Correcting the propagation of step singularities on uneven meshes with anti-diffusive schemes: application to 1D Euler equations

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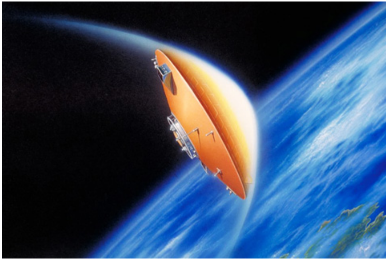

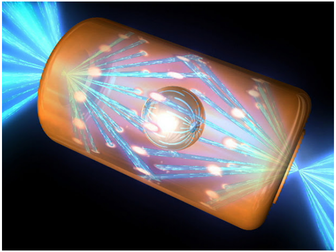

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Context and motivations

↪ Applying shock-capturing schemes to "real" (industrial) settings

- "low" order (order 2)
- "poor" mesh regularity
- "ugly" equations of state
- "strong" shocks and multiphysics.

↪ Work horse of CFD: Godunov approach [1]

REA algorithm (reconstruct, evolve, average)

- flow solution represented as piecewise constant states
- each pair of neighbouring states constitutes a Riemann problem (solution may be found exactly)
- Results from these Riemann problems can be averaged to update the numerical solution

[1] S.K. Godunov. Mat. Sb. (1959). Russian Math. Surv. (1962).

Context and motivations

- Sufficient to find approximate solutions[2] (ensuring they still contain important nonlinear physics)

  $\hookrightarrow$ Familly of approximate Riemann solvers (not listed here)

$\hookrightarrow$ While considered as very robust they can fail! (sometimes spectacularly!)

- J. Quirk[3] provided a list of possible failures (great Riemann solver debate):
  - expansion shocks
  - negative internal energies
  - slowly moving shocks
  - carbuncle phenomenon
  - kinked mach stems
  - odd-even decoubling
  - ...

[2] P.L Roe. Ann. Rev. Fluid Mech., (1986).
[3] J.J. Quirk. Nasa Report (1992).

Outline

1. Wrong shock propagation with uneven meshes: numerical illustrations
2. Qualitative analysis
3. Possible solutions: anti-diffusive schemes
4. Numerical results
5. Conclusion, perspectives and open questions

Problem setings

1D Euler equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0, \\ \partial_t(E) + \partial_x((E + p)u) = 0. \end{cases}$$

$\hookrightarrow$ Interested in the capture of sharp discontinuities.

$\hookrightarrow$ In the present work: propagation of shock waves on regular meshes and meshes with local refinement

Figure: Representation of a regular mesh (red) and a mesh with local refinement (green) ($\Delta x_{i+1}/\Delta x_i = r$ with $r = 0.9$ (left) and $r = 1/0.9$ (right)).

A numerical illustration (strong shock) 1/2

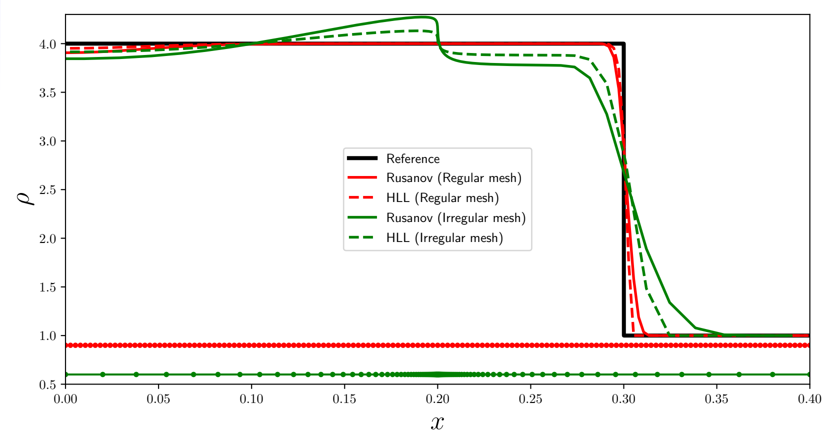
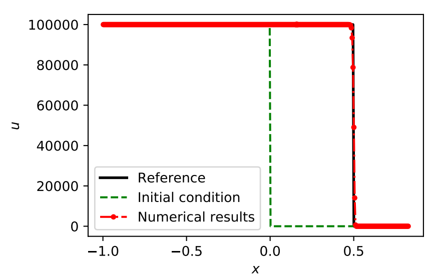


Figure: Shock profile obtained with a regular mesh (red) and a mesh with local refinement (green) ($\Delta x_{i+1}/\Delta x_i = r$ with $r = 0.9$ (left) and $r = 1/0.9$ (right)).

