v_j^l - v_{2k}^{l+1}.$$

Prediction operator: *details*

Polynomial accuracy

$$\left|\mathbf{d}^{l}\right| \leq C\, 2^{-l} \left|\mathbf{v}^{\prime}\right|_{L^{\infty}(V_j^l)} .$$

Main property for MR process:

- Solution with locally bounded o-th order derivatives [A. Cohen *et al.* (1992)];

$$|\mathbf{d}^{l}| = 0.$$

- Decay with 2^{-l} for solutions smooth enough;
- Significantly high *detail* values within singularities.

Multiresolution transform:

$$\mathbf{D}^l = \left\{ d_j^l,\ 0 \le j \le N_l \right\}, \quad \text{with } N_l = (2^{N_{dim}} - 1)\ 2^{N_{dim}(l-1)}$$

$$\mathbf{v}^{(l+1)} \longmapsto \left(\mathbf{v}^l,\ \mathbf{D}^{l+1} \right).$$

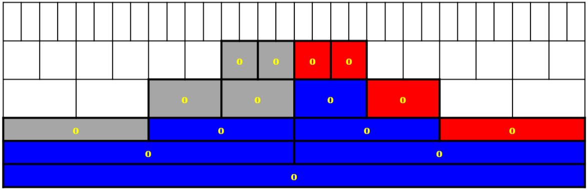
One to one transformation: from *leaves* down to the root

$$\mathcal{M} : \mathbf{v}^L \longmapsto \left(\mathbf{v}^0, \mathbf{D}^1, \ldots, \mathbf{D}^L \right) = \mathbf{M}^L.$$

$$\begin{tikzcd}
\bar{v}_L \arrow[r, leftrightarrow] \arrow[dr, leftrightarrow] & \bar{v}_{L-1} \arrow[r, leftrightarrow] \arrow[dr, leftrightarrow] & \bar{v}_{L-2} \arrow[r, leftrightarrow] \arrow[dr, leftrightarrow] & \cdots \arrow[r, leftrightarrow] \arrow[dr, leftrightarrow] & \bar{v}_1 \arrow[r, leftrightarrow] \arrow[dr, leftrightarrow] & \bar{v}_0 \\
 & d_{L-1} & d_{L-2} & \cdots & d_1 & d_0
\end{tikzcd}$$

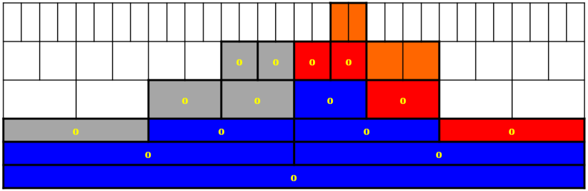
Thresholding and Tree pruning/enlargement, graded Tree:

- Thresholding: $\left|\mathbf{d}^{l}\right|_{L_1} < \varepsilon_l \Rightarrow$ cell discarded;



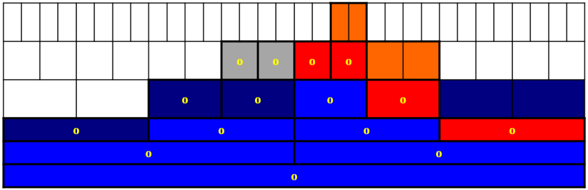
Thresholding and Tree pruning/enlargement, graded Tree:

- Thresholding: $\left|\mathbf{d}^l\right|_{L_1} < \varepsilon_l \Rightarrow$ cell discarded;
- Enlarge the tree for foreseeing discontinuity: $\left|\mathbf{d}^l\right|_{L_1} \geq \varepsilon_l$ and $\left|\mathbf{d}^l\right|_{L_1} \geq 2^p\, \varepsilon_l$



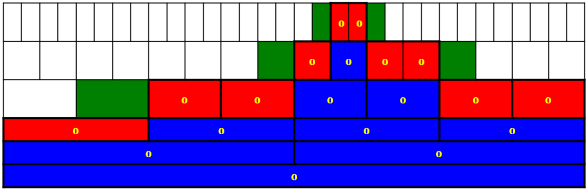
Thresholding and Tree pruning/enlargement, graded Tree:

