MOOD: An *a posteriori* paradigm to stabilize high accurate numerical schemes.

"Multi-dimensional Optimal Order Detection"

Direct Arbitrary-Lagrangian-Eulerian context

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Many thanks to my collaborators on MOOD

... and welcome to the furure ones !

Italy

W.Boscheri, M.Dumbser, O.Zanotti — Trento

Czech Republik

P.Vachal, M.Kucharik, R.Liska — CVUT, Prague

Portugal

S.Clain, G.Machado, R.Pereira — Braga

U.S.A.

M.Shashkov — Los Alamos, NM

France

S.Diot, J-.P. Braeunig, C.Fochesato, R.Motte, M.Peybernes, R.Poncet — CEA
G.Blanchard — Toulouse

Summary of the talk

Introduction and general philosophy of a posteriori MOOD paradigm

Reminder on MOOD for Eulerian FV schemes

Detection criteria in the Hydrodynamics and (Relativistic) MHD contexts. MultiD test problems on (un)structured meshes. Efficiency and performances compared to classical WENO code

MOOD for ALE FV schemes

Detection criteria in an hydrodynamics mesh moving context. 2D/3D test problems.

Conclusion and perspectives

MOOD : Multi-dimensional Optimal Order Detection

Prelims

Context

MOOD concepts stated and developed during S.Diot's PhD (2009-2012) with S.Clain (U. do Minho, Portugal). Full implementation and testing for [1-3] has been done by S.Diot.

Design principles

- Genuinely multidimensional Eulerian finite volume on unstructured meshes
- Arbitrary high-order polynomial reconstruction
- Detect the 'optimal polynomial degree' (stable, robust, accurate)

Bibliography

[1] S. Diot, R. Loubère, S. Clain, The MOOD method in the three-dimensional case, Int. J. Numer. Meth. FLUIDS (2013).
[2] S.D, R.L, S.C, Improved detection criteria for the MOOD on unstructured meshes, Comput. Fluids 64 (2012) 43-63.
[3] S.D, R.L, S.C, A high-order finite volume method... (MOOD), J. Comput. Phys. 230 (2011)

MOOD : Multi-dimensional Optimal Order Detection

Prelims

MOOD as an a posteriori limiting procedure

The general idea of testing a candidate solution at t^{n+1} revealed fruitful in other contexts $\Rightarrow$ ADER-$\mathbb{P}_N\mathbb{P}_M$ code of M.Dumbser is the starting point for large testing campagne.

Other systems

- Hydrodynamics (HD) equations
- Magneto-HD (MHD) and RMHD
- Baer-Nunziato, kinetic (on going work)

Other frameworks

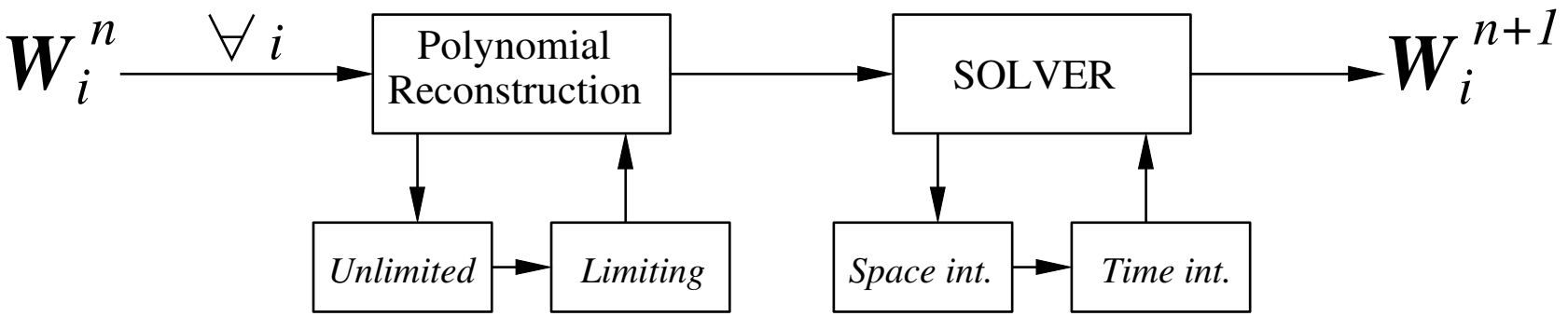
- Eulerian Finite Volumes (FV)
- Arbitrary-Lagrangian-Eulerian (ALE) FV
- Subcell limiting in FE DG methods

Bibliography

[4] R.L, M.Dumbser, S.D, A New Family of High Order Unstructured MOOD and ADER Finite Volume Schemes for Multidimensional Systems of Hyperbolic Conservation Laws , 2014, CiCP 16 (3), pp. 718-763
[5] M.Dumbser, O.Zanotti, R.Loubère, S.Diot, A posteriori subcell limiting of the discontinuous Galerkin finite element method for hyperbolic conservation laws, J. Comput. Phys. 278, 2014, pp 47-75
[6] W.Boscheri, M.Dumbser, R.Loubère, Multi-dimensional direct Arbitrary-Lagrangian-Eulerian high accurate ADER-MOOD finite volume schemes, submitted 2014
[7] W.Boscheri, M.Dumbser, R.Loubère, 3D Arbitrary-Lagrangian-Eulerian high accurate ADER-MOOD finite volume schemes for general conservative and non-conservative hyperbolic systems, to be submitted 2014-2015.

Philosophy

Generic High-Order/Accurate Finite Volume scheme

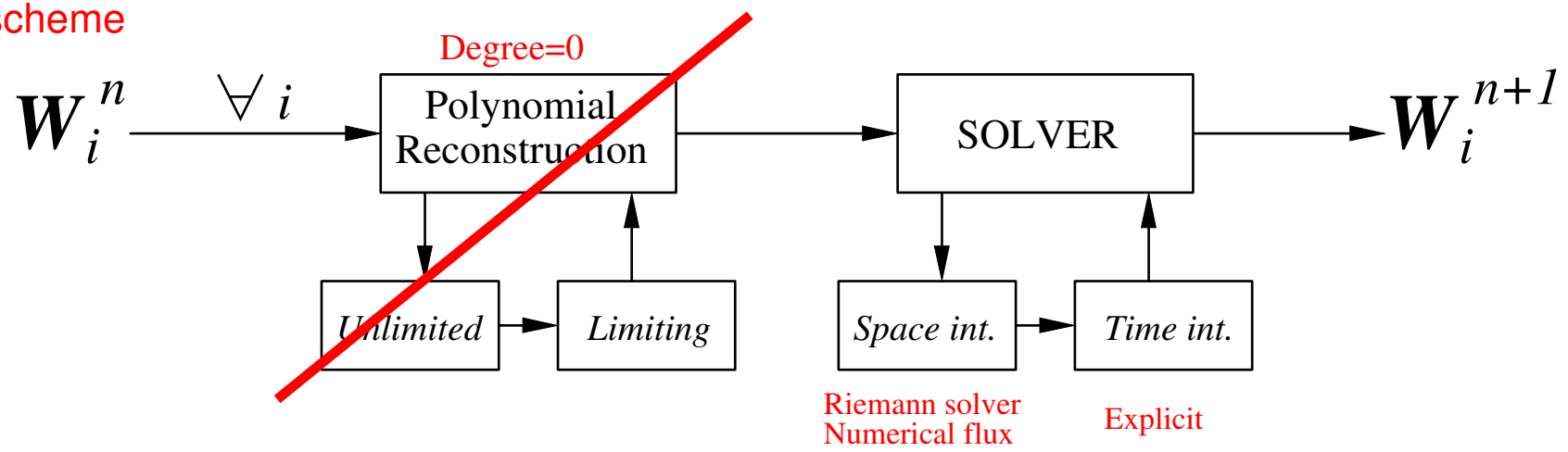


High accuracy

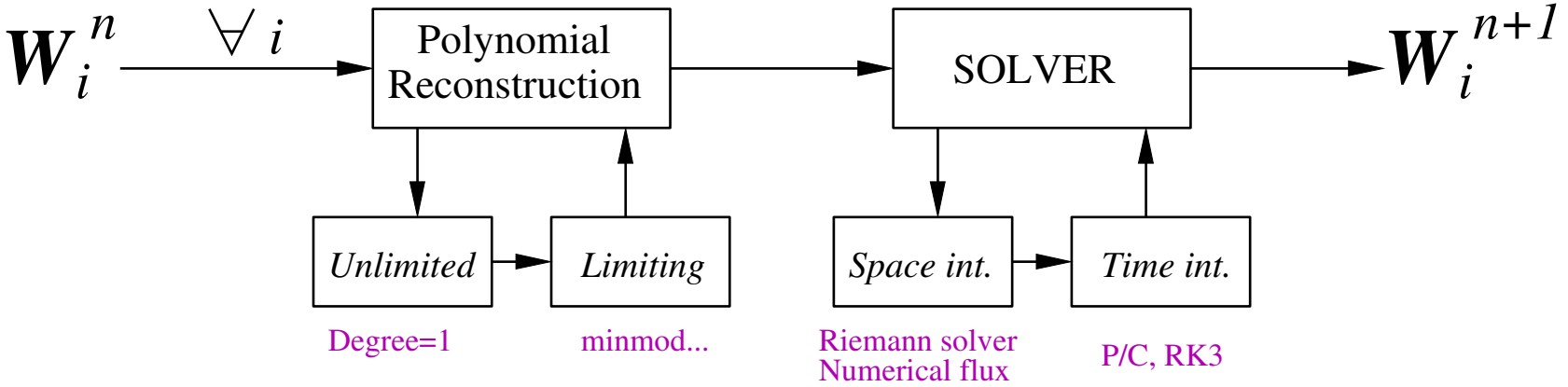
- Accuracy in space due to unlimited reconstructions of state variable to feed the fluxes
- Accuracy in time due to iterations (Predic./Correct., Runge-Kutta)
- Stabilization due to 'limiting'
- Need high accuracy for space/time (numerical) integrations

Philosophy

FV scheme

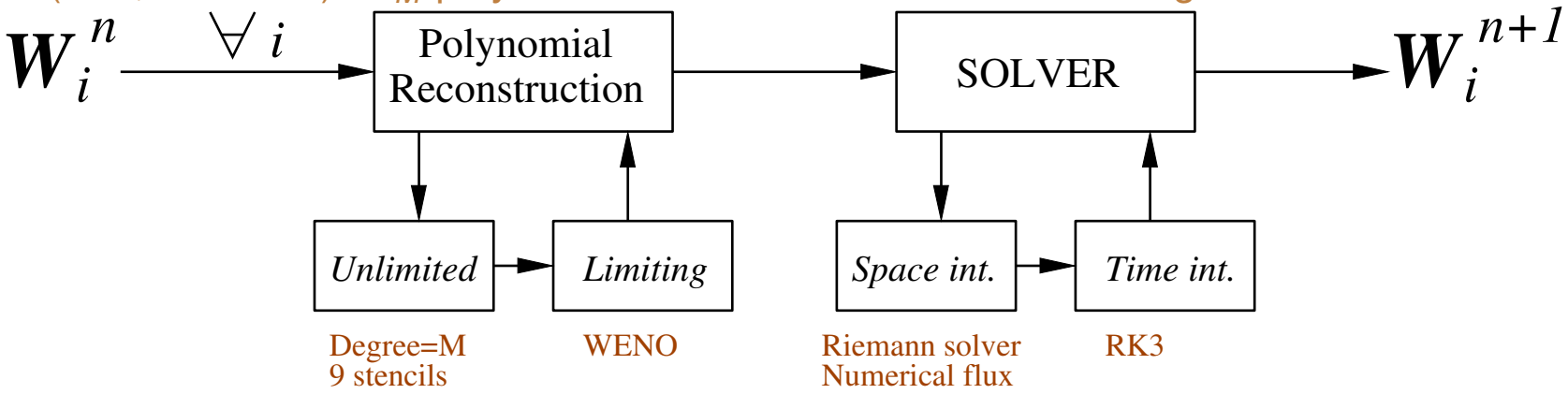


MUSCL (Kolgan, Van Leer. . .) scheme : $\mathbb{P}_1$ reconstruction + limiter to enforce bounds

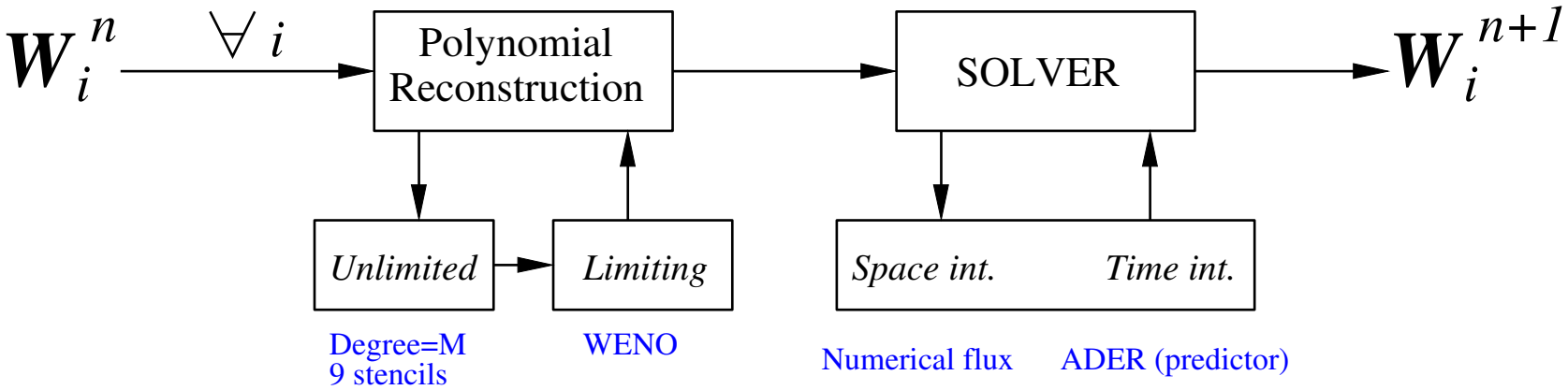


Philosophy

WENO (Shu, Osher. . .) : $\mathbb{P}_M$ polynomials + non-linear combination to get ENO behavior



$\mathbb{P}_0\mathbb{P}_M$ (Dumbser, Munz, Toro. . .) : $\mathbb{P}_M$ reconstructions + ADER



Philosophy

MOOD : Multi-dimensional Optimal Order Detection

Most limiting strategies are based on an *a priori* process (i.e based on $\boldsymbol{W}_i^n$ only)

1. 'Worst case scenario' – Over/undershoot of reconstructions are premisses of oscillations !
2. 'Precautional principle' – I preventively must act to avoid creation of new extrema
3. 'Prediction capability' – Given $\boldsymbol{W}_i^n$ I know when/how/where my scheme will misbehave

However

1. 'Worst case scenario' – Increase of mean value does not imply occurence of an oscillation
2. 'Precautional principle' – Is it always/often legitimate to act ?
3. 'Prediction capability' – Can I predict the scheme reactions when applied on a NL system ?

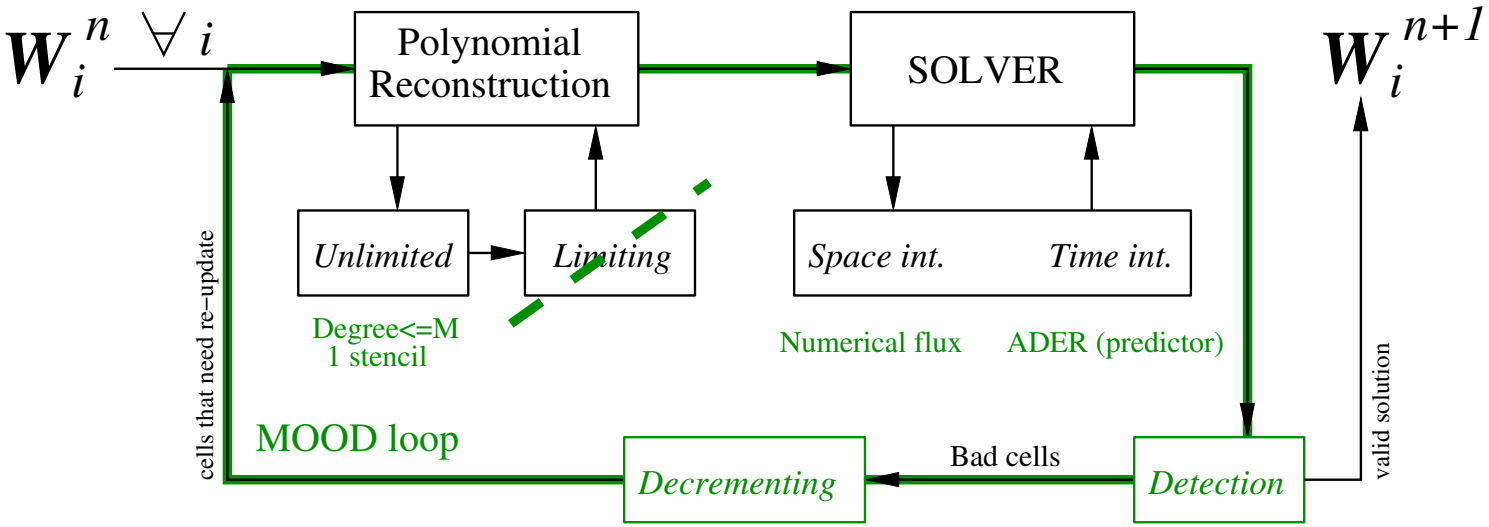
A posteriori MOOD paradigm

1. compute $\boldsymbol{W}_i^{n+1}$ with unlimited reconstructions ;
2. *a posteriori* Detect if $\boldsymbol{W}_i^{n+1}$ locally fails ;
3. Localy to i Decrement the order of accuracy of reconstructions. Re-update these cells.