$\hookrightarrow$ For this given mesh: Failure of almost all (Godunov and others) schemes!

A numerical illustration 2/2



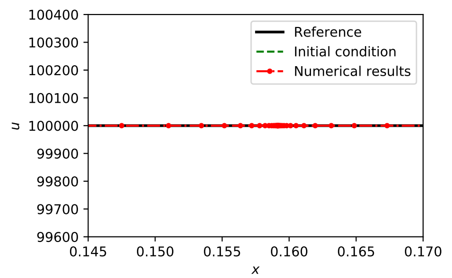


Figure: Profile obtained with the Burger equation and zoom on the mesh refinement (right).

$\hookrightarrow$ The numerical artefact does not appear in the case of scalar equations.

$\hookrightarrow$ Seems to be independent of the numerical scheme.

Second Noh artefact 1/2

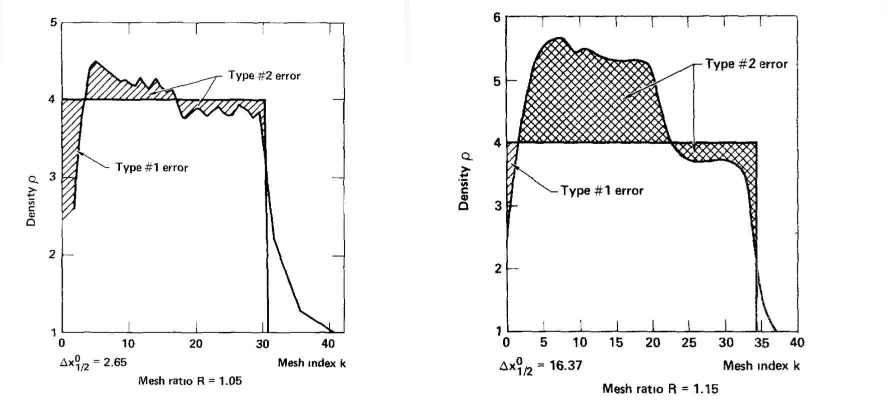


Figure: Density profiles reported by Noh[4] (strong shock).

[4] W.F. Noh. Journal of Computational Physics. 72, 78-120 (1978).

Second Noh artefact[5] 2/2

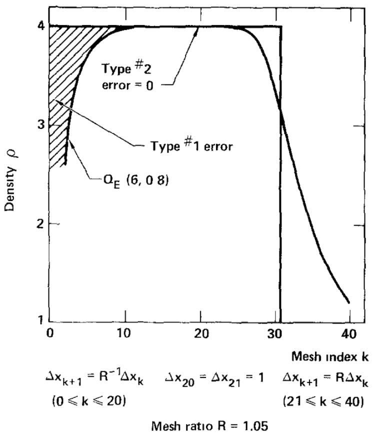


Figure: Density profiles reported by Noh (case of an adapted artificial viscosity for constant shock width).

[5] W.F. Noh. Journal of Computational Physics. 72, 78-120 (1978).

Qualitative analysis (still working on it)

Simplified HLL scheme (opposite and constant velocities in the underlying approximate Riemann solver)

$$\partial_t U_i + \frac{F(U_{i+1}) - F(U_{i-1})}{2\Delta x_i} - a\frac{U_{i+1} - 2U_i + U_{i-1}}{2\Delta x_i} = 0,$$

where

$$^tU = (\rho, \rho u, E), \qquad {}^tF(U) = (\rho u, \rho u^2 + p, (E+p)u).$$

Modified equations

$$\partial_t U_i + \left(\frac{r + 2 + 1/r}{4}\right)(\partial_x F(U))_i - \frac{a}{2}\left(r - \frac{1}{r}\right)(\partial_x U)_i - \frac{a\Delta x_i}{16}\left((1+r)^2 + (1+\frac{1}{r})^2\right)(\partial^2_{xx} U)_i = \mathcal{O}(\Delta x_i^2),$$

- Consistency problem with non uniform meshes
- But consistency recovered on uniform states (upstream and downstream)
- Noh's test connects uniform states but depends on dissipation length scale
- Validity of this consistency analysis on shocks? Other analysis required for shocks.

