

# Stable and accurate compressive interface capturing advection schemes

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# Objective

Derive stable and accurate conservative finite volumes scheme for advection problems on a bounded domain  $\Omega \subset \mathbb{R}^d$ ,  $d = 2, 3$ ,

$$\begin{aligned}\partial_t y + \mathbf{a} \cdot \nabla y &= 0, \quad \text{on } \Omega \times (0, T], \\ y(., t = 0) &= y^0(.) \in \Omega.\end{aligned}$$

assuming a divergence-free velocity field  $\mathbf{a}$ , for an initial function  $y^0 : \Omega \rightarrow \{0, 1\}$  having a finite number of measurable discontinuity lines.

See it as an alternative approach to interface reconstruction algorithms (VOF, Youngs, ...)

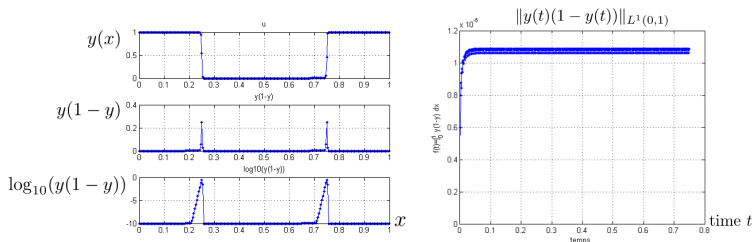
- ▶ Look for full SIMD parallel algorithm (multithreading)
- ▶ Simple coding / debugging
- ▶ Easily deal with an arbitrary number of materials
- ▶ Ability to extend to 3D computations
- ▶ Ability to easily extend to general unstructured meshes
- ▶ Ability to derive predictive performance models

# Testing classical MUSCL-type 2nd-order schemes

- ▶ Slope limiter theory has been designed to achieve spatial 2nd-order or higher order accuracy with TVD property [Sweby, ...]
- ▶ Moreover some slope limiters provide a compressive property on step-shaped functions
- ▶ !: some of them appear to be overcompressive (superbee, ultrabee), creating spurious staircase steps.
- ▶ Behaviour on multidimensional advection problems has to be clarified ...

# Capturing discontinuities with standard flux limited schemes

Pure 1D advection MUSCL scheme with *superbee* limiter :



- ▶ Discontinuities are spread over  $O(10)$  points up to the  $10^{-10}$  numerical accuracy ;
- ▶ !: the spreading is CFL-dependent ;
- ▶ But the spreading stays bounded over time.

NB : Limited downwind [Després-Lagoutière 2001-] provides better results: discontinuities are spread over 1 point at most in 1D.

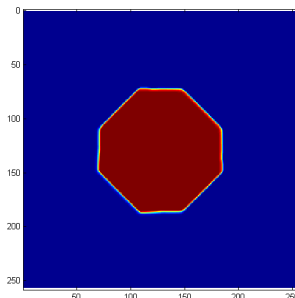
# Multidimensional experiments using advection schemes

## Artefacts and instabilities

1. One can observe geometrical artefacts using compressive solvers (limited downwind, VOFIRE, superbee, ...)
2. Strange attractors/spatial patterns for Cartesian meshes : disks become octagons or diamonds under a uniform velocity field, ...
3. Spurious interface instabilities “zigzag”

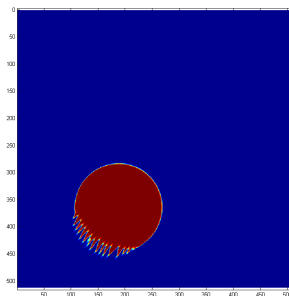
Some attempts to fix artefacts and instabilities: [alternative longitudinal reconstruction by Michel, Tran et al. 2010, ...], but more numerical diffusion.

# Common artefacts and interface instabilities - Examples



An initial disk advected into a uniform velocity field in the diagonal direction rapidly evolves toward an octagon or diamond shape [remarked by Després-Lagoutière for limited downwind]. It does not depend on the mesh size. Here, cartesian mesh  $256 \times 256$ , Courant number = 0.3, superbee limiter.

# Common artefacts and interface instabilities - Examples



“Zigzag” interface instabilities of an initial disk into a pure rotating velocity vector field. This does not depend on the mesh size. Here, cartesian mesh  $512 \times 512$ , Courant number = 0.3, superbee limiter.