Philosophy

MOOD : Multi-dimensional Optimal Order Detection

MOOD : $\mathbb{P}_{\leq M}$ reconstruction with *a posteriori* detection and decrementing



- Decrementing consists in reducing the polynomial degree by 1 or more
- Independent of mesh structure, maximal order, solver, numerical fluxes
- One conservative polynomial reconstruction per cell, per degree, per variable
- Worst case scenario : degree drops to 0 $\Rightarrow$ FV scheme
- Some properties easily ensured (for instance positivity)
- Relatively non invasive to existing solvers

Philosophy

MOOD : Basics questions

1. *Constraints for the candidate solution (for the code to be able to compute next timestep) ?* Given a system of PDEs what are the minimal requirements demanded to a numerical solution to avoid prematurely termination of the simulation ($\simeq$ admissible states) $\rightarrow$ Physical Admissibility Detection (PAD) criteria.

   Example : *hydrodynamics with perfect gas EOS :* $\rho_i > 0$, *and* $E_i - \frac{1}{2}\mathbf{v}_i^2 > 0$.

2. *Parachute/bullet-proof scheme ?* This is the scheme to be trust, it always provides a bullet-proof solution and avoid code crashing.

   Example : *first-order FV scheme.*

3. *Cascade of schemes ?* From the most accurate scheme (accurate and prone to instability) to the bullet-proof scheme (inaccurate but robust).

   Example : $\mathbb{P}_M \longrightarrow \mathbb{P}_2 \longrightarrow \mathbb{P}_0$ *unlimited reconstructions with* $M = 3$ *or* 5.

4. *Constraints for a candidate solution to be acceptable ?* Must ensure the stability of the solution, and some 'important' features (that the developer can choose) $\rightarrow$ Numerical Admissibility Detection (NAD) criteria.

   Example : *(hydro) relaxed Discrete Maximum Principle (DMP) + local regularity u2 detection process on density variable.*

ADER $\mathbb{P}_N\mathbb{P}_M$ generic framework

General hyperbolic systems with source and non-conservative products

The $\mathbb{P}_N\mathbb{P}_M$ framework Dumbser, Balsara, Toro, Munz. JCP, 227, 2008. is a unified framework for the construction of one step FV and DG schemes for systems like

$$\mathbf{Q}_t + \nabla \cdot \mathbf{F}(\mathbf{Q}, \nabla\mathbf{Q}) + \mathbf{B}(\mathbf{Q}) \cdot \nabla\mathbf{Q} = \mathbf{S}(\mathbf{Q}),$$

ADER $\mathbb{P}_N\mathbb{P}_M$ generic discretization and code

Discrete one-step ADER scheme : integration of the PDE over the space-time control volume $K_i \times [t^n; t^{n+1}]$, Gauss theorem, introduction of a numerical flux $\mathcal{G}_{ij} \cdot \mathbf{n}_{ij}$ and insertion of the local predictor solution $\mathbf{q}_h$ into the computation of numerical fluxes at the element boundaries in normal direction $\mathbf{n}_{ij}$ leads to the conservative, high order accurate one-step FV scheme :

$$\mathbf{Q}_i^{n+1} = \mathbf{Q}_i^n - \frac{1}{|K_i|} \sum_{K_j \in \nu_i} \int_{t^n}^{t^{n+1}} \int_{\partial K_{ij}} \mathcal{G}_{ij}(\mathbf{q}_h^-, \mathbf{q}_h^+) \cdot \mathbf{n}_{ij} \, dS \, dt.$$

High-order predictor $\mathbf{q}_h$ based on one $\mathbb{P}_M$ (central stencil).

As such there is no limiting procedure $\rightarrow$ MOOD paradigm in substitution

"Toy" code : multiD structured/unstructured MPI ADER $\mathbb{P}_N\mathbb{P}_M$ war machine of Dumbser et al.

MOOD For Eulerian Finite Volume schemes

Context of Eulerian Finite Volume schemes

Assumption : Access to a general high order FV code
Proposition : remove any kind of limiter and stabilize it with a MOOD loop
Needs : define the PAD, NAD, the parachute scheme and the cascade.
$\Longrightarrow$ This depends on the system of PDEs one solves.

Numerical study

Our reference code is ADER-WENO of arbitrary order of accuracy on 2D/3D structured or unstructured grids.
Comparison between ADER-MOOD and ADER-WENO codes is carried out.

MOOD For Eulerian Finite Volume schemes

0 : Advection equation

Detection criteria, cascade, parachute

Detection criteria follows from the underlying physics, cascade and parachute are user choices

Detection criteria : Discrete Maximum Principle (DMP) as 1^{st} filter

Candidate sol. $\boldsymbol{W}_i^\star$ fulfills the DMP ? $\min_{j\in\overline{\nu}(i)}(\boldsymbol{W}_i^n, \boldsymbol{W}_j^n) \leq \boldsymbol{W}_i^\star \leq \max_{j\in\overline{\nu}(i)}(\boldsymbol{W}_i^n, \boldsymbol{W}_j^n)$

If detection is strict on $\{\text{DMP}\} \Rightarrow 2^{nd}$-order error at smooth extrema $\Rightarrow$ DMP violation must be allowed at smooth extrema to reach higher orders !

Detection citeria : u2 as 2^{nd} filter $\rightarrow$ distinguish discontinuities from smooth extrema

A solution violating the DMP is nonetheless acceptable if

$$\mathcal{W}_i^{min}\mathcal{W}_i^{max} > 0 \quad \text{(Non oscill. detect.)} \quad \text{and} \quad \left|\frac{\mathcal{W}_i^{min}}{\mathcal{W}_i^{max}}\right| > 1-\varepsilon = 1/2 \quad \text{(Num.Smoothn. detect.)}$$

where $\mathcal{W}_i^{min}=\min_{j\in\overline{\nu}(i)}(\mathcal{W}_j, \mathcal{W}_i)$, $\mathcal{W}_i^{max}=\max_{j\in\overline{\nu}(i)}(\mathcal{W}_j, \mathcal{W}_i)$ with $\mathcal{X}_j = \partial_{xx}\boldsymbol{W}_j^{rec}$, $\mathcal{Y}_j = \partial_{yy}\boldsymbol{W}_j^{rec}$, $\mathcal{Z}_j = \partial_{zz}\boldsymbol{W}_j^{rec}$ with $\boldsymbol{W}_j^{rec} \in \mathbb{P}^2$

MOOD For Eulerian Finite Volume schemes

1 : Hydrodynamics system of conservation laws

Detection criteria

- PAD : $\rho_i > 0$, and $\varepsilon_i > 0$
- NAD : DMP+u2 on conservative variables, NaN

Cascade, Parachute

Cascade $\mathbb{P}_3 \longrightarrow \mathbb{P}_1^{\text{LIM}} \longrightarrow \mathbb{P}_0$. Parachute scheme $\mathbb{P}_0$.

Numerical results from

[4] R.L, M.Dumbser, S.Diot, A New Family of High Order Unstructured MOOD and ADER FV Schemes, 2014, CiCP 16, 718-763

MOOD For Eulerian Finite Volume schemes

1 : Hydrodynamics system of conservation laws - Isentropic Vortex in 2D

On this smooth problem comparison of ADER-MOOD and ADER-WENO codes.
Both methods behave alike but MOOD is less expensive (CPU time and memory). Effective 4th order of accuracy are obtained.

	ADER-MOOD $\mathbb{P}_3 \longrightarrow \mathbb{P}_1^{lim} \longrightarrow \mathbb{P}_0$					**ADER-WENO** $\mathbb{P}_0\mathbb{P}_3$				
N_x	CPU	L^2 error		L^∞ error		CPU	L^2 error		L^∞ error	
24	1.31	2.65E-02	—	3,33E-02	—	1.15	4.49E-02	—	3.24E-02	—
32	1.00	1.08E-02	3.12	1.29E-02	3.29	1.25	1.13E-02	4.78	1.17E-02	3.54
64	1.07	7.19E-04	3.91	6.76E-04	4.26	1.28	7.23E-04	3.97	6.76E-04	4.11
128	1.06	4.14E-05	4.12	4.19E-05	4.01	1.30	4.14E-05	4.13	4.19E-05	4.01
Expected order			4		4			4		4

Here the CPU times are normalized according to the unlimited $\mathbb{P}_0\mathbb{P}_3$ scheme.

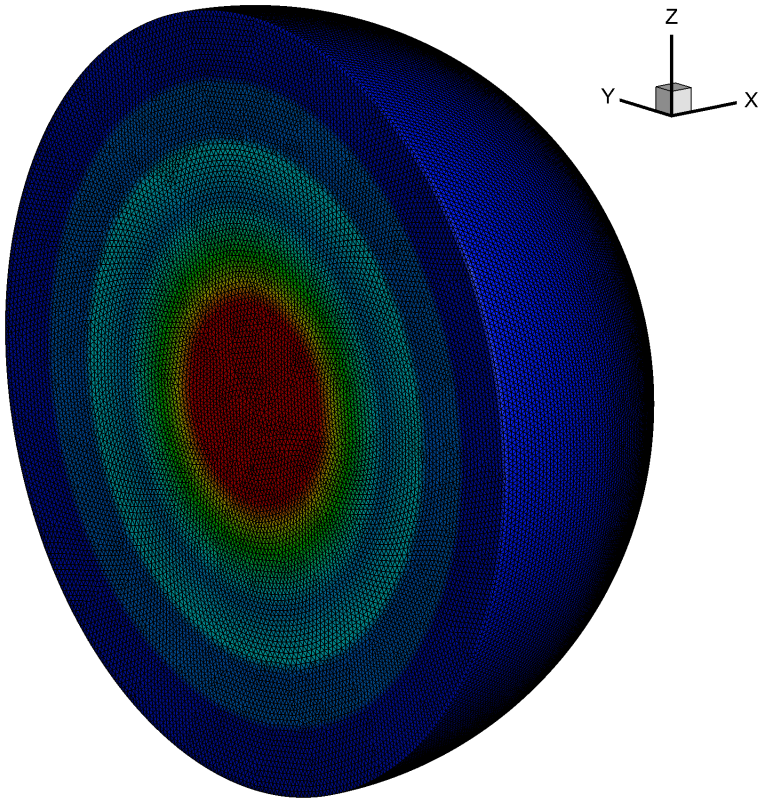
$N_x = 64$	Memory (MB)	CPU time (s)
ADER-WENO	233	314
ADER-MOOD	76	277
Ratio	3	1.13

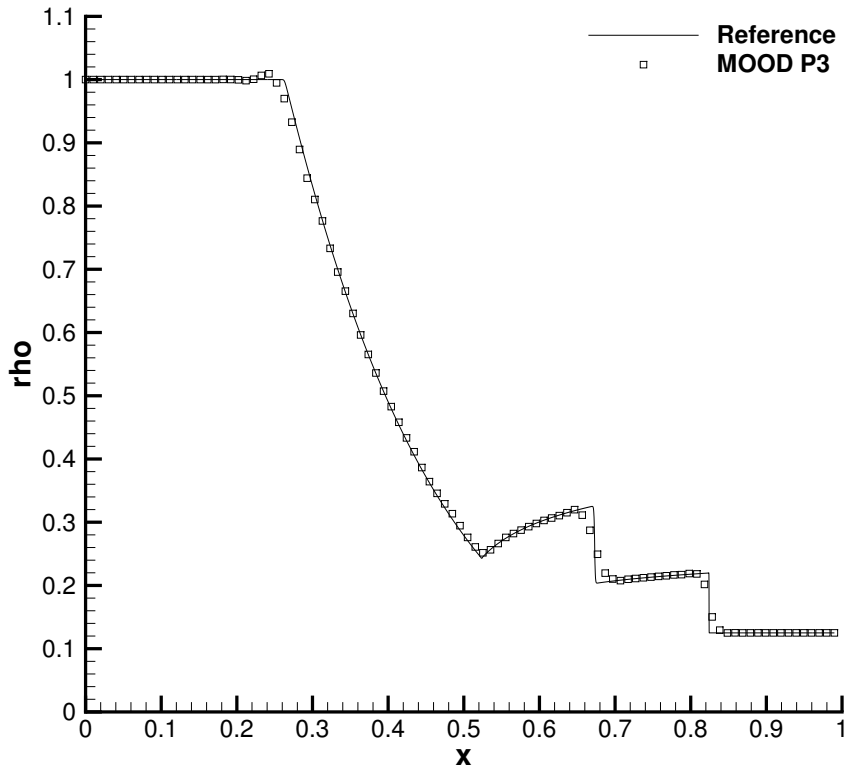
Run on a single CPU core of an Intel i7-2600 processor with 3.4 GHz of clock speed and 12 GB of RAM

MOOD For Eulerian Finite Volume schemes

1 : Hydrodynamics system of conservation laws - Explosion problem in 3D

3D explosion problem at $t_{\text{final}} = 0.2$ on $3,464$ millions of tetrahedra.





MOOD For Eulerian Finite Volume schemes

1 : Hydrodynamics system of conservation laws - Explosion problem in 3D

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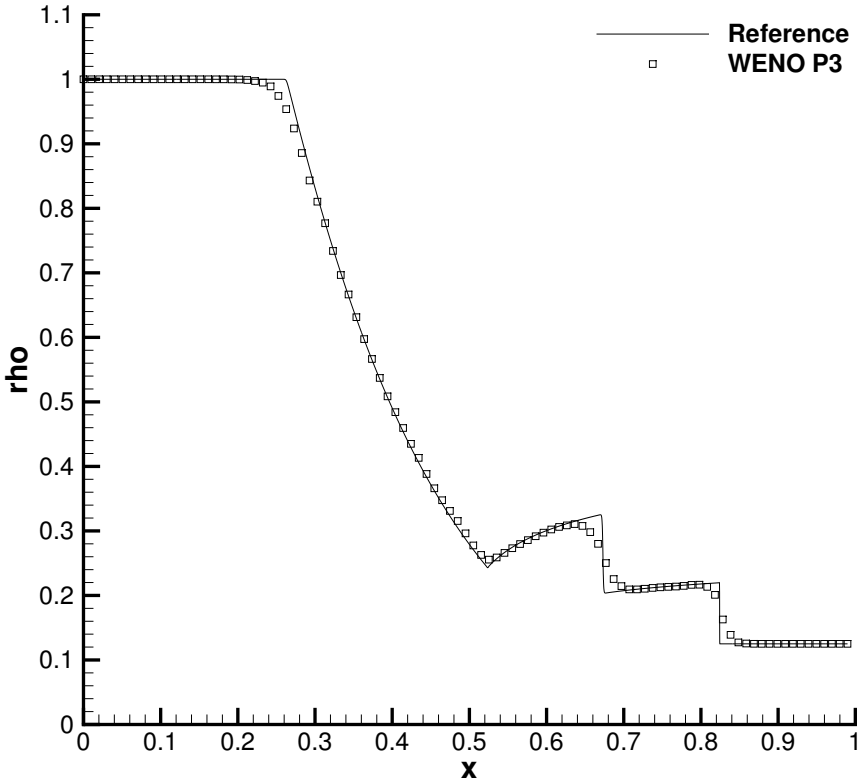
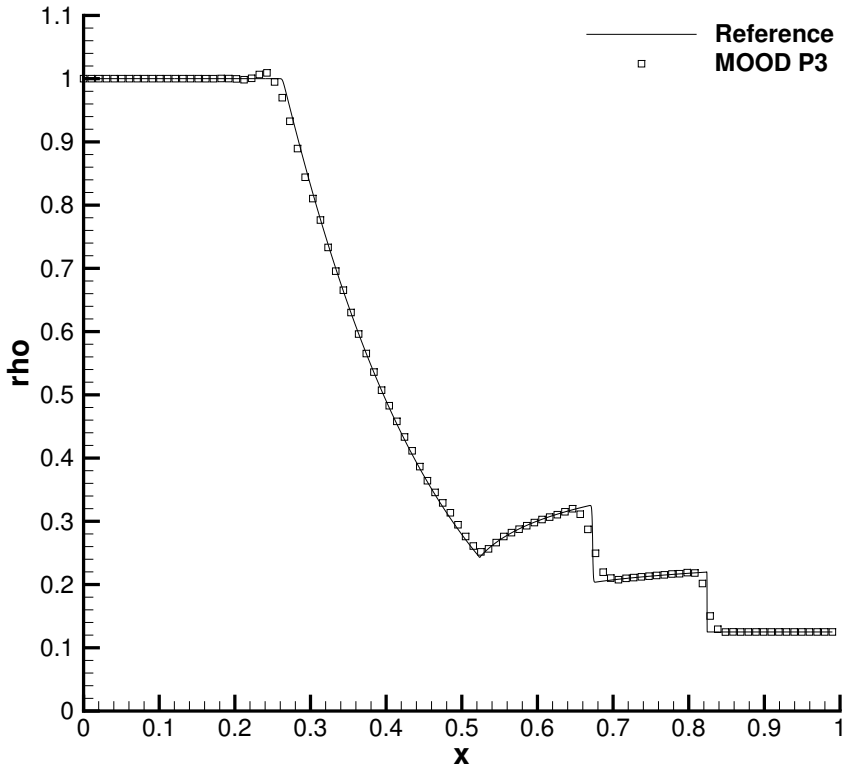




MOOD is 1.28 times faster and uses 3.28 less memory than WENO approach (512 processors).