- Thresholding: $\left|\mathbf{d}^l\right|_{L_1} < \varepsilon_l \Rightarrow$ cell discarded;
- Enlarge the tree for foreseeing discontinuity: $\left|\mathbf{d}^l\right|_{L_1} \geq \varepsilon_l$ and $\left|\mathbf{d}^l\right|_{L_1} \geq 2^p\, \varepsilon_l$
- Building graded tree:
  if $(j,l) \in \widetilde{\Lambda}_{\varepsilon_l}$ then $(j/2+q, l-1) \in \widetilde{\Lambda}_{\varepsilon_l}$; $q \in [-s, +s]$



Thresholding and Tree pruning/enlargement, graded Tree:

- Thresholding: $\left|\mathbf{d}^l\right|_{L_1} < \varepsilon_l \Rightarrow$ cell discarded;
- Enlarge the tree for foreseeing discontinuity: $\left|\mathbf{d}^l\right|_{L_1} \geq \varepsilon_l$ and $\left|\mathbf{d}^l\right|_{L_1} \geq 2^p\,\varepsilon_l$
- Building graded tree:
  if $(j,l) \in \widetilde{\Lambda}_{\varepsilon_l}$ then $(j/2+q, l-1) \in \widetilde{\Lambda}_{\varepsilon_l}$; $q \in [-s,+s]$
- Add virtual *leaves* for flux conservation



Thresholding: control

Approximation MR operator: $\mathcal{A}_{\Lambda_{\varepsilon_l}}$

$$\|\mathbf{v}^L - \mathcal{A}_{\Lambda_{\varepsilon_l}} \mathbf{v}^L\| = C \sum_{|\mathbf{d}^l| < \varepsilon_l} |\mathbf{d}^l| \, 2^{-N_{dim} l}$$

Control of the thresholding effect Harten (1994):

$$\varepsilon_l = 2^{N_{dim} \cdot (l-L)} \; \varepsilon$$

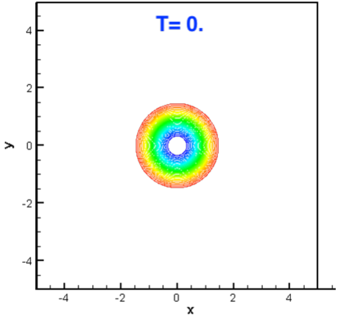
Knowing ε : $\|\mathbf{v}^L - \mathcal{A}_{\Lambda_{\varepsilon_l}} \mathbf{v}^L\| \le C\varepsilon$

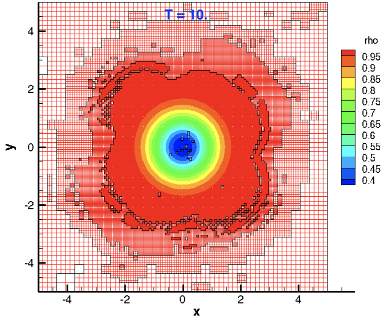
2D Vortex advection: solution

Strong vortex propagated at 45° by a supersonic flow:

$$(\delta u, \delta v) = \frac{\varepsilon}{2\pi} e^{0.5(1-r^2)}(-y, x) \;\; ; \;\; \delta T = -\frac{(\gamma - 1)\varepsilon^2}{8\pi^2} e^{0.5(1-r^2)} \;\; ; \;\; \delta S = 0.$$

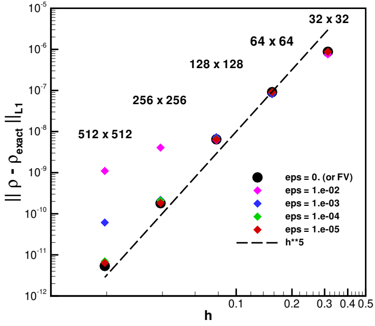
$\varepsilon = 5$; $(\rho, u, v, P) = (1, 1, 1, 1)$ and $(x \times y) = [-5, 5] \times [-5, 5]$