# Origin of instabilities / artefacts

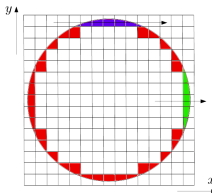
1. Spatial patterns: due to the **one-dimensional nature of slope limiting** process, generating some  $x$ - and  $y$ - flux imbalances with some loss of accuracy.
2. **Linear instability** of some compressive limiters (ex: downwind scheme).
3. NB: do not forget instability sources due to a bad **discretization in time** !

Equivalent equation of the first-order explicit Euler scheme :

$$\partial_t y + \mathbf{a} \cdot \nabla y + \frac{\Delta t}{2} \nabla \cdot (\mathbf{a} \otimes \mathbf{a} \nabla y) = 0.$$

4. At the discrete level, fraction profiles  $y$  are **smooth in the tangent direction of the interface**  $\implies$  do not compress too much, otherwise staircase steps may appear !

# Requirement for the low-diffusive advection scheme



- ▶ The solver has to be overcompressive in the normal direction to the interface.
- ▶ The solver should be 2nd-order accurate in tangent directions.
- ▶ The limiter has to preserve the gradient direction  $\nabla y$  (normal direction) for accuracy.
- ▶ High order accuracy in time (RK2 integration for example).

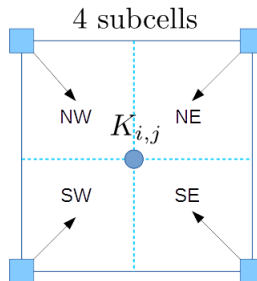
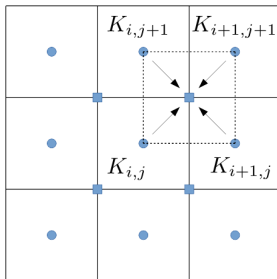
→ Our choice: multidimensional limiting process (MLP) strategy [ideas from FEM-TVD by Kuzmin-Turek 2003, MLP by Yoon et al. 2005, Kim et al 2005, ...].

# Multidimensional Limiting Process (MLP)

1. First estimate the local cell gradient  $(\nabla^h y)_{i,j}$
2. Consider piecewise-linear local approximation :

$$\mathcal{J}^h y(\mathbf{x}) = y_{i,j} + \phi_{i,j} (\nabla^h y)_{i,j} (\mathbf{x} - \mathbf{x}_{i,j}), \quad 0 \leq \phi_{i,j} \leq 1.$$

3. Limit the slope in order not to create new local extrema at the cell corners
4. Reconstruct a piecewise constant subcell solution
5. Compute the advective fluxes at the edges



# Low diffusive advection scheme (2)

i) Gradient predictor step

$$\begin{aligned}(\nabla y)_{ij} &\approx \frac{1}{|K_{ij}|} \int_{K_{ij}} \nabla y(x, y) dx dy \\ &= \frac{1}{|K_{ij}|} \int_{\partial K_{ij}} y \boldsymbol{\nu} d\sigma.\end{aligned}$$

Simpson formula :

$$\int_{A_{i+1/2,j}} y dy \approx \frac{h}{6} y_{i+1/2,j+1} + \frac{2h}{3} y_{i+1/2,j} + \frac{h}{6} y_{i+1/2,j-1}$$

where

$$y_{i+1/2,j} = \frac{y_{ij} + y_{i+1,j}}{2}.$$

$\Rightarrow$  We get the 8-point scheme

$$(\nabla^h y)_{i,j} \approx \frac{1}{h} \left( \begin{array}{l} \frac{1}{12}(y_{i+1,j+1} - y_{i-1,j+1}) + \frac{1}{3}(y_{i+1,j} - y_{i-1,j}) + \frac{1}{12}(y_{i+1,j-1} - y_{i-1,j-1}) \\ \frac{1}{12}(y_{i+1,j+1} - y_{i+1,j-1}) + \frac{1}{3}(y_{i,j+1} - y_{i,j-1}) + \frac{1}{12}(y_{i-1,j+1} - y_{i-1,j-1}) \end{array} \right)$$

# Low-diffusive advection scheme (3)

ii) Gradient “limitation” **correction step**: for each cell  $K_{i,j}$ , consider

$$\mathcal{J}^h y(\mathbf{x}) = y_{i,j} + \phi_{i,j} (\nabla^h y)_{i,j} (\mathbf{x} - \mathbf{x}_{i,j}), \quad \phi_{i,j} \geq 0.$$