MOOD For Eulerian Finite Volume schemes

2 : Ideal Magneto-Hydrodynamics (MHD)

System of PDEs - 3D NL hyperbolic systems of conservation laws

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho\mathbf{v}\\ \rho E\\ \mathbf{B}\\ \psi\end{pmatrix}+\nabla\cdot\begin{pmatrix}\rho\mathbf{v}\\ \rho\mathbf{v}\mathbf{v}+\left(p+\frac{1}{8\pi}\mathbf{B}^2\right)\mathbf{I}-\frac{1}{4\pi}\mathbf{B}\mathbf{B}\\ \mathbf{v}\left(\rho E+p+\frac{1}{8\pi}\mathbf{B}^2\right)-\mathbf{v}\cdot\frac{1}{4\pi}\mathbf{B}\mathbf{B}\\ \mathbf{B}\mathbf{v}-\mathbf{v}\mathbf{B}+\psi\mathbf{I}\\ c_h^2\mathbf{B}\end{pmatrix}=0 \tag{1}$$

$$p=(\gamma-1)\left(\rho E-\frac{1}{2}\rho\mathbf{v}^2-\frac{1}{8\pi}\mathbf{B}^2\right),\qquad \nabla\cdot\mathbf{B}=0. \tag{2}$$

Generalized Lagrangian multiplier ψ divergence cleaning from [Munz *et al.* Hyperbolic divergence cleaning for the MHD equations. JCP, 175 (2002)]

Detection criteria, Cascade, Parachute

PAD : Ensure $\rho > 0$, $p > 0$ (not easy for highly magnetized flow field !)
NAD : Ensure *DMP* + *u*2. Check NaN
Cascade $\mathbb{P}_3 \longrightarrow \mathbb{P}_1^{\text{LIM}} \longrightarrow \mathbb{P}_0$. Parachute scheme FV $\mathbb{P}_0$.

Numerical results from

[4] R.L, M.Dumbser, S.Diot, A New Family of High Order Unstructured MOOD and ADER FV Schemes, 2014, CiCP 16, 718-763

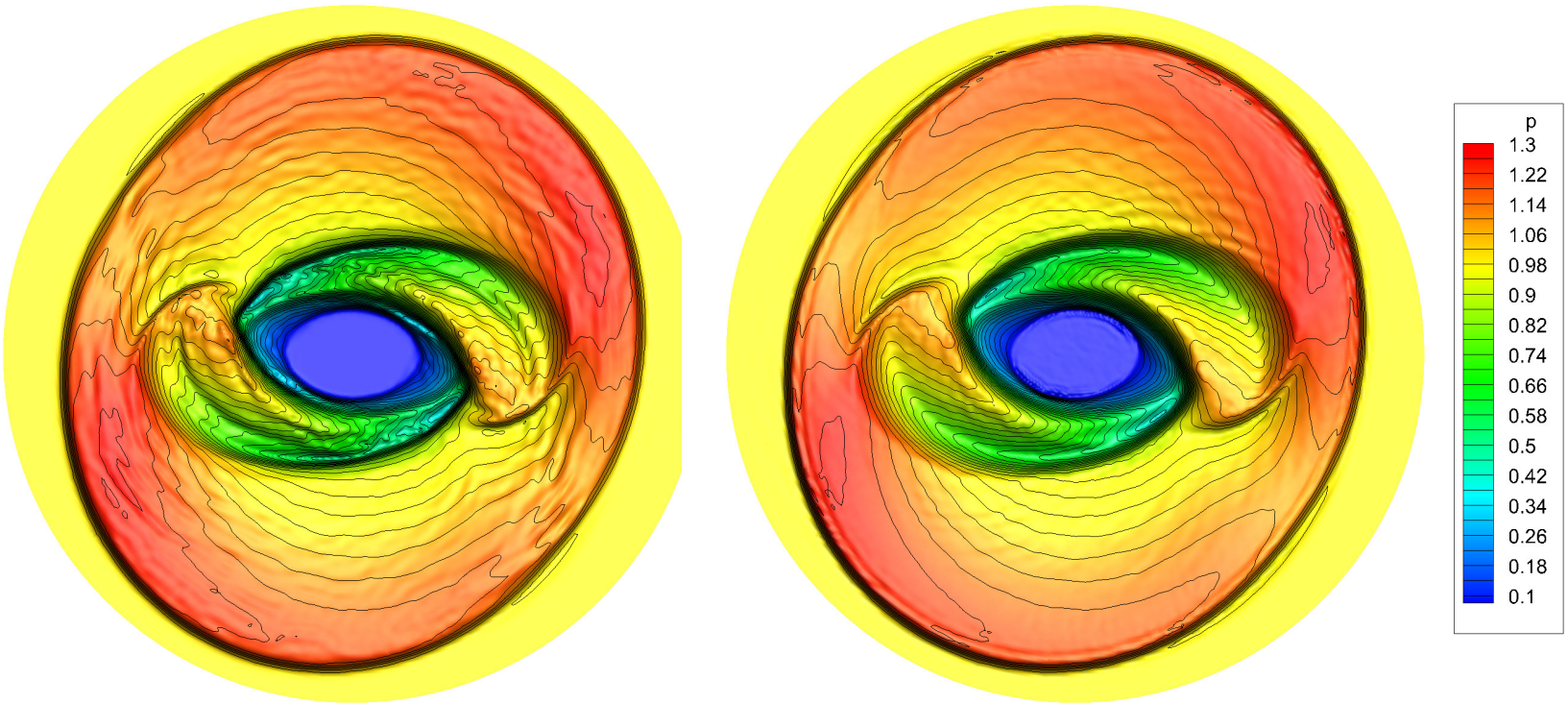
MOOD For Eulerian Finite Volume schemes

2 : Ideal Magneto-Hydrodynamics (MHD)

2D rotor problem — 106930 adapted triangles - $\gamma = 1.4$ - [Balsara JCP 149 (1999)]

$$\rho = \begin{cases} 10 & 0 \leq r \leq 0.1 \\ 1 & 0.1 < r \leq 0.5 \end{cases} \qquad p = 1, \qquad v = \omega \cdot r = 1 \text{ at } r = 0.1 \qquad \mathbf{B} = (2.5, 0, 0)^T$$

ADER-WENO $\mathbb{P}_0\mathbb{P}_3$ **ADER-MOOD** $\mathbb{P}_3 \rightarrow \mathbb{P}_1^{lim} \rightarrow \mathbb{P}_0$



$\Longrightarrow$ leads to 2.51 ratio saving in memory, 1.14 saving in CPU time

MOOD For Eulerian Finite Volume schemes

3 : Relativistic magnetohydrodynamics (RMHD)

Relativistic MHD - 3D NL hyperbolic system - Fairly ugly and dirty system of equations !

$$\partial_t \mathbf{Q} + \nabla \cdot \mathbf{F} = 0$$

The RMHD system is $\mathbf{Q} = \begin{pmatrix} D \\ \mathbf{q} \\ E \\ \mathbf{B} \\ \psi \end{pmatrix} = \begin{pmatrix} \gamma\rho \\ \gamma w_{tot}\mathbf{v} - b^0\mathbf{b} \\ \gamma^2 w_{tot} - b^0 b^0 - p_{tot} \\ \mathbf{B} \\ \psi \end{pmatrix}$. The flux tensor $\mathbf{F} = \begin{pmatrix} \gamma\rho\mathbf{v} \\ \gamma^2 w_{tot}\mathbf{v}\mathbf{v} - \mathbf{b}\mathbf{b} + p_{tot}\mathbf{I} \\ \gamma^2 w_{tot}\mathbf{v} - b^0\mathbf{b} \\ \mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v} + \psi\mathbf{I} \\ c_h^2\mathbf{B} \end{pmatrix}$.

EOS : $e = \rho + \frac{p}{\Gamma - 1}$, Lorentz factor : $\gamma = \frac{1}{\sqrt{1-\mathbf{v}^2}}$, and further quantities are $b^0 = \gamma\,(\mathbf{v}\cdot\mathbf{B})$, $\mathbf{b} = \frac{\mathbf{B}}{\gamma} + \gamma\mathbf{v}\,(\mathbf{v}\cdot\mathbf{B})$,

$|b|^2 = \frac{\mathbf{B}^2}{\gamma} + (\mathbf{v}\cdot\mathbf{B})^2$ give total enthalpy and total pressure $w_{tot} = e + p + |b|^2$, $p_{tot} = p + \frac{1}{2}|b|^2$. Divergence-free $\nabla \cdot \mathbf{B} = 0$

Primitive variables (and flux tensor $\mathbf{F}$) can not be expressed in a closed analytical form in terms of the conserved quantities !

Primitive $\mathbf{W} = \{(\rho, \mathbf{v}, p, \mathbf{B}), \psi\} \longrightarrow$ Conservatives $\mathbf{Q}$ done numerically (Newton or bisection) but can fail : $\mathbf{W}(\mathbf{Q})$.

Detection criteria, Cascade, Parachute

PAD : Ensure $\rho > 0$, $p > 0$, $|\mathbf{v}| < 1$ and NAD : Ensure $DMP + u2$, NaN and success of $\mathbf{W}(\mathbf{Q})$.
Cascade $\mathbb{P}_3 \longrightarrow \mathbb{P}_1^{\text{LIM}} \longrightarrow \mathbb{P}_0$. Parachute scheme $\mathbb{P}_0$.

Numerical results from

[4] R.L, M.Dumbser, S.Diot, A New Family of High Order Unstructured MOOD and ADER FV Schemes, 2014, CiCP 16 , 718-763

Relativistic version of the MHD rotor problem

The rotor has a radius of $R_i = 0.1$ and is spinning with an angular frequency of $\omega = 9.95$, (maximal toroidal velocities of $v = 0.995 \sim 1$ speed of light).
Density $\rho = 10$ inside the rotor and $\rho = 1$ in the fluid at rest. Pressure $p = 1$ and magnetic field $\mathbf{B} = (1, 0, 0)^T$.
Lorentz factor is very high ($\gamma \approx 10$).
Unstructured mesh made of 106930 triangles (small mesh).
High order methods encounter difficulties with pressure positivity.

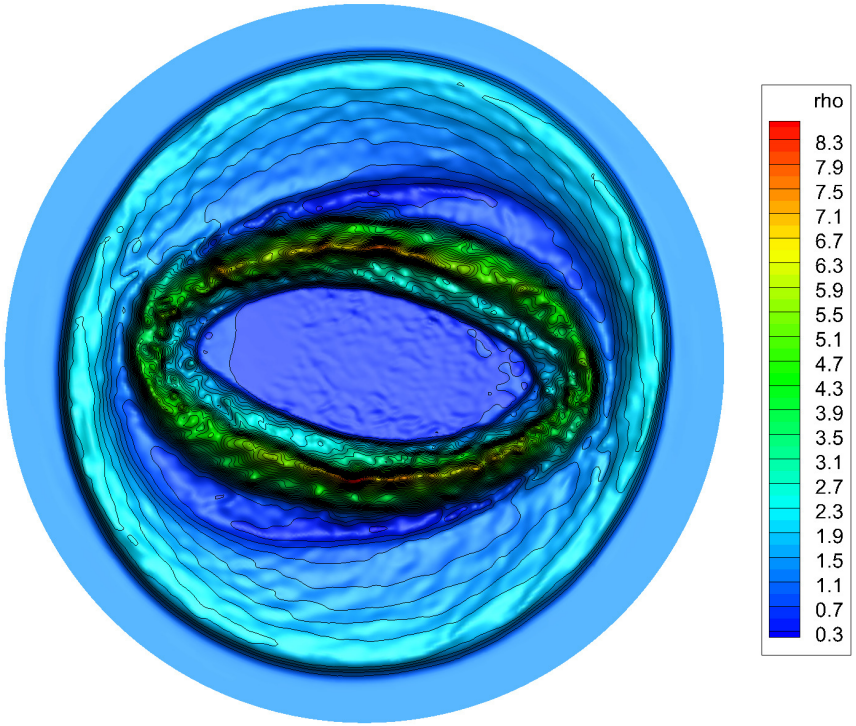
Note

The Lorentz Factor is the factor by which time, length, and "relativistic mass" change for an object while that object is moving.

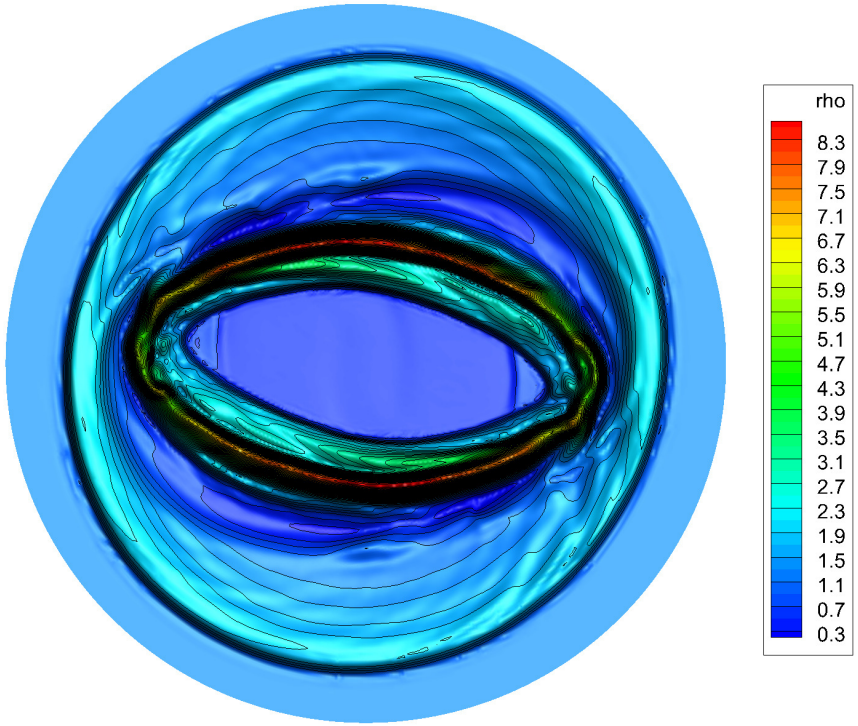
MOOD For Eulerian Finite Volume schemes

3 : Relativistic magnetohydrodynamics (RMHD)