Isolated shock wave

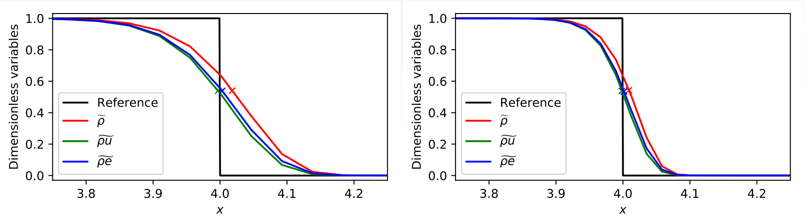
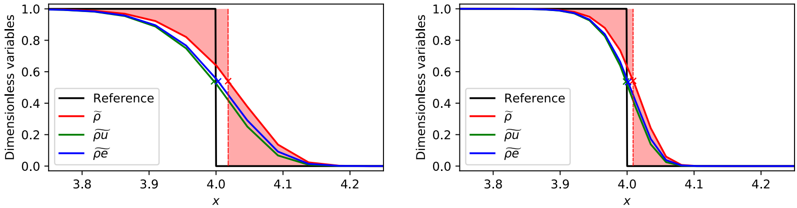


Figure: Dimensionless shock profiles with 200 cells (left) and 400 cells (right).



$\hookrightarrow$ The crosses represent the frame origin in which the red surface vanishes (computed numerically).

$\hookrightarrow$ As the mesh cells varie so the shock lengths and the distance between the shock profiles.

Rankine-Hugoniot conditions (?)

- Isolated shock traveling with a constant velocity.

Reference frame (Galilean) centered on the shock wave is considered

$\hookrightarrow$ System writes under the same form (Galilean invariance).

Discrete space integration between an abscissa before and after (upstream / downstream) the shock

$$\sum_{x_a}^{x_b}\left(\partial_t U + \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x_i}\right) = \frac{d}{dt}\left(\sum_{x_a}^{x_b} U\right) + [F(U)]_{x_a}^{x_b} = 0.$$

In the case of a mesh with a constant space step Δx: no numerical viscosity variation.

$\hookrightarrow$ no shock profile variation, $\qquad [F(U)]_{x_a}^{x_b} = 0.$

$\hookrightarrow$ discrete Rankine-Hugoniot conditions are recovered.

Progressive mesh: the shock length varies. The time derivative does not vanish. Discrete Rankine-Hugoniot conditions are not correctly enforced.

What can we do?

- The numerical viscosity of standard (Godunov, Staggered, ...) schemes, (which usually give strong stability properties) leads, in the case of uneven meshes, to the second Noh artefact.

A first idea:

- Modify the numerical viscosity to enforce the correct Rankine-Hugoniot conditions

$$\frac{d}{dt}\left(\sum_{x_a}^{x_b} U\right) = 0, \qquad [F(U)]_{x_a}^{x_b} = 0.$$

$\hookrightarrow$ Seems challenging (non-local conditions)!

Present investigation strategies

- Anti-diffusive numerical schemes when shock waves are involved.

Possible solutions: anti-diffusive schemes

↪ Anti-diffusive approaches have been investigated for the capture of sharp discontinuities.

Investigated numerical methods

- Random Choice Method[6] (RCM)
- Hybrid Godunov-Random Choice method[7] (RCM-Godunov)
- ALE conservative anti-diffusive method (ACA)
- Interface reconstruction strategy[8] (collaboration with C. Chalons) (not presented here)

[6] A.J. Chorin. J. Comput. Phys. (1976) / P. Colella. J. Sci. Stat. Comput. (1985).
[7] C. Chalons, P. Goatin. Interf. Free Bound. (2008) / C. Fiorini. PhD thesis (2018)
[8] N. Aguillon, C. Chalons. M2AN (2016). / B. Després, F. Lagoutière, J. Sci. Comput. (2001).