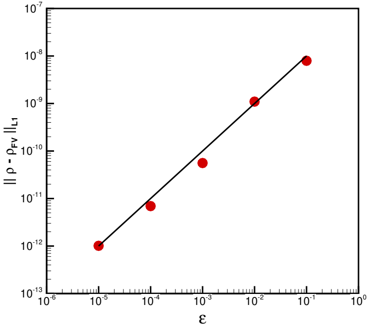


Euler 2D Vortex advection: Error analysis

Error / Exact solution

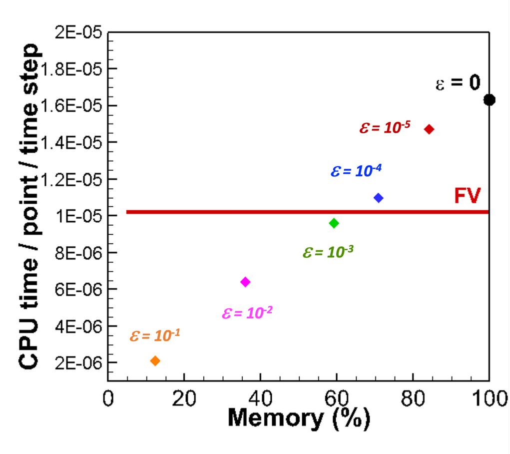


Perturbation Error $T = 10$



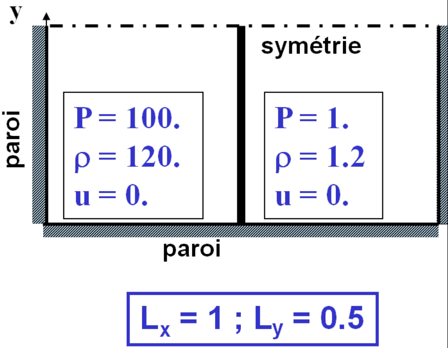
Euler 2D Vortex advection: Effciency

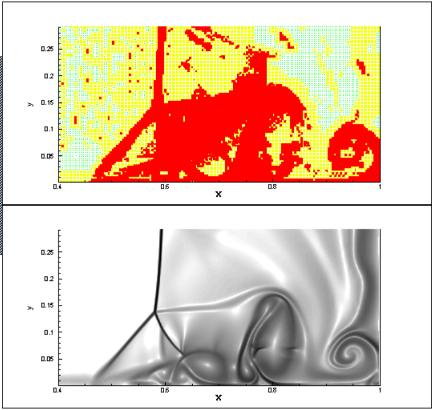
- CPU($\varepsilon = 0$) = 2.$\times$ CPU(FV)
- Memory Compression: $\forall\varepsilon$
  - $\varepsilon > 10^{-3}$: 60 % (FV)
  - $\varepsilon > 10^{-2}$: 35 % (FV)
- $\varepsilon > 10^{-3} \Rightarrow$ CPU Gains if 50 % FV-Mem saved



2D Viscous shock tube: MR 9 grid levels, $\varepsilon = 10^{-2}$, $s = 1$

$T = 1.$

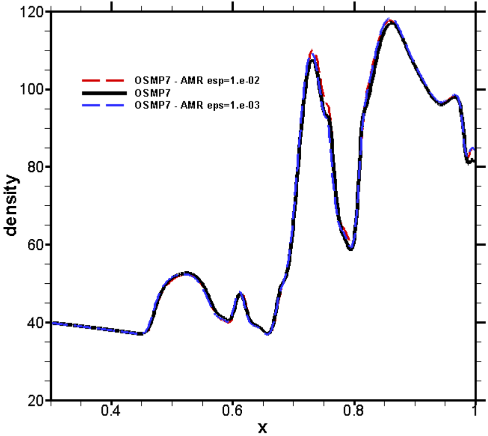




$\varepsilon = 10^{-2} \Rightarrow$ **Memory compression = 70 %; CPU ratio: t^{MR}/t^{FV} = 20 %**