WENO



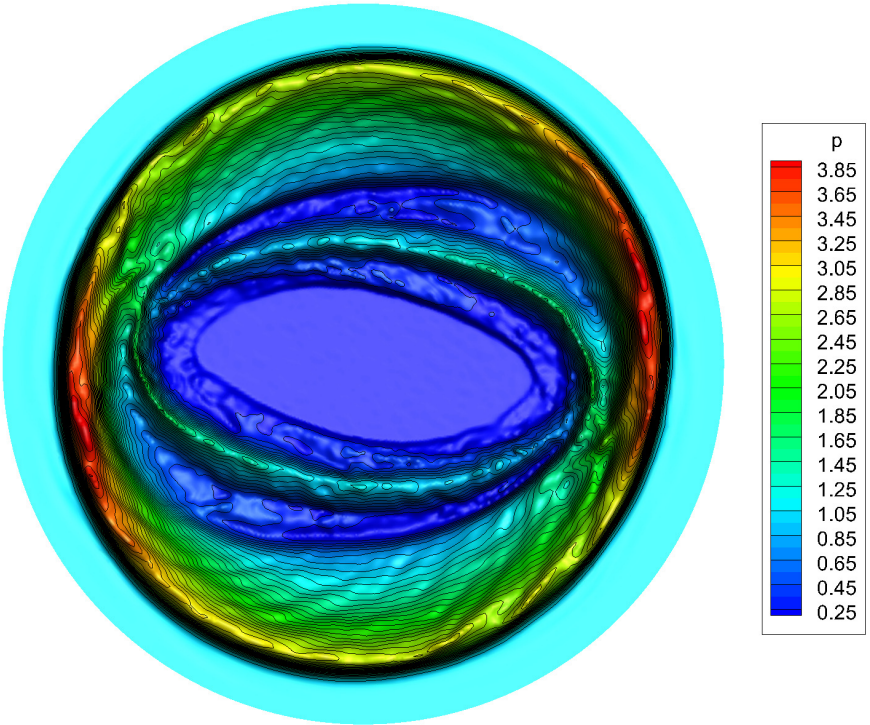
MOOD



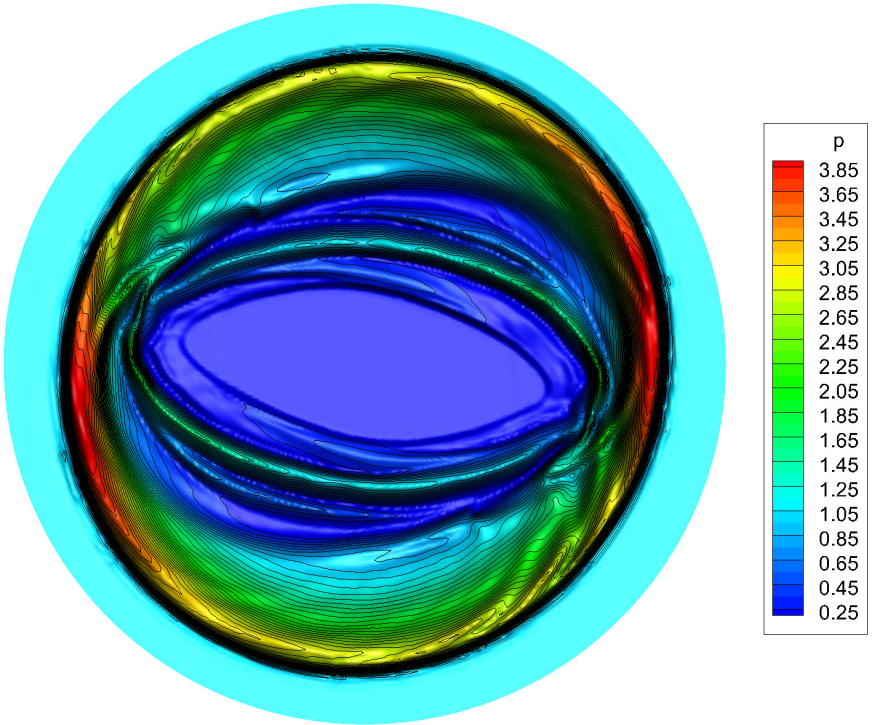
MOOD For Eulerian Finite Volume schemes

3 : Relativistic magnetohydrodynamics (RMHD)

WENO



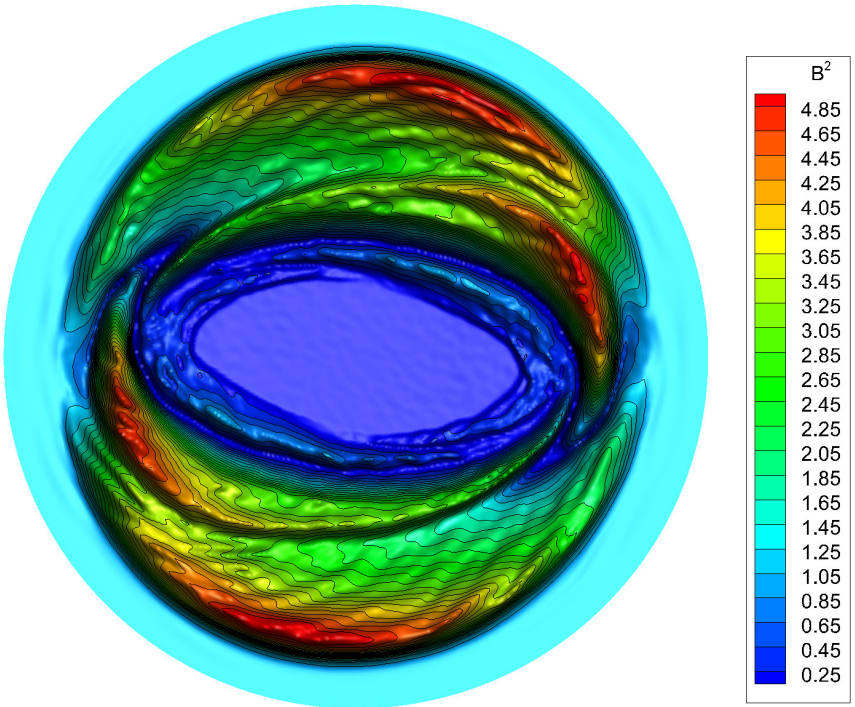
MOOD



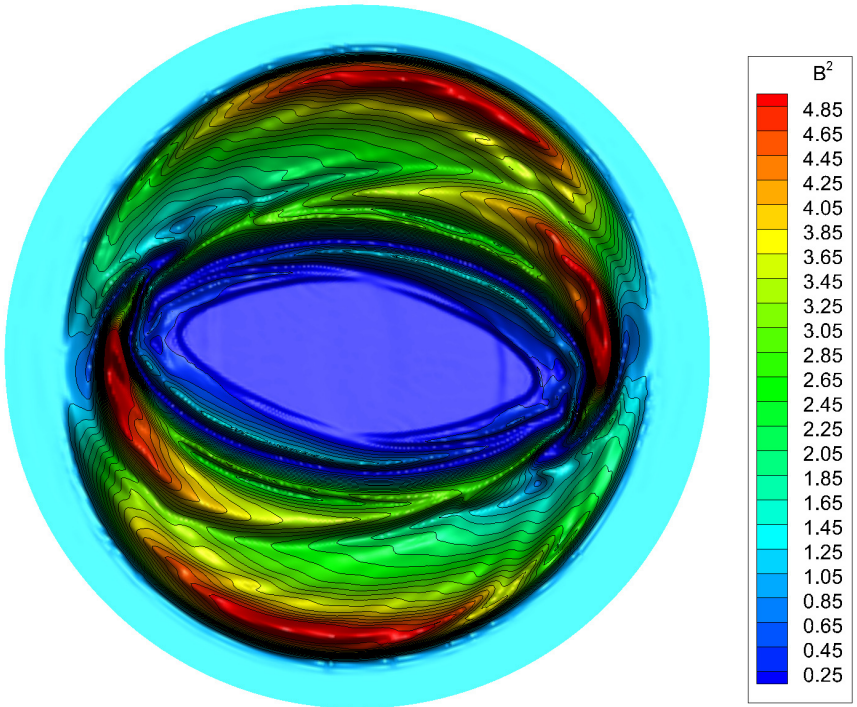
MOOD For Eulerian Finite Volume schemes

3 : Relativistic magnetohydrodynamics (RMHD)

WENO



MOOD



MOOD For Eulerian Finite Volume schemes

Systematic CPU time and memory consumption study

MOOD implemented into a 3D $\mathbb{P}_N\mathbb{P}_M$ ADER-WENO MPI // code dedicated to solve

$$\mathbf{Q}_t + \nabla \cdot \mathbf{F}(\mathbf{Q}, \nabla\mathbf{Q}) + \mathbf{B}(\mathbf{Q}) \cdot \nabla\mathbf{Q} = \mathbf{S}(\mathbf{Q}).$$

MOOD avoids too many reconstruction compared to WENO. For such a general code the reconstruction represents $\sim$ 60% of the work (CPU and memory).

Tests on 1 CPU core (Intel i7-2600 proc. 3.4 GHz, 12 GB of RAM) to avoid overheat due to MPI //.

Test case	**CPU time [s]**			**Memory [GB]**		
	WENO	MOOD	Ratio	WENO	MOOD	Ratio
2D vortex	313.8	276.7	1.13	233.55	76.10	3.07
2D Double Mach	5425	3327	1.63	2.14	0.628	3.41
3D Sod	46606	27283	1.70	13.44	2.464	5.98
3D Explosion*	1791.6	1399.0	1.28	460.5	140.6	3.28
2D Orszag-Tang vortex	15602	16599	0.94	2.536	1.002	2.53
2D MHD rotor	3315	2902	1.14	1.991	0.793	2.51
2D RMHD rotor	17434	18098	0.96	1.993	0.794	2.51

* run made on 521 CPU using MPI.

Memory consumption drops by a factor 2.5 $\rightarrow$ 6. CPU is better only for simple systems of PDEs.

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Context of direct ALE schemes

Assumption : Access to a general high order direct ALE-WENO code for Hydrodynamics equations
Proposition : remove any kind of limiter and stabilize with a MOOD loop
Needs : ensure mesh validity and physically relevant solution, stable and accurate.

Numerical study

Our reference code is ADER-ALE of arbitrary order of accuracy with WENO limiting on 2D/3D unstructured grids W.Boscheri *et al* [*]

Bibliography

[*] W. Boscheri and M. Dumbser. An Efficient Quadrature-Free Formulation for High Order ALE ADER-WENO Finite Volume Schemes on Unstructured Meshes. Journal of Scientific Computing, online april 2015.

W.Boscheri, M.Dumbser, R. Loubère, Direct Arbitrary-Lagrangian-Eulerian ADER-MOOD Finite Volume Schemes for Multidimensional Hyperbolic Conservation Laws, submitted 2014.

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Hydrodynamics equations on moving grid

Let $\mathbf{Q} = (\rho, \rho u, \rho v, \rho w, \rho E)$ be the vector of conserved variables with ρ the fluid density, $\mathbf{v} = (u, v, w)$ the velocity vector and ρE the total energy density. A general formulation reads

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \underline{\underline{\mathbf{F}}}(\mathbf{Q}) = 0, \qquad \mathbf{x} \in \Omega \subset \mathbb{R}^3, t \in \mathbb{R}_0^+, \tag{3}$$

where $\underline{\underline{\mathbf{F}}} = (\mathbf{f}, \mathbf{g}, \mathbf{h})$ is the conservative nonlinear flux tensor given by

$$\mathbf{f} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u(\rho E + p) \end{pmatrix}, \quad \mathbf{g} = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ v(\rho E + p) \end{pmatrix}, \quad h = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w(\rho E + p) \end{pmatrix}. \tag{4}$$

The system is closed by the EOS of an ideal gas $p = (\gamma - 1)\left(\rho E - \frac{1}{2}\rho \mathbf{v}^2\right) = (\gamma - 1)\rho\varepsilon$

p is the fluid pressure and γ the ratio of specific heats. Let furthermore $\varepsilon = \left(E - \frac{1}{2}\mathbf{v}^2\right)$ be the specific internal energy. Provided that an admissible fluid state is considered, that is to say $\rho > 0$ and $\varepsilon > 0$, then the speed of sound is given by $c = \sqrt{\frac{\gamma p}{\rho}} = \sqrt{\gamma(\gamma - 1)\varepsilon}$.

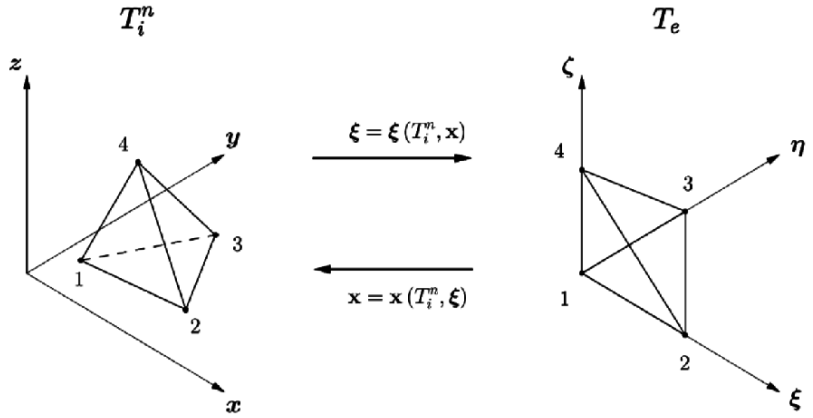
MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Moving tetrahedrization

$\Omega(t) \subset \mathbb{R}^3$ is discretized at any time level t^n by a set of moving and deforming tetrahedral elements T_i^n. N_E denotes the total number of elements and the tetrahedrization $\mathcal{T}_\Omega^n$ of the domain is

$$\mathcal{T}_\Omega^n = \bigcup_{i=1}^{N_E} T_i^n. \tag{5}$$

We assume that the mesh configuration continuously changes in time. There exists a mapping between the physical element T_i^n to a reference element T_e via a local reference coordinate system $\xi - \eta - \zeta$



The spatial reference element T_e is the unit tetrahedron. $\boldsymbol{\xi} = (\xi, \eta, \zeta)$ and $\mathbf{x} = (x, y, z)$ are the vector of the spatial coordinates in the reference system and the position vector in the physical system, respectively. Let $\mathbf{X}_{k,i}^n = (X_{k,i}^n, Y_{k,i}^n, Z_{k,i}^n)$ be the vector of physical spatial coordinates of the k-th vertex of tetrahedron T_i^n

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Finite volume data and polynomial reconstruction

High order accurate in space and time

High accuracy is obtained with polynomial reconstructions (space) and ADER scheme (time).

Finite volume data

Finite volume scheme data are represented at a given time t^n At each t^n within the control volume T_i^n the mean value of the state vector $\mathbf{Q}_i^n$ is

$$\mathbf{Q}_i^n = \frac{1}{|T_i^n|} \int_{T_i^n} \mathbf{Q}(\mathbf{x}, t^n)\, d\mathbf{x}, \tag{6}$$

Polynomial reconstruction of degree $M >> 1$

(Originally Boscheri *et al* used WENO in 2D/3D for unstructured mesh.)
The reconstruction operator generates piecewise polynomials $\mathbf{w}_h(\mathbf{x}, t^n)$ of degree M for each element T_i^n considering a unique central reconstruction stencil $\mathcal{S}_i$. $\mathcal{S}_i$ is composed of a number of n_e neighbor elements.

Note : n_e must be larger than the smallest possible number $\mathcal{M} = (M+1)(M+2)(M+3)/6$ needed to reach the nominal order of accuracy $M+1$. Here $n_e \simeq 2\mathcal{M}$ (2D) or $n_e \simeq 3\mathcal{M}$ (3D).

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Finite volume data and polynomial reconstruction

Polynomial reconstruction of degree $M >> 1$

Orthogonal Dubiner-type basis functions $\psi_l(\xi, \eta, \zeta)$ on the reference tetrahedron T_e

$$\mathbf{w}_h(\mathbf{x}, t^n) = \sum_{l=1}^{\mathcal{M}} \psi_l(\boldsymbol{\xi}) \hat{\mathbf{w}}_{l,i}^n := \psi_l(\boldsymbol{\xi}) \hat{\mathbf{w}}_{l,i}^n, \tag{7}$$

$\hat{\mathbf{w}}_{l,i}^n$ are the unknown degrees of freedom.
We require integral conservation for the reconstruction on each element T_j^n belonging to stencil $\mathcal{S}_i$ leading to an overdetermined linear system of equations solved using a least squares technique (LSQ).

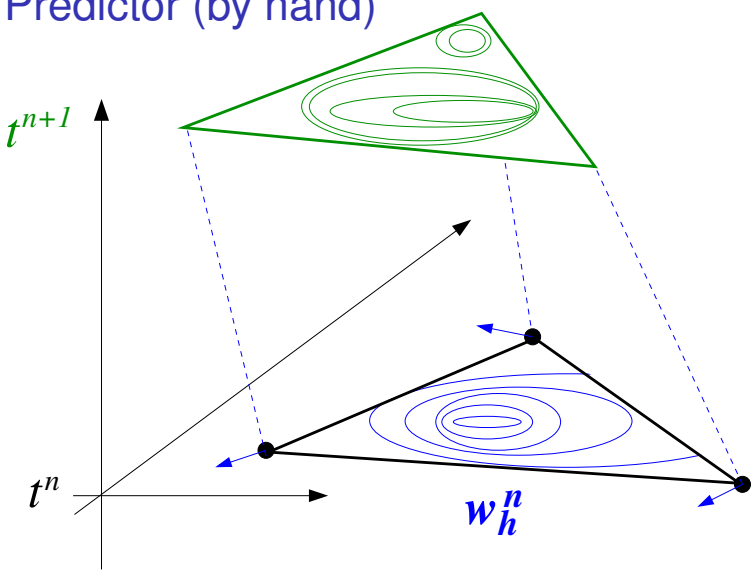
MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Local space-time Galerkin predictor on moving mesh

Basics

The reconstructed polynomials $\mathbf{w}_h(\mathbf{x}, t^n)$ computed at the current time t^n are evolved for one time step *locally* within each element $T_i(t)$ without requiring any neighbor interaction $\Longrightarrow$ piecewise space-time polynomials of degree M, denoted by $\mathbf{q}_h(\mathbf{x}, t)$.