Corner values :

$$\hat{y}_{i+1/2,j+1/2} = y_{i,j} + (\nabla^h y)_{i,j} (\mathbf{x}_{i+1/2,j+1/2} - \mathbf{x}_{i,j})$$

Local extrema limitation at  $\mathbf{x}_{i+1/2,j+1/2}$  :

$$\bar{y}_{i+1/2,j+1/2} = \max(y_{i,j}, y_{i+1,j}, y_{i,j+1}, y_{i+1,j+1}),$$

$$\underline{y}_{i+1/2,j+1/2} = \min(y_{i,j}, y_{i+1,j}, y_{i,j+1}, y_{i+1,j+1}).$$

We expect that

$$\underline{y}_{i+1/2,j+1/2} \leq \mathcal{J}^h y(\mathbf{x}_{i+1/2,j+1/2}) \leq \bar{y}_{i+1/2,j+1/2},$$

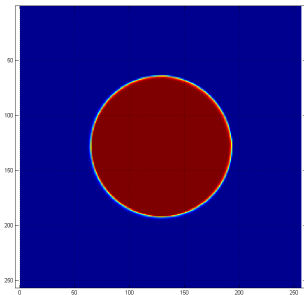
$\implies$  We find a  $\phi_{i+1/2,j+1/2}$ . Repeat for each corner. We get:

$$\phi_{i,j} = \min(\phi_{i+1/2,j+1/2}, \phi_{i+1/2,j-1/2}, \phi_{i-1/2,j+1/2}, \phi_{i-1/2,j-1/2}).$$

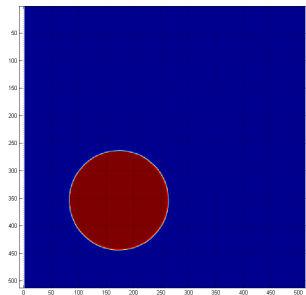
## Remark. Should $\phi$ be less than 1 ?

- ▶ Actually we do not ask for  $\phi_{i,j}$  to be less than 1 (as commonly used).
- ▶ Why ? Because the gradient prediction may underestimate the gradient intensity because of the 8-point discrete formula.
- ▶ The constraint  $\phi_{i,j} \leq 1$  creates too much numerical diffusion.
- ▶ Most important is the Local Extrema Diminishing (LED) process + compressive process in our case.

# Using MLP, artefacts and instabilities disappear ...



(a)

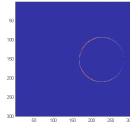
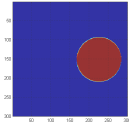


(b)

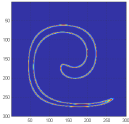
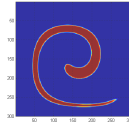
- (a): large-time evolution of an initial disk with uniform diagonal velocity.  
(b): evolution of an initial disk into a pure rotating field after few disk revolutions.

# Validating on the Kothe-Rider advection case, mesh $300^2$

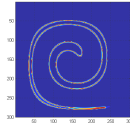
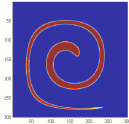
(t=0)



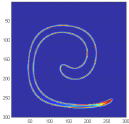
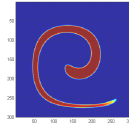
(t=3)



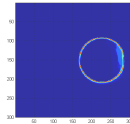
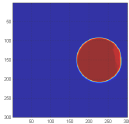
(t=6)



(t=9)

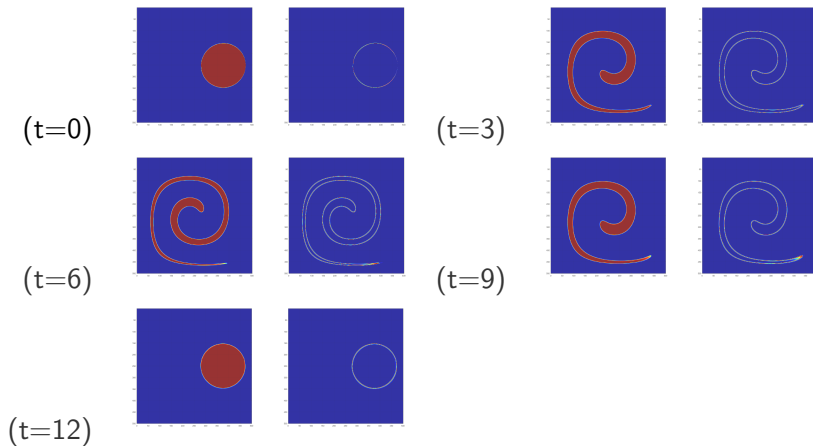


(t=12)