Approximate Riemann solver

Riemann problem for hyperbolic system of conservation laws

$$\partial_t U + \partial_x F(U) = 0,$$

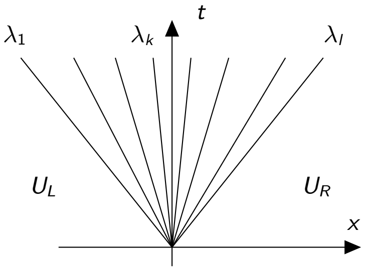
with $U \in \mathbb{R}^m, x \in \mathbb{R}, t > 0$. Initial conditions

$$U(t=0,x) = \begin{cases} U_L & \textit{if} \quad x < 0, \\ U_R & \textit{if} \quad x > 0. \end{cases}$$

$\hookrightarrow$ Self-similarity of the exact Riemann solution $U(x/t, U_L, U_R)$

Approximate Riemann solver

$$U^{\mathcal{R}}(x/t, U_L, U_R) = \begin{cases} U_1^\star = U_L & \text{if} \quad x/t < \lambda_1, \\ \vdots & \\ U_k^\star & \text{if} \quad \lambda_{k-1} < x/t < \lambda_k \\ \vdots & \\ U_{l+1}^\star = U_R & \text{if} \quad x/t > \lambda_l. \end{cases}$$



Harten, Lax and van Leer formalism

Godunov-type scheme

$$U_i^{n+1} = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \mathcal{U}(t^{n+1}, x) dx,$$

$$\mathcal{U}(t^{n+1}, x) = U^{\mathcal{R}} \left(\frac{x - x_{i+1/2}}{t^n + \Delta t}, U_i^n, U_{i+1}^n \right) \quad \text{if } \ x \in [x_i, x_{i+1}].$$

Consistency with the integral form of the hyperbolic system[9]

$$F(U_R) - F(U_L) = \sum_{k=1}^{l} \lambda_k (U_{k+1}^\star - U_k^\star).$$

Entropy integral relation

$$G(U_R) - G(U_L) \leq \sum_{k=1}^{l} \lambda_k \left(\eta(U_{k+1}^\star) - \eta(U_k^\star) \right),$$

where $(\eta(U), G(U))$ is an entropy-entropy flux pair ($\eta(U)$ a convex function).

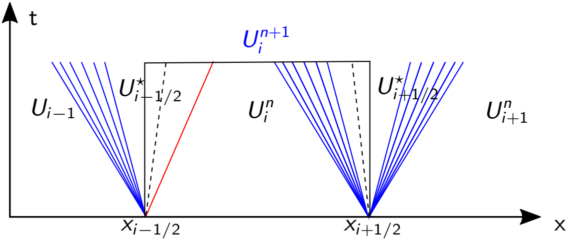
[9] A. Harten, P. Lax, B. Van Leer. Siam Review (1983).

Anti-diffusive strategy: Random Choice formalism[10]

- *Step a.* Resolution of the Riemann problem at each interface (step similar to the Godunov method).

  $\hookrightarrow$ Must be exact in the case of an isolated shock wave.

- *Step b (Pick up step).* Numerical solution picked at random (or quasi-random) (while Godunov method considers an average) in the local solutions of Riemann problems.



[10] A.J. Chorin. J. Comput. Phys. (1976) / P. Colella. J. Sci. Stat. Comput. (1985).

Step a. Euler equations with an HLL scheme

$\hookrightarrow$ Standard HLL approximate Riemann solver with Roe velocities[11].

HLL intermediate state[12]

$$U^\star = \frac{\lambda_3 U^R - \lambda_1 U^L - (F(U^R) - F(U^L))}{\lambda_3 - \lambda_1}.$$

$\hookrightarrow$ Choice of λ_1 and λ_3 critical when capturing isolated shock waves.