Predictor (by hand)



Element-local weak space-time formulation of the governing PDE.
An isoparametric approach is adopted, the mapping between the physical space-time coordinate x and the reference space-time coordinateξ is represented by the same basis functions θ_k

$$\left\langle \theta_k, \frac{\partial \theta_l}{\partial \tau} \right\rangle \widehat{\mathbf{q}}_{l,i} = - \langle \theta_k, \theta_l \rangle \, \Delta t \, \widehat{\mathbf{P}}_{l,i}. \qquad (8)$$

Mass and stiffness space-time matrices.

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Non local mesh Motion

Nodal solver from Després [ARMA 05], Maire *et al* [SISC 07]

As Lagrangian as possible !
A suitable Lagrangian *node solver* technique assigns a *unique* velocity vector $\overline{\mathbf{V}}_k$ accurately representing an almost Lagrangian velocity, therefore leading to the new *Lagrangian coordinates*

$$\mathbf{x}_k^{Lag} = \mathbf{x}_k^n + \Delta t \, \overline{\mathbf{V}}_k, \tag{9}$$

Relaxation to maintain geometrical quality

We rely on a local *rezoning algorithm* which produces $\mathbf{x}_k^{Rez}$ (Laplacian smoothing).
The final node position

$$\mathbf{x}_k^{n+1} = \mathbf{x}_k^{Lag} + \omega_k \left(\mathbf{x}_k^{Rez} - \mathbf{x}_k^{Lag} \right), \tag{10}$$

where ω_k is a node-based coefficient associated to the deformation of the Lagrangian grid over the time step Δt, see Loubere *et al* [JCP 11]

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Finite volume final formulation

Space-time divergence operator

The governing PDEs are reformulated using a space-time divergence operator $\tilde{\nabla}$

$$\tilde{\nabla} \cdot \tilde{\mathbf{F}} = \mathbf{0}, \qquad \tilde{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}, \frac{\partial}{\partial t} \right)^T, \ \tilde{\mathbf{F}} = (\mathbf{f}, \mathbf{g}, \mathbf{h}, \mathbf{Q}) \text{ space-time flux tensor} \tag{11}$$

The new state vector $\mathbf{Q}^{n+1}$ is evaluated by integrating over a *four-dimensional* space-time control volume $\mathcal{C}_i^n = T_i(t) \times \left[t^n; t^{n+1} \right]$

$$\int_{\mathcal{C}_i^n} \tilde{\nabla} \cdot \tilde{\mathbf{F}} \, d\mathbf{x}dt = \mathbf{0} \implies \int_{\partial \mathcal{C}_i^n} \tilde{\mathbf{F}} \cdot \tilde{\mathbf{n}} \, dS = \mathbf{0}, \tag{12}$$

(Gauss theorem leads to a sum of the fluxes computed over the *three-dimensional* manifold $\partial \mathcal{C}_i^n$ (the boundary of the 4D space-time control volume) given by the initial and final configuration of the tetrahedron at times t^n and t^{n+1}, respectively, as well as by the evolution of each lateral face of element $T_i(t)$ within the timestep.)

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Finite volume final formulation

High order direct ALE FV scheme

Final discretization

$$|T_i^{n+1}|\,\mathbf{Q}_i^{n+1} = |T_i^n|\,\mathbf{Q}_i^n - \sum_{T_j \in \mathcal{N}_i} \int_{\partial C_{ij}^n} \tilde{\mathbf{F}}_{ij} \cdot \tilde{\mathbf{n}}_{ij}\, d\mathbf{x}dt. \tag{13}$$

The integral on the RHS computed using Gaussian quadrature of sufficient precision on a reference element.
The discontinuity of the predictor solution $\mathbf{q}_h$ is resolved by a numerical flux function $\tilde{\mathbf{F}}_{ij} \cdot \tilde{\mathbf{n}}_{ij}$ (robust Rusanov type scheme or a less diffusive Osher type flux).

CFL constrain

$$\Delta t_{CFL} = \text{CFL} \min_{T_i^n} \frac{d_i}{|\lambda_{\max,i}|}, \qquad \forall T_i^n \in \Omega^n, \tag{14}$$

$|\lambda_{\max,i}|$ is the maximum absolute value of the eigenvalues from $\mathbf{Q}_i^n$ in T_i^n.
Δt is also restricted by a maximal cell compression coefficient.

MOOD For Direct Arbitrary-Lagrangian-Eulerian Schemes (ALE) schemes

Stabilization *a posteriori*

Previously

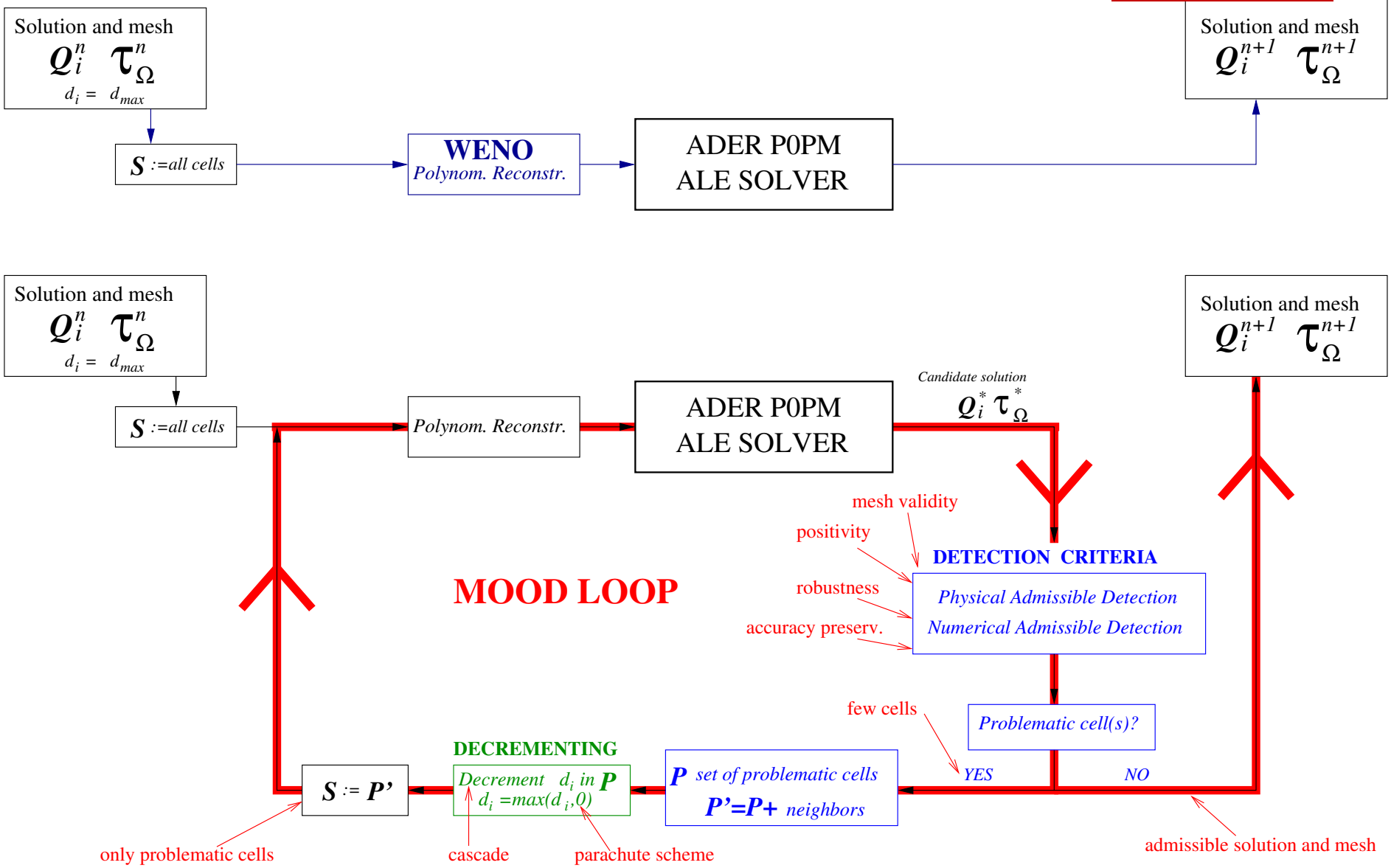
Boscheri *et al* used WENO reconstructions for $\mathbf{w}_h(\mathbf{x}, t)$.
Here we use a MOOD loop, unique stencil, decrement M if invalid solution is observed.

Detection criteria

PAD : $\rho_i^* > 0, \varepsilon_i^* > 0$, and $|T_i^*| > 0$ (valid mesh)
NAD : DMP+U2 on conservative variables, NaN

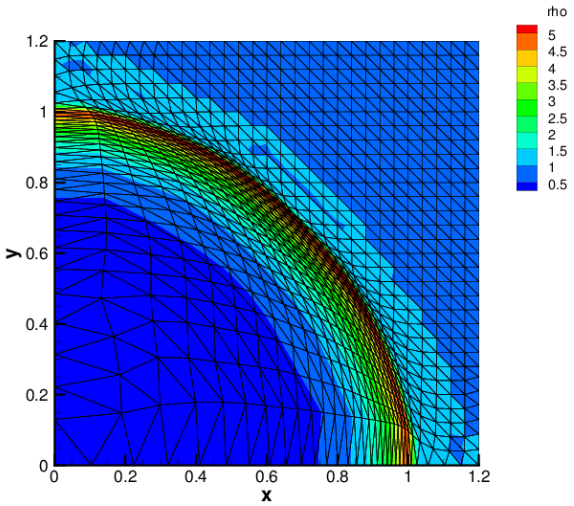
Cascade of schemes and parachute scheme

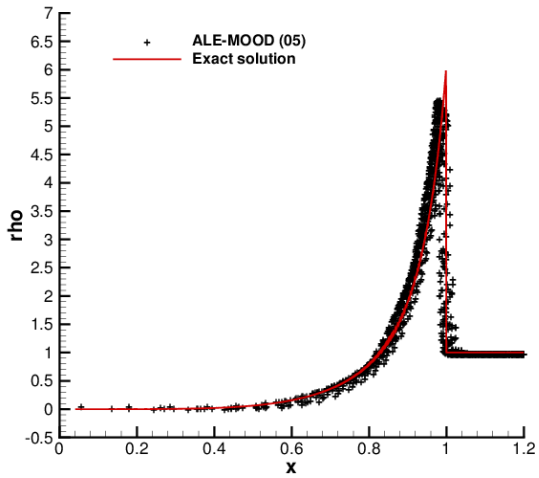
$\mathbb{P}_M \rightarrow \mathbb{P}_1^{lim} \rightarrow \mathbb{P}_0$ (usually $M = 4$). FV $\mathbb{P}_0$ scheme as parachute.

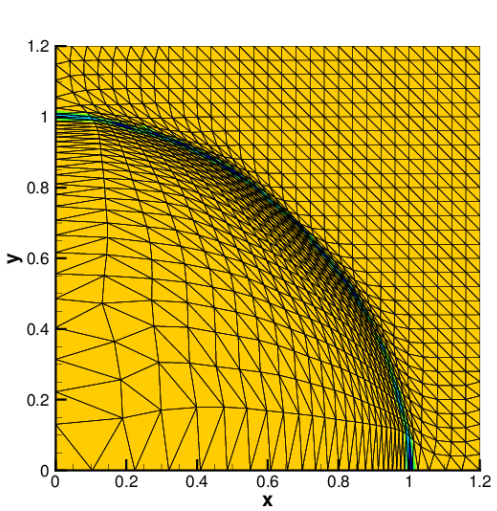

Solution and mesh
Q_i^n τ_Ω^n
$d_i = d_{max}$
S :=all cells
WENO
Polynom. Reconstr.
ADER P0PM
ALE SOLVER
Solution and mesh
Q_i^{n+1} τ_Ω^{n+1}
Solution and mesh
Q_i^n τ_Ω^n
$d_i = d_{max}$
S :=all cells
Polynom. Reconstr.
ADER P0PM
ALE SOLVER
Candidate solution
Q_i^* τ_Ω^*
Solution and mesh
Q_i^{n+1} τ_Ω^{n+1}
MOOD LOOP
mesh validity
positivity
robustness
accuracy preserv.
DETECTION CRITERIA
Physical Admissible Detection
Numerical Admissible Detection
few cells
Problematic cell(s)?
YES
NO
admissible solution and mesh
DECREMENTING
Decrement d_i in P
$d_i = max(d_i, 0)$
P set of problematic cells
$P'=P+$ neighbors
$S := P'$
only problematic cells
cascade
parachute scheme