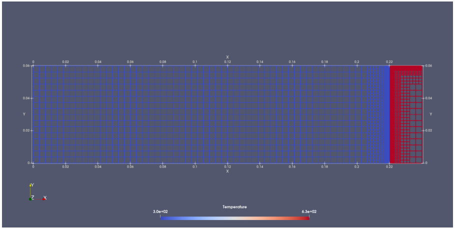
2D Viscous shock tube: video MR 9 grid levels, $\varepsilon = 10^{-2}$, $s = 1$

MR - 9 grid levels: (1024 $\times$ 512) - Reference: FV-OSMP7 (1000 $\times$ 5000)

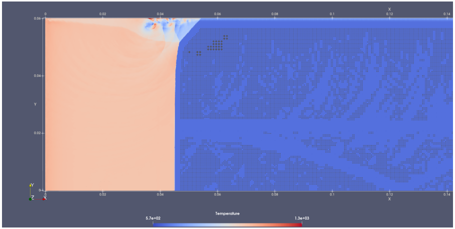


Tube: MR 8 levels (16×4 trees $= 4096 \times 1024$), $\varepsilon = 10^{-3}$, $s = 1$

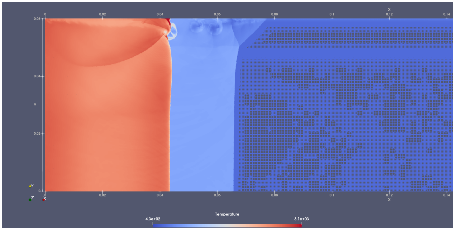
$t = 0$ s; 99.5 % compression



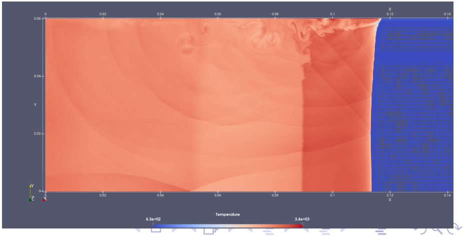
$t = 40 \times 10^{-5}$ s; 80 % compression



$t = 45 \times 10^{-5}$ s; 78 % compression

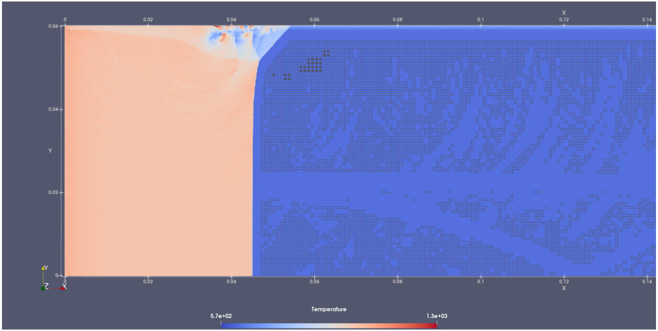


$t = 50. \times 10^{-5}$ s; 77 % compression



Tube: MR 8 levels (16×4 trees $\equiv 4096 \times 1024$), $\varepsilon = 10^{-3}$, $s = 1$

OpenMP: 32 cores - parallelization delicate for grid adaption.



- **Multiresolution technique:**
  - Assess capability of the adaptive multiresolution technique for compressible viscous flows;
  - Accuracy controled by the perturbation error: threshold parameter ($\varepsilon \lesssim 10^{-3}$)
  - Must be coupled with high-order numerical scheme;
  - Attractive approach because of a priori error control;
  - Powerful but hard to handle: Speed up if Mem. < 50 %;
- **Work in progress:**
  - Couled with Immersed Boundary conditions;
  - Emphasize on parallel algorithm:
    - Reflect on an efficient data organization;
    - Hard task for effective load balancing;
    - See SAMURAI software.