# Validating on the Kothe-Rider, mesh $500^2$



# Extending the approach for multimat hydrodynamics

- ▶ Assume isobaric isothermal closure mixture models
- ▶ MUSCL + limiters on variables  $p$ ,  $T$ ,  $\mathbf{u}$ ,  $y_k$
- ▶ Compute edge pressure  $p_A$  and temperature  $T_A$  at the edge  $A$  (high-order upwind)
- ▶ Compute species densities  $(\rho_k)_A = \rho_k(p_A, T_A)$
- ▶ Compute  $(y_k)_A$  with the MLP approach
- ▶ Compute  $\tau_A = \sum_k (y_k)_A (\tau_k)_A$
- ▶ Compute internal energies  $e_A = e_A(((y_k)_A)_k, T_A)$ . Compute  $E_A$ .
- ▶ Total and partial mass flux computations :

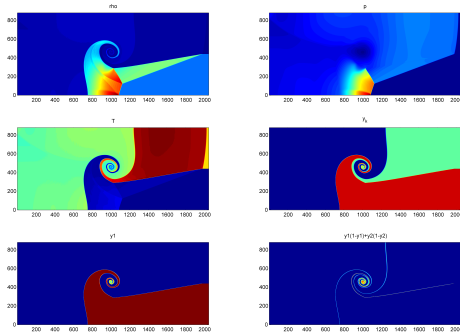
$$(\Phi_\rho)_A = \rho_A (\mathbf{v} \cdot \boldsymbol{\nu})_A, \quad (\Phi_{\rho y_k})_A = (y_k)_A (\Phi_\rho)_A, \quad \text{etc....}$$

# A remark on the choice of variables for gradient limitations

Why the choice of the variables to limit is so important ?

1. Try to correctly capture contact discontinuities
2. This means no spurious oscillations on both pressure and normal velocity through contact discontinuities

# Validating the advection approach for compressible hydrodynamics



**Figure:** Triple point (perfect gases) using a collocated Lagrange+remap solver + low diffusive interface capturing advection scheme. Results are comparable with those computed with ALE centered (collocated) schemes.

# Zoom-in of the vortex region

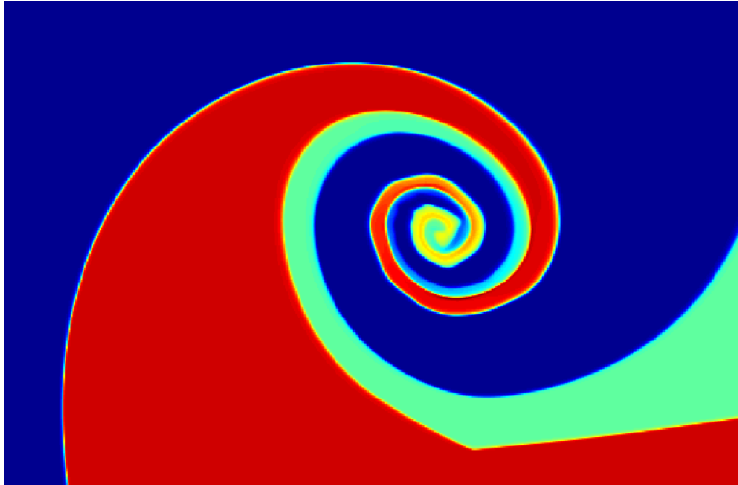


Figure: Triple point triple, mesh 2048x878

# Concluding remarks & perspectives

1. The approach shows accuracy and artefacts are mainly erased
2. First extension to hydrodynamics succeeded ...
3. ... but MLP is also necessary on variables like  $\rho$  or  $T$  in order not to create interface artefacts.

## Future works:

1. Extension to unstructured meshes
2. Find more compressive limiters
3. Experiments on stiffer EOS (e.g. air-water, cf for example [Champmartin-De Vuyst JCP 2013])
4. Data and memory management for many materials
5. Performance modeling (roofline, Execution Cache Model, [Gasc, De Vuyst, Motte, Peybernes, Poncet, ISC 2015, PARCO 2015]) and performance comparison with IR algorithms.

- ▶ LRC MESO joint lab between CMLA and CEA DAM DIF