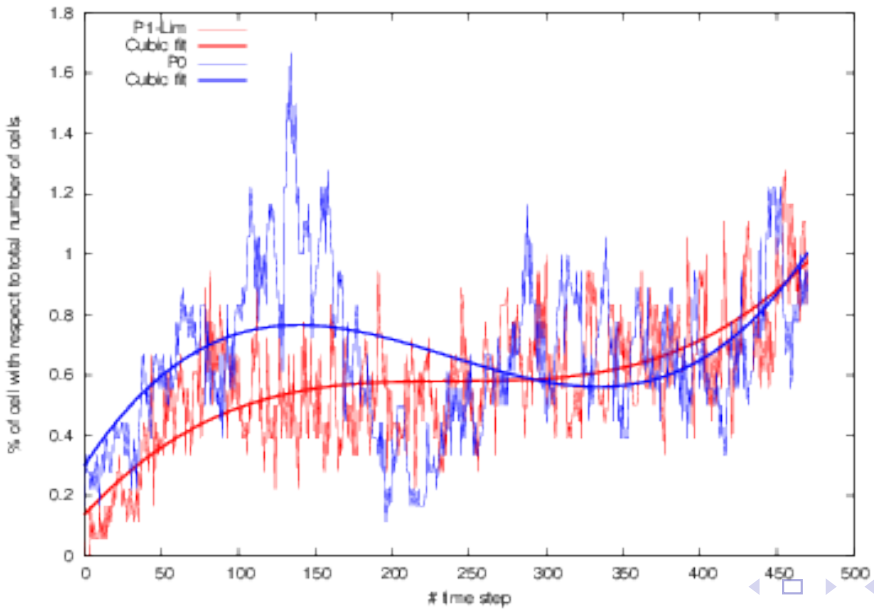
MOOD For Direct ALE schemes

Sedov problem : point explosion in 2D



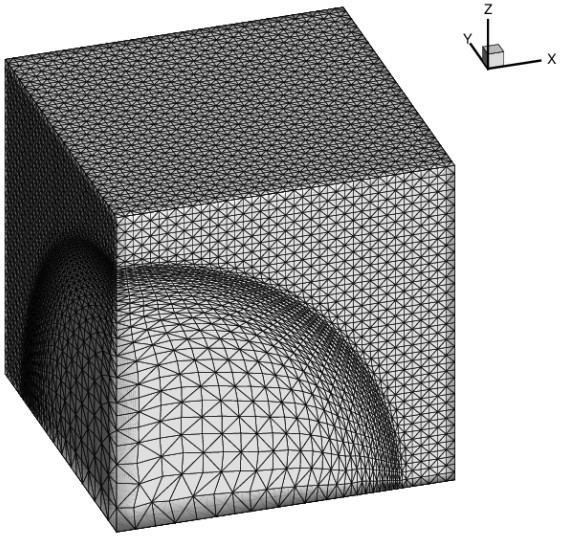


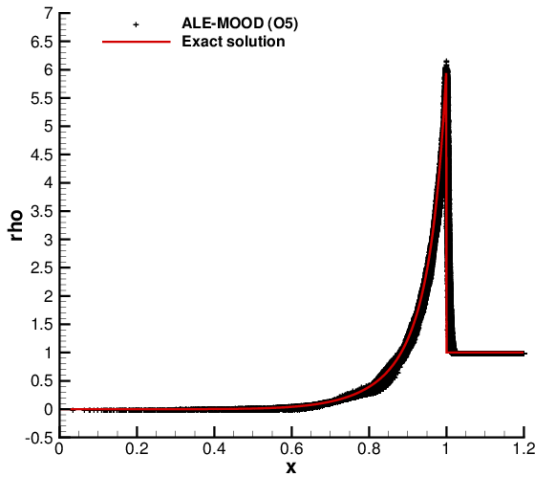


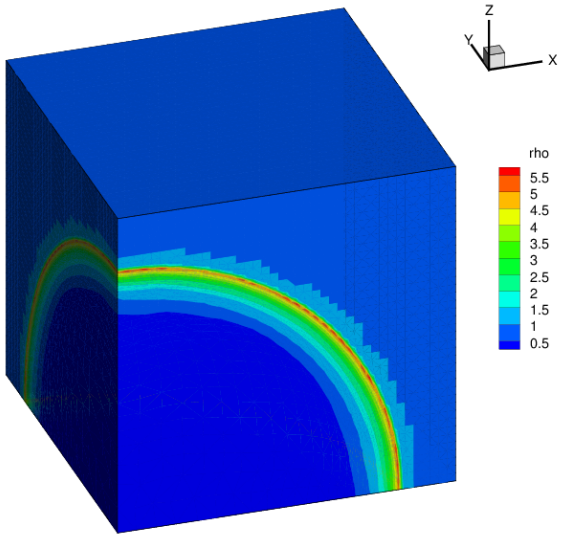


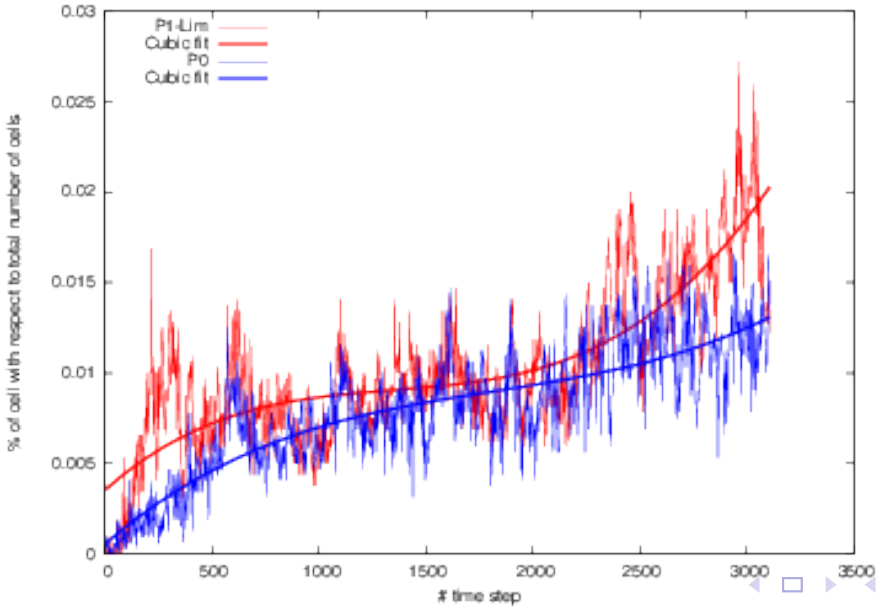
MOOD For Direct ALE schemes

Sedov problem : point explosion in 3D



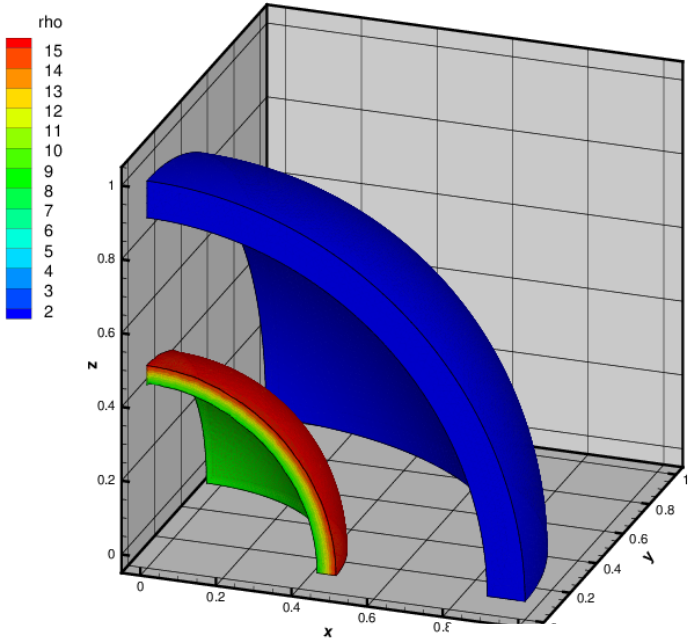


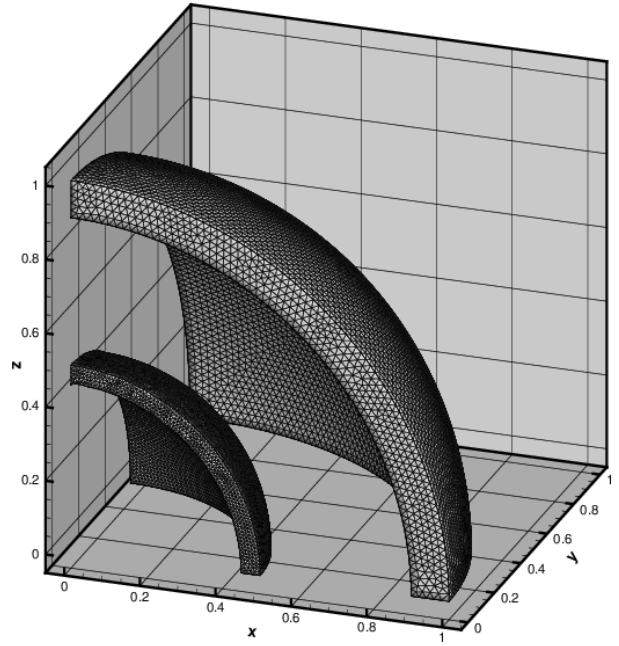


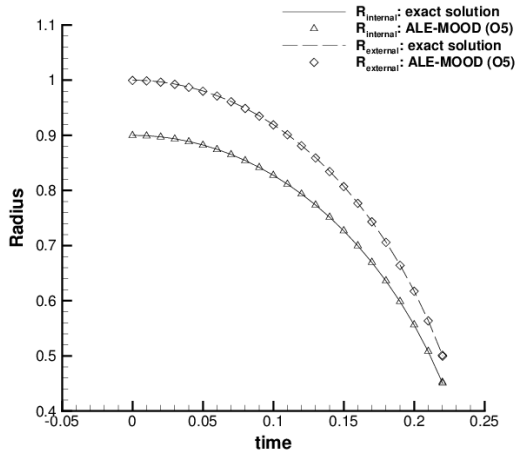


MOOD For Direct ALE schemes

Kidder problem : isentropic compression in 3D

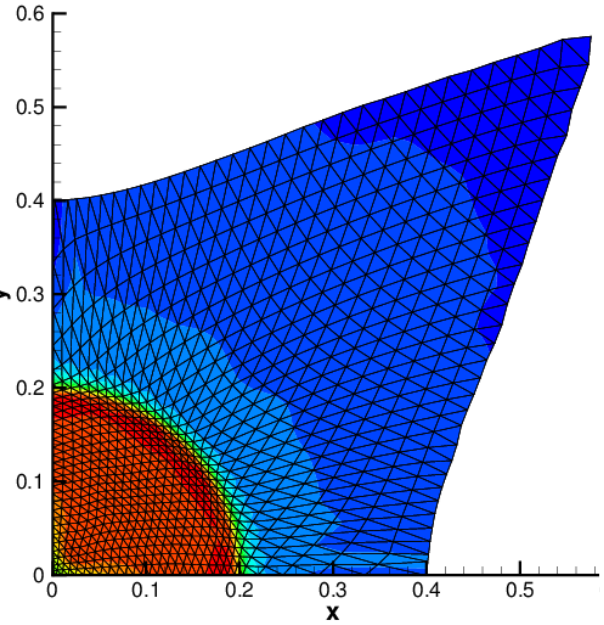


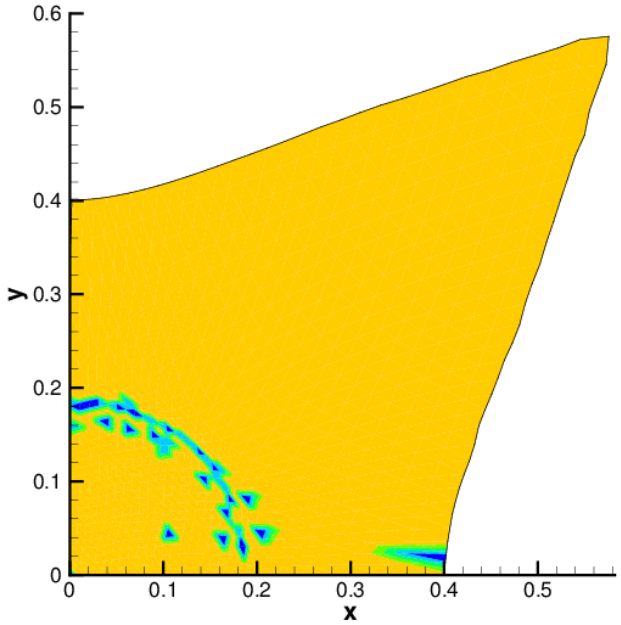


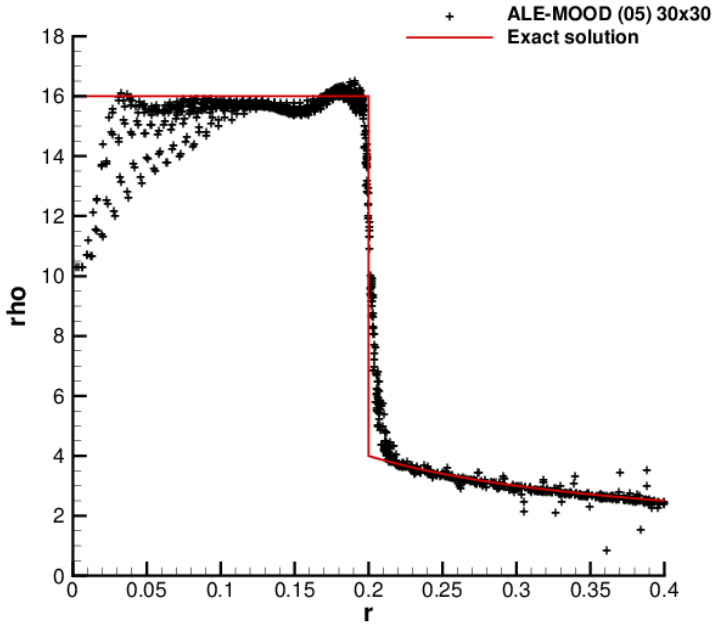


MOOD For Direct ALE schemes

2D Noh problem : infinity strenght diverging shock 2×30^2 cells

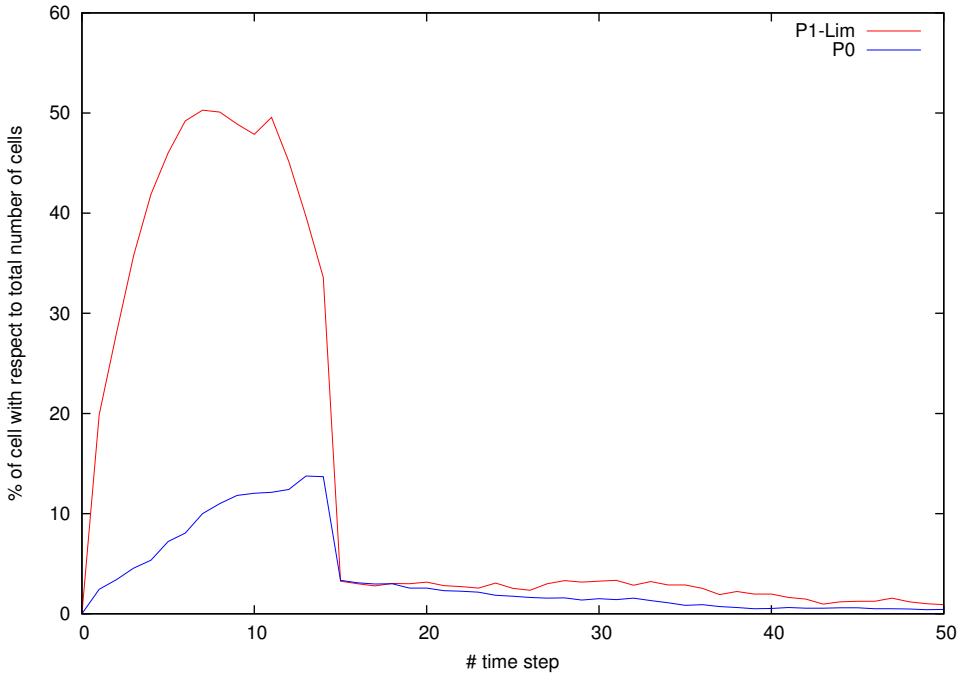


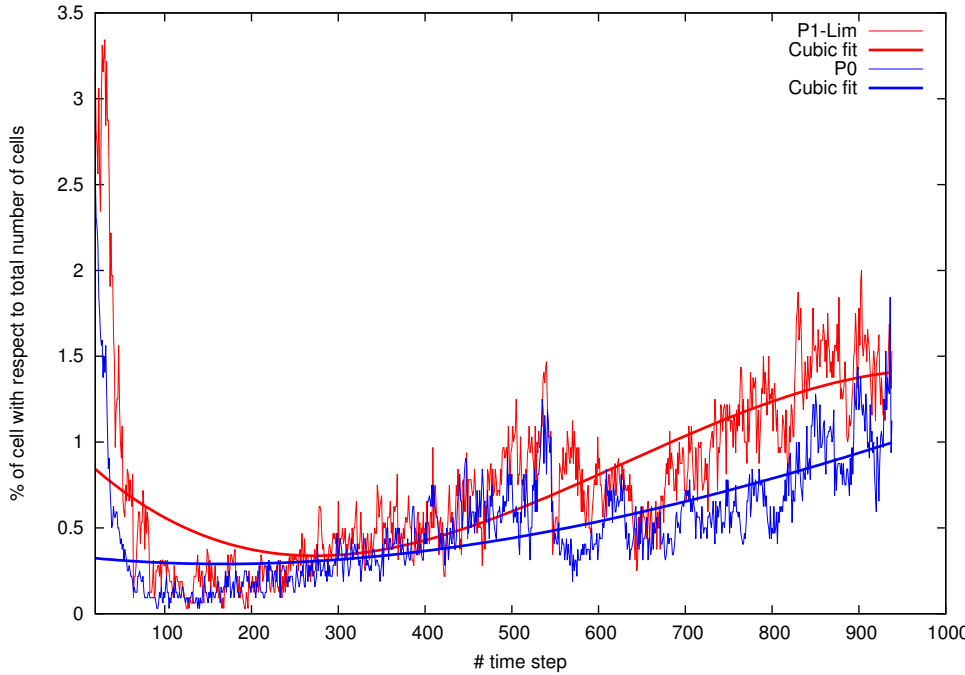




MOOD For Direct ALE schemes

2D Noh problem : 2×30^2 cells

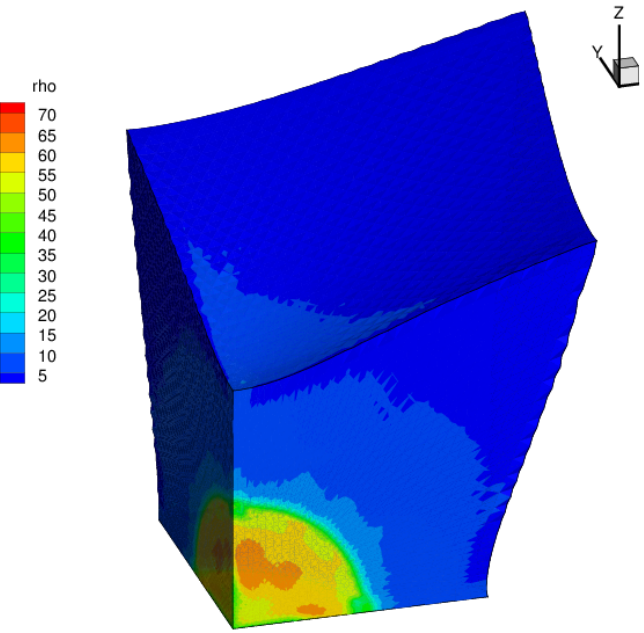


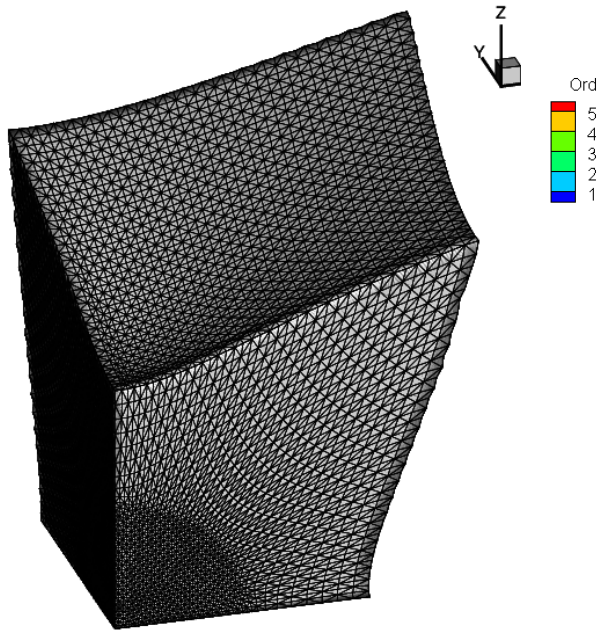


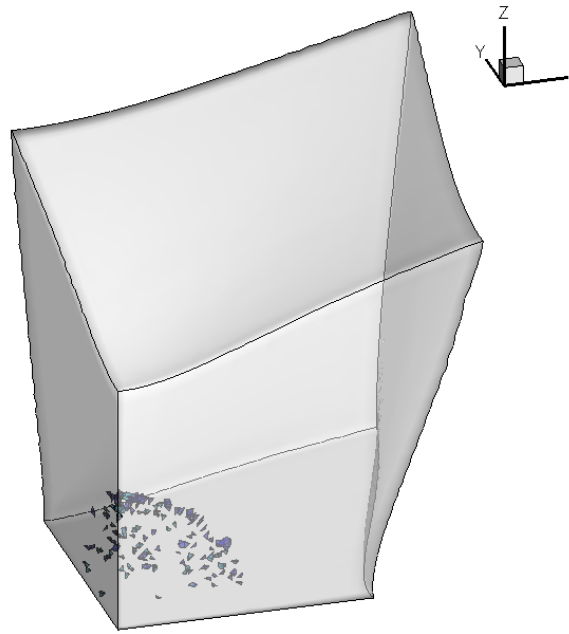
Problematic cells detected (first 50 cycles (left), next ones (right))

MOOD For Direct ALE schemes

3D Noh problem : 32×10^4 cells

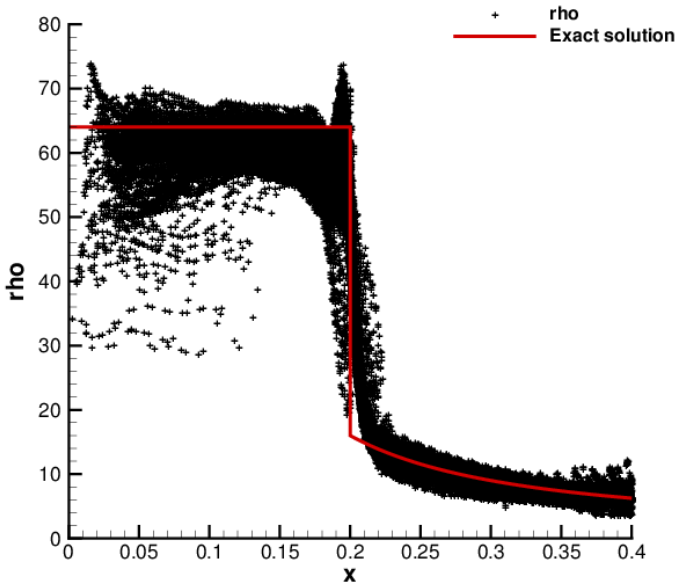


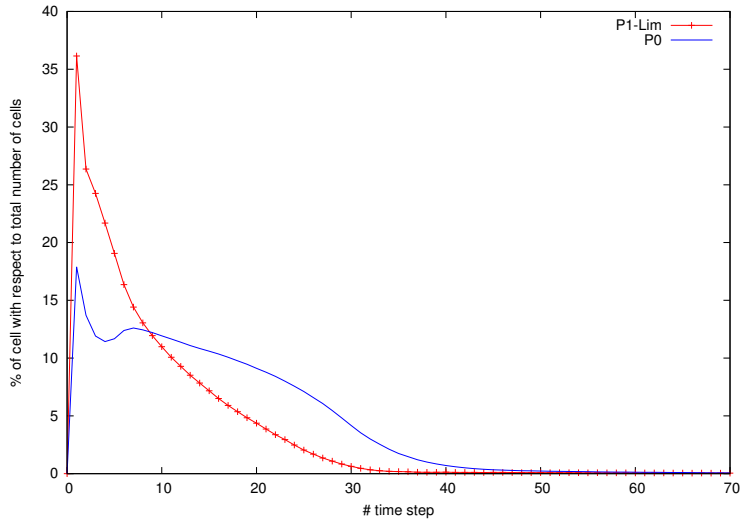


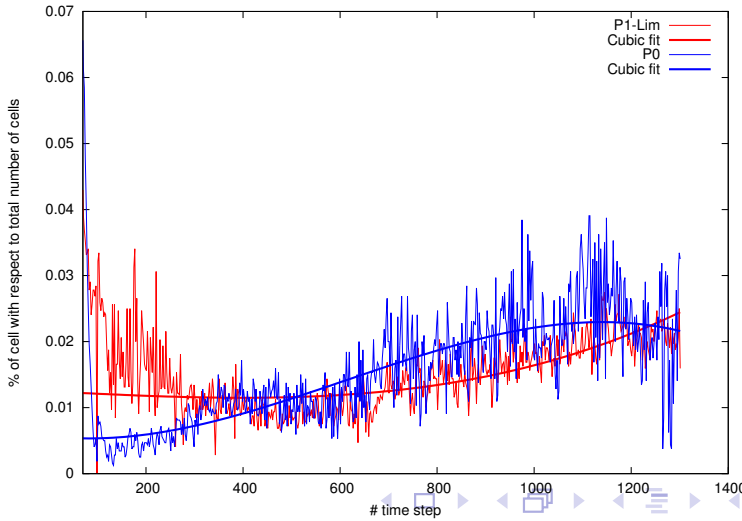


MOOD For Direct ALE schemes

3D Noh problem : 32×10^4 cells

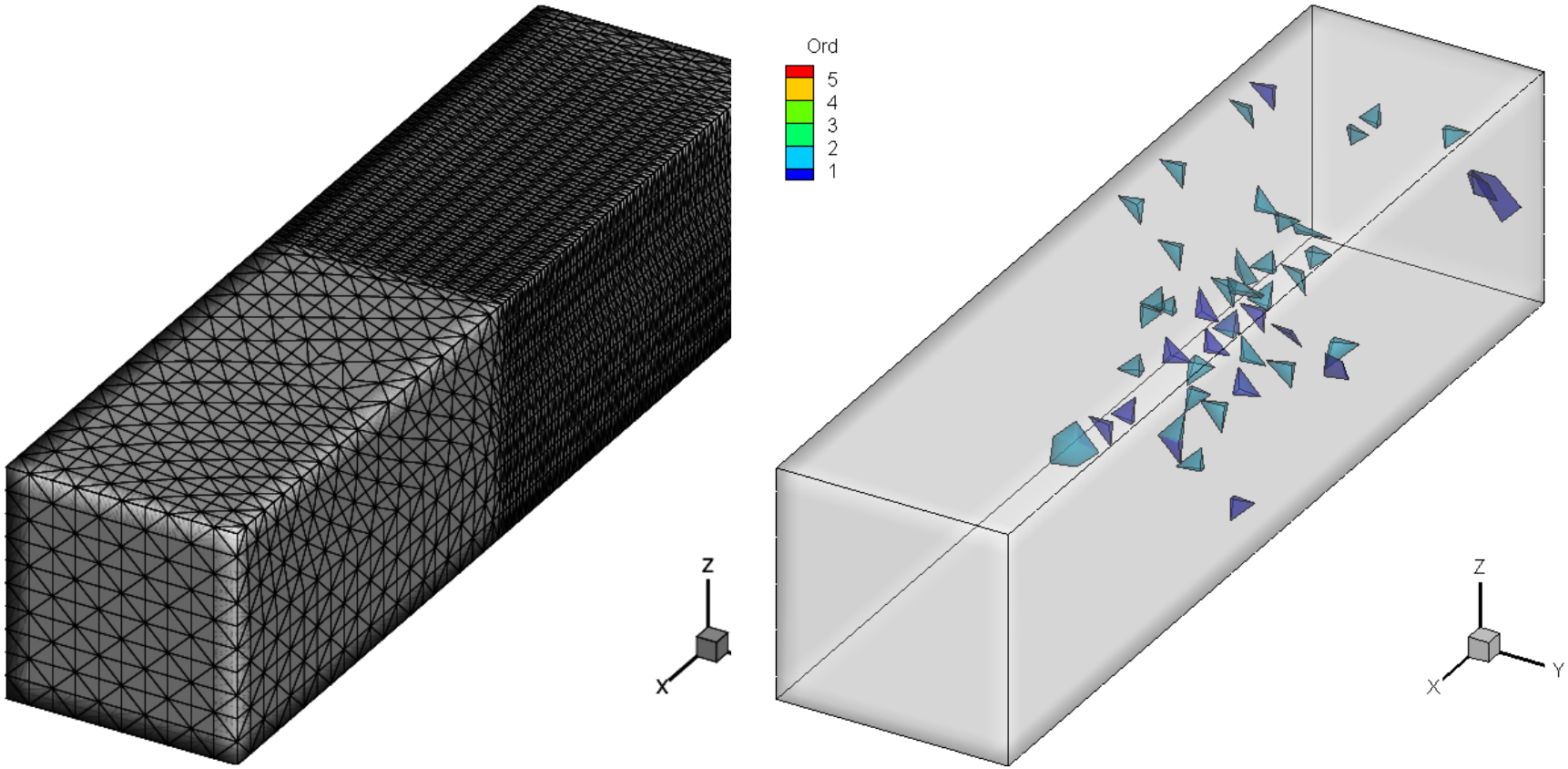






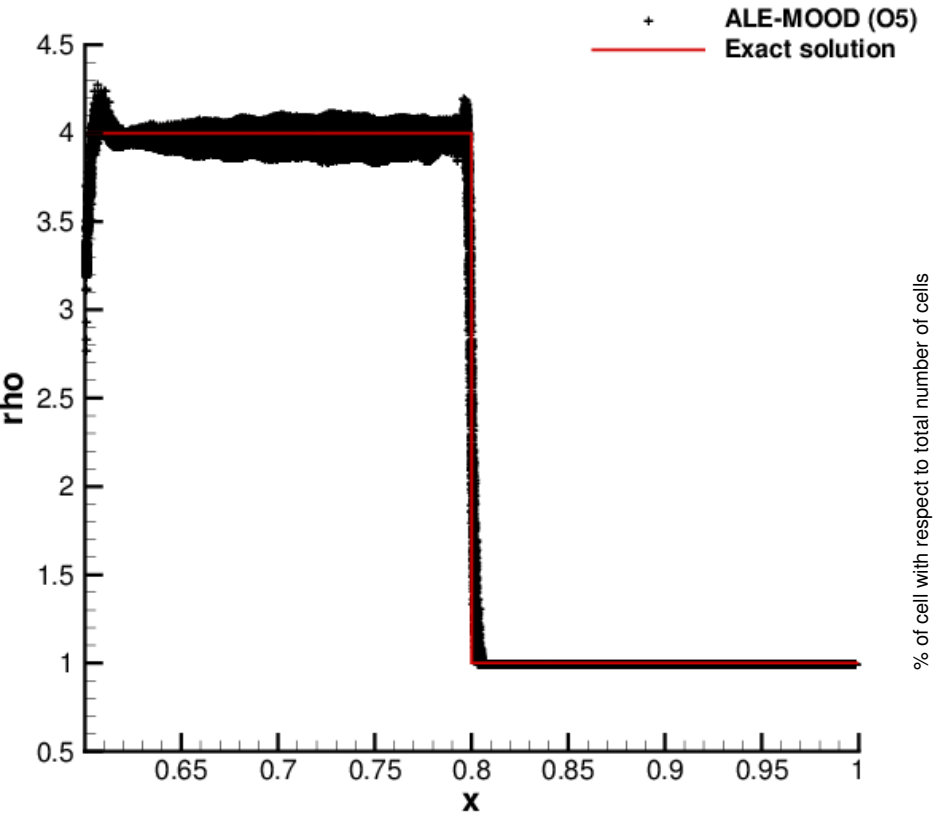
MOOD For Direct ALE schemes

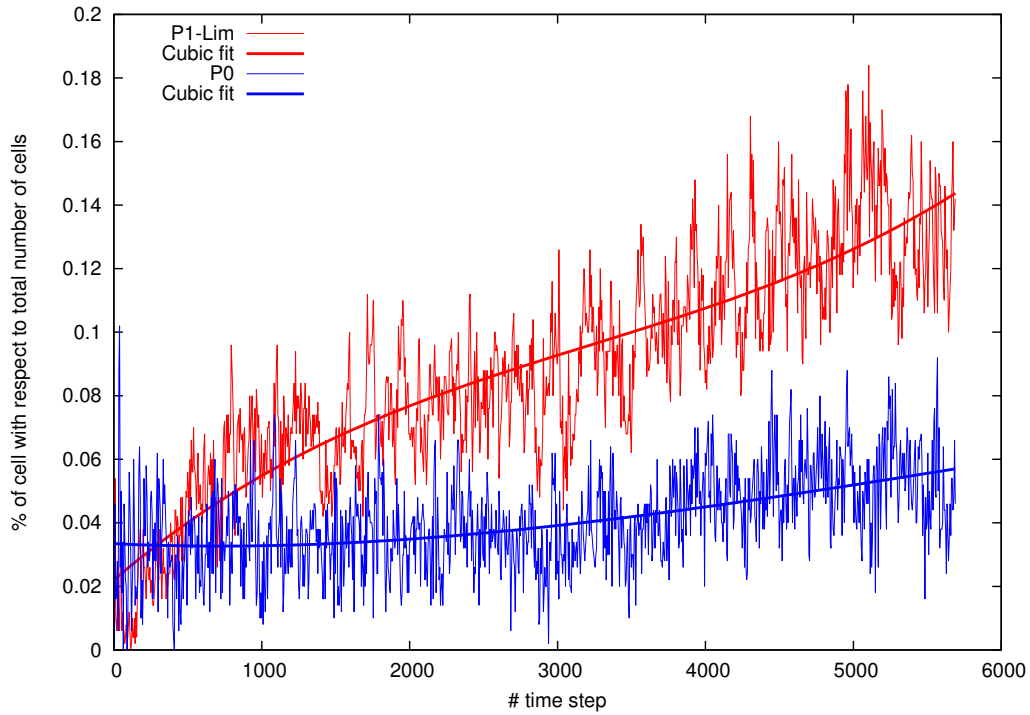
3D Saltzmann problem : 5×10^4 cells



MOOD For Direct ALE schemes

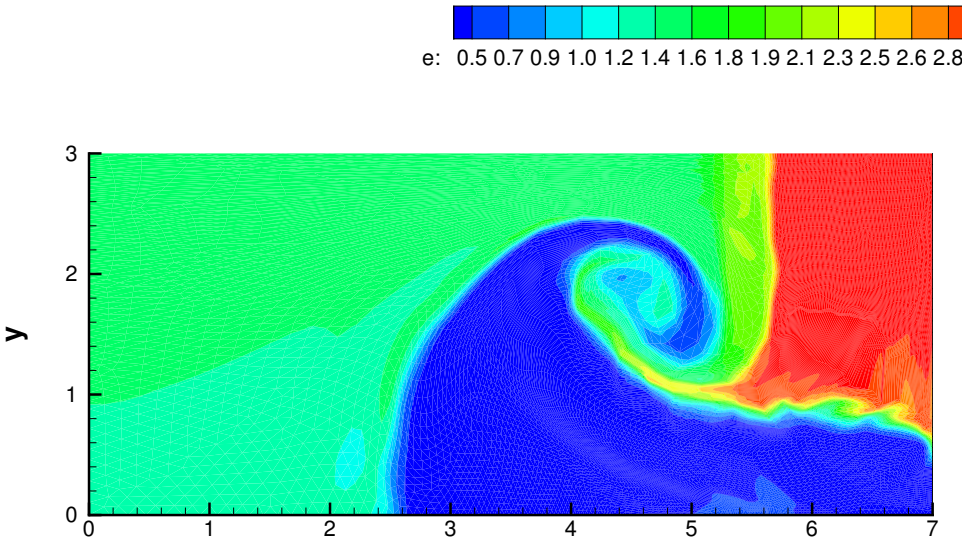
3D Saltzmann problem : 5×10^4 cells

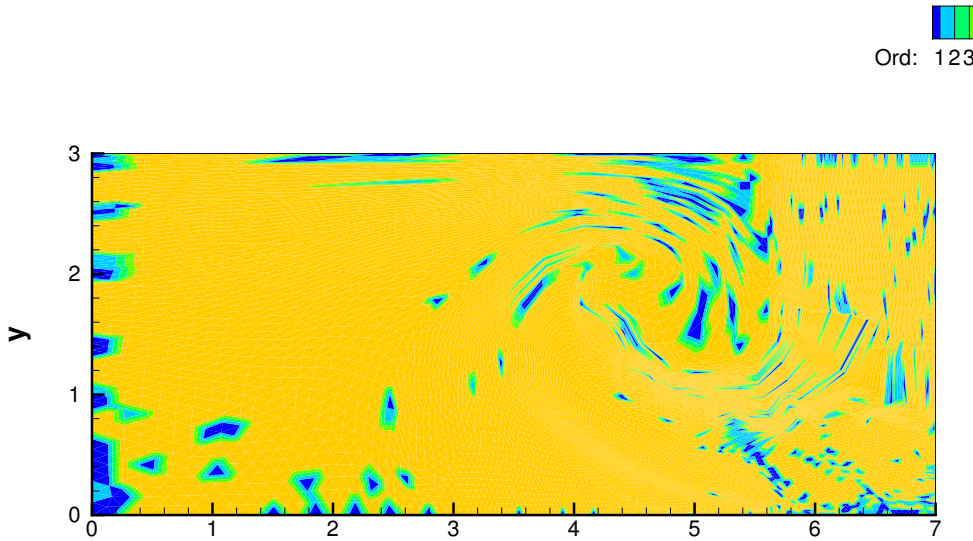


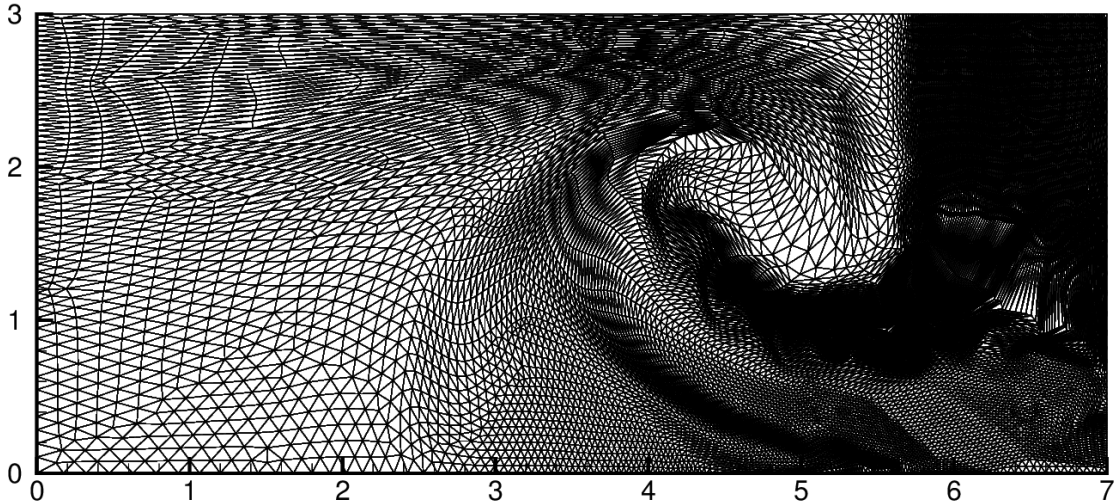


MOOD For Direct ALE schemes

2D triple point problem : 19098 cells

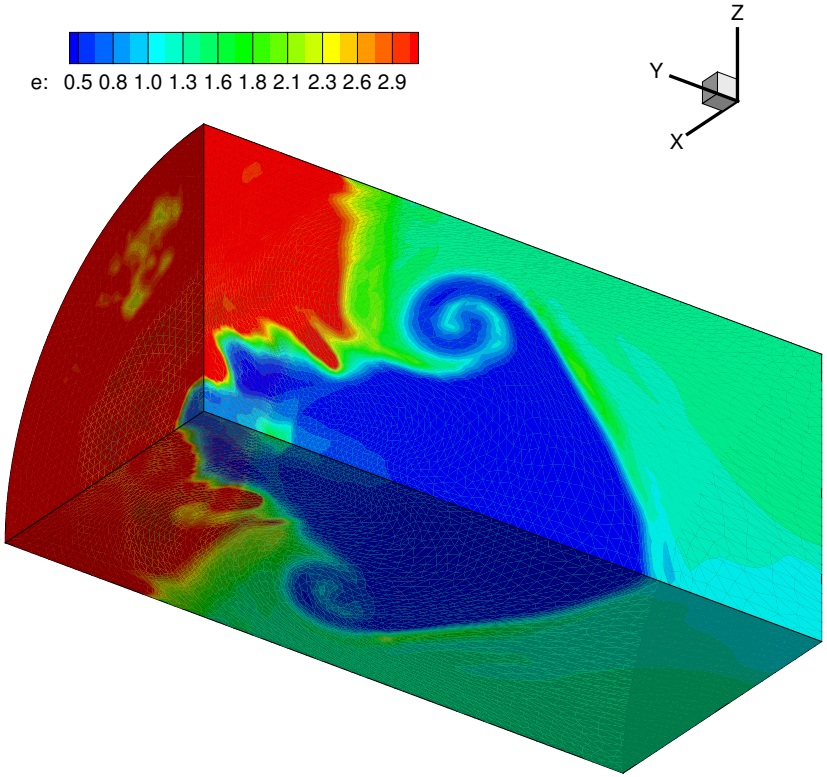


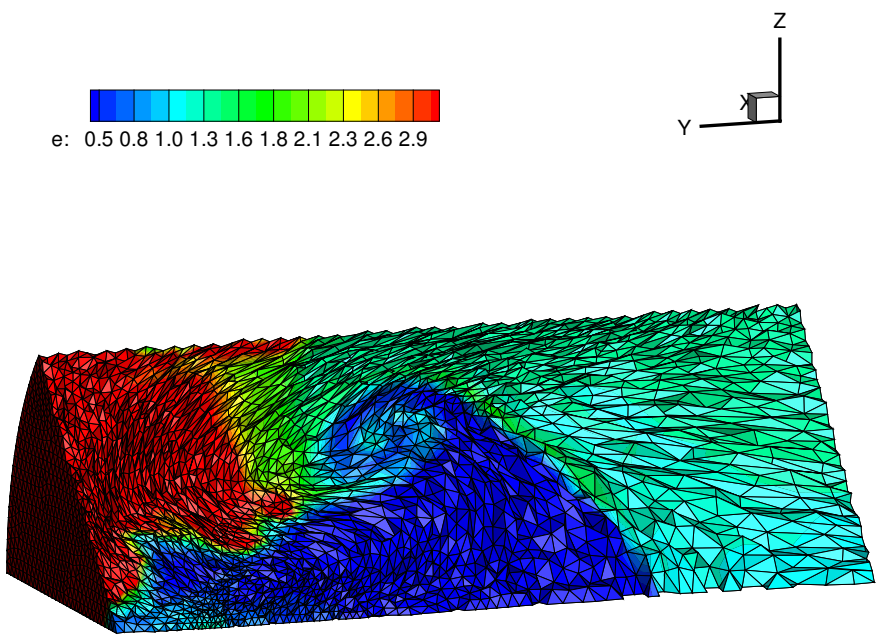




MOOD For Direct ALE schemes

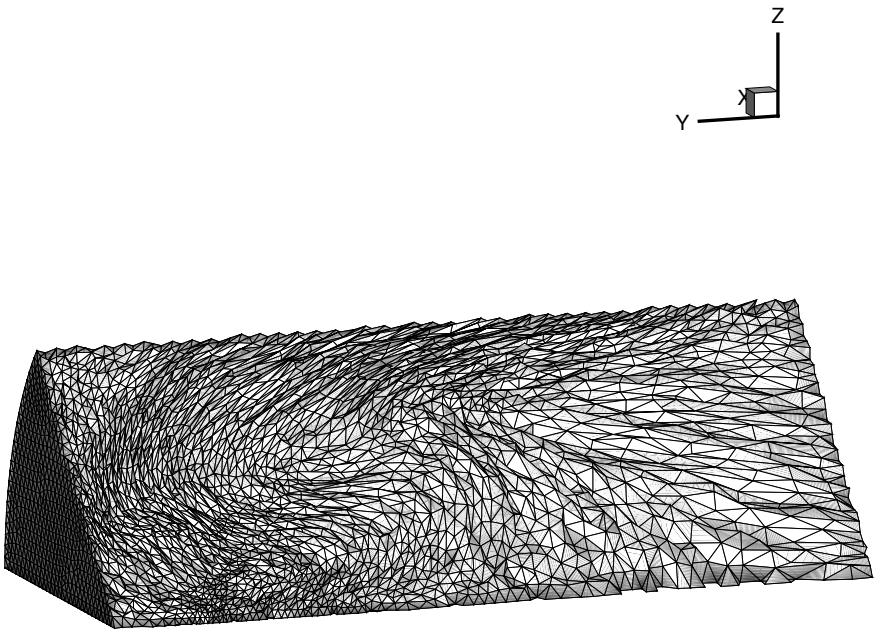
3D triple point problem : 304246 cells

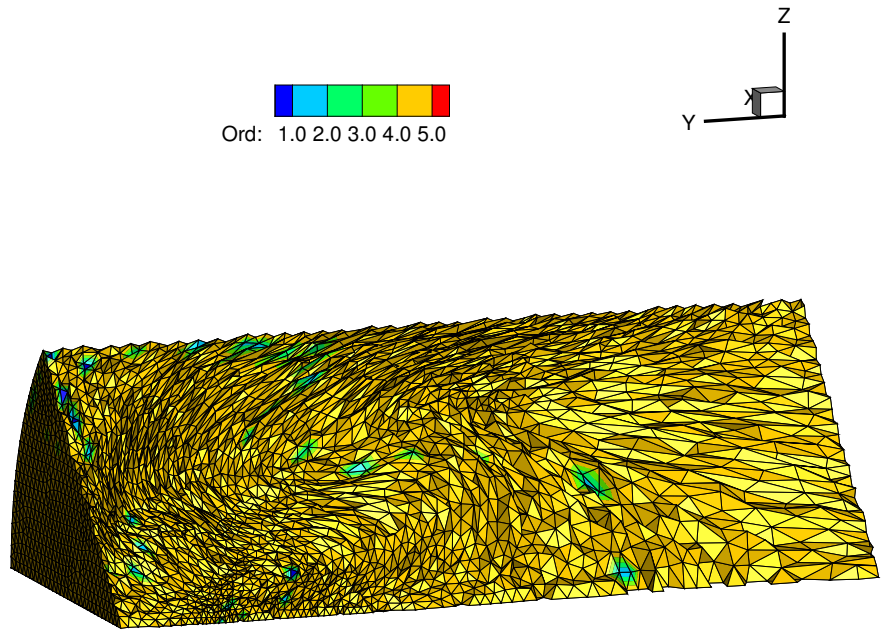




MOOD For Direct ALE schemes

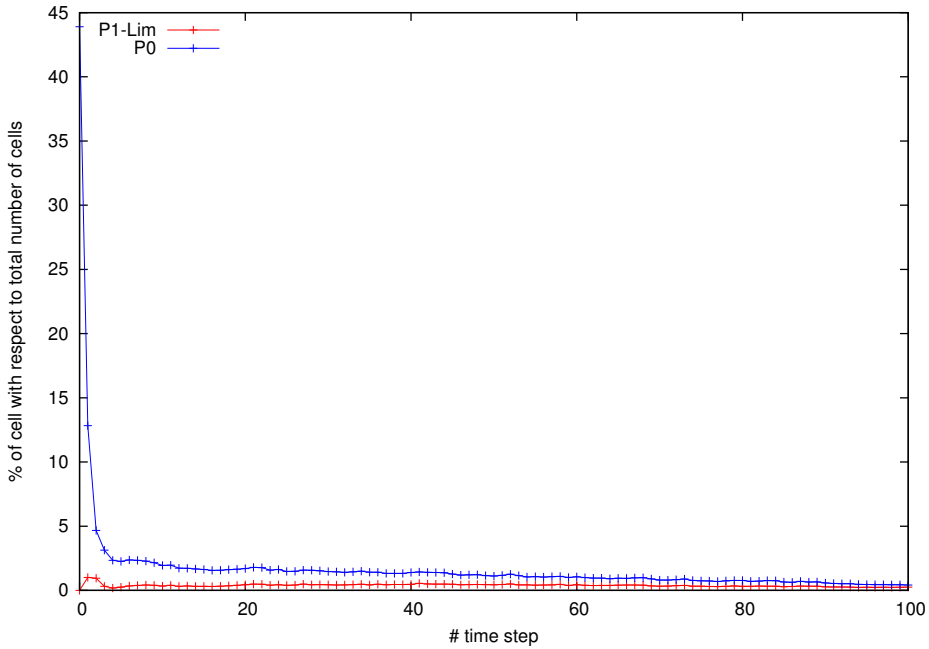
3D triple point problem : 304246 cells

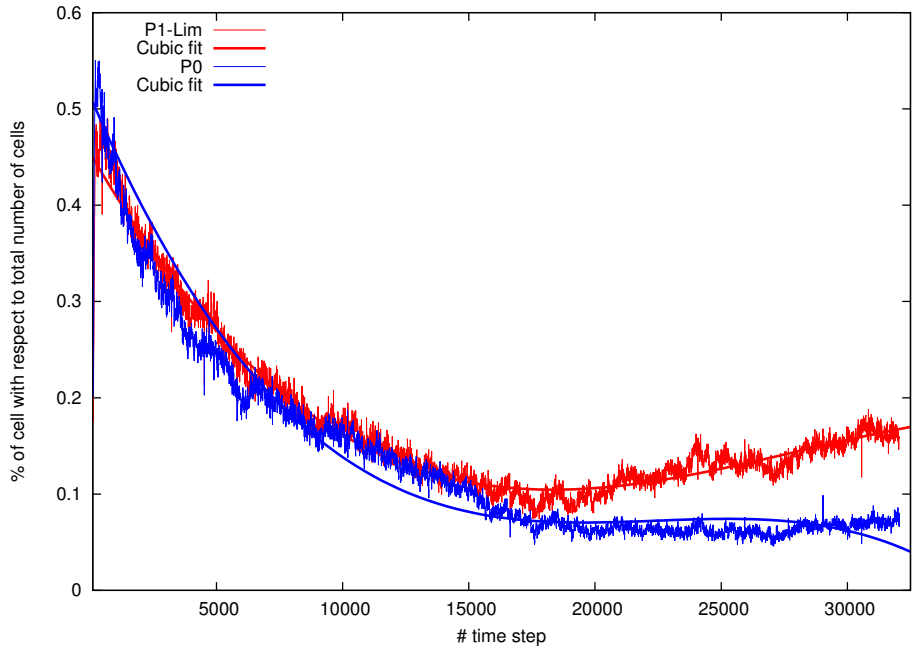




MOOD For Direct ALE schemes

3D triple point problem : 304246 cells





MOOD For Direct ALE schemes

Comparison WENO/MOOD in 3D

3D Tests	N_E $\times 10^4$	**ALE-WENO-$\mathbb{P}_0\mathbb{P}_4$** CPU time $\times 10^{-2}$s	**ALE-WENO-$\mathbb{P}_0\mathbb{P}_4$** Memory $\times 10^4$MB	**ALE-MOOD-$\mathbb{P}_0\mathbb{P}_4$** CPU time $\times 10^{-2}$s	**ALE-MOOD-$\mathbb{P}_0\mathbb{P}_4$** Memory $\times 10^4$MB	**WENO/MOOD** Acc.	**WENO/MOOD** Sav.
Sod	7.1	37.89	1.55	15.16	0.85	2.50	1.83
Sedov	32.0	7.67	2.59	3.26	1.52	2.35	1.70
Noh	32.0	6.83	2.55	3.12	1.54	2.19	1.66
Kidder	11.2	7.92	1.84	2.19	0.98	3.64	1.87
Saltz.	5	10.53	0.050	4.14	0.027	2.54	1.85
Tpoint	30.4	34.10	3.28	14.09	1.94	2.42	1.69
					Average	**2.6**	**1.8**

Summary of CPU time needed to update one cell within one timestep ($\times 10^{-2}$ in seconds) and memory consumption (in MB). ALE-WENO-$\mathbb{P}_0\mathbb{P}_4$ versus ALE-MOOD-$\mathbb{P}_0\mathbb{P}_4$ schemes. Last two columns : ratio between the CPU times ("acceleration") and the memory consumption ("saving").

Conclusion

a posteriori MOOD paradigm for direct ALE FV schemes

- High-order finite volume scheme genuinely beyond 2nd order (up to 6th tested)
- Based on a unique high degree polynomial reconstruction per degree per cell on conservative variables
- ADER in time
- Coupled with a 'detection procedure' and a 'polynomial degree decrementing'
- Elligibility of the solution based on a set of properties that YOU want to consider to declare a numerical solution to be 'good' (ex : DMP, positivity, physical bounds, etc.)
- Compare favorably with state of the art (ALE ADER WENO) in 2D 3D unstructured
- MOOD adapts to //, other hyperbolic systems

Future extensions

Stiff source terms and non-conservative products (compressible multi-phase flows).

Perspectives

Thank you for your attention

Acknowledgments

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Where does it come from ?

a priori or *a posteriori*

J.S.Baehr `http://www.iep.utm.edu/apriori` *"A priori" and "a posteriori" refer primarily to how, or on what basis, a proposition might be known. In general terms, a proposition is knowable a priori if it is knowable independently of experience, while a proposition knowable a posteriori is knowable on the basis of experience. The distinction between a priori and a posteriori knowledge thus broadly corresponds to the distinction between empirical and nonempirical knowledge.*