Roe averages

$$\lambda_1 = \tilde{u} - \tilde{c}, \qquad \lambda_3 = \tilde{u} + \tilde{c},$$

$$\tilde{u} = \frac{\sqrt{\rho^L} u^L + \sqrt{\rho^R} u^R}{\sqrt{\rho^L} + \sqrt{\rho^R}}, \qquad \tilde{H} = \frac{\sqrt{\rho^L} H^L + \sqrt{\rho^R} H^R}{\sqrt{\rho^L} + \sqrt{\rho^R}}, \qquad \tilde{c} = \sqrt{(\gamma - 1)(\tilde{H} - \tilde{u}^2/2)}.$$

$\hookrightarrow$ Exact capture of an isolated shock wave.

[11] P.L. Roe. J. Comput. Phys. (1981).

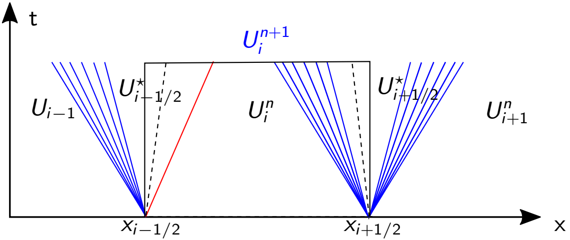
[12] A. Harten, P. Lax, B. Van Leer. Siam Review (1983).

Step b. Pick up step

Updated numerical solution picked at random (or quasi-random)

$$U_i^{n+1} = \begin{cases} U^\star_{i-1/2}, & \text{if } \ 0 \le \theta^n \le \lambda_{3,i-1/2}\Delta t/\Delta x, \\ U^n_{i+1/2}, & \text{if } \ \lambda_{3,i-1/2}\Delta t/\Delta x \le \theta^n \le 1 + \lambda_{1,i+1/2}\Delta t/\Delta x \\ U^\star_{i+1/2}, & \text{if } \ 1 + \lambda_{1,i+1/2}\Delta t/\Delta x \le \theta^n \le 1, \end{cases}$$

where θ^n is chosen at random (or quasi-random) in the interval $[0, 1]$.



$\hookrightarrow$ The quality of the numerical method strongly depends on the random numbers[13] generator.

[13] E.F. Toro. Spinger (1997).

Pick up step

- Parameters θ^n chosen as the Van der Corput Pseudo-Random sequence[14]

$$\theta^n = \sum_{k=0}^{m} i_k 2^{-(k+1)}, \qquad n = \sum_{k=0}^{m} i_k 2^k,$$

where i_k found by binary expansion of the integer n.

- During the sampling procedure (step b): no numerical diffusion involved (not the case with the average procedure in the Godunov method).

$\hookrightarrow$ Strong stability issues with this scheme (spurious oscillations).

$\hookrightarrow$ Objective: more robust than RCM while preserving the anti-diffusive character.

[14] P. Colella. PhD thesis (1978) / J. Sci. Stat. Comput. (1982).

Hybrid Random-Choice-Godunov method[15]

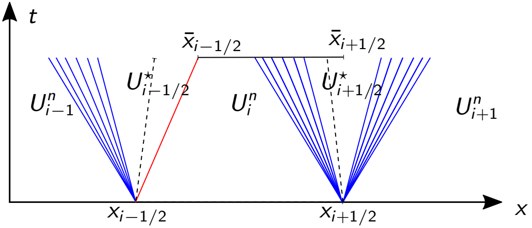
- Step a (unchanged). Approximate Riemann solver exact for isolated shock waves (HLL approximate solver with Roe velocities).

- Step b. Average step on a new mesh (temporary virtual mesh)

$\hookrightarrow$ The virtual mesh is defined to follow the shock wave (not uniform)

$$\bar{x}^n_{i-1/2} = x_{i-1/2} + \sigma^n_{i-1/2} \Delta t^n.$$

$\hookrightarrow$ averaging procedure not performed on the physical mesh (as with the standard Godunov methods) but on the virtual mesh.



[15] C. Chalons, P. Goatin. Interf. Free Bound. (2008) / C. Fiorini. PhD thesis (2018)

Average procedure

Quantities on the virtual mesh

$$\bar{U}_i^{n+1} = \frac{\Delta x}{\Delta x_i} U_i^n + \frac{\Delta t}{\Delta x_i} \left((F_{i+1/2} - F_{i-1/2}) - \sigma_{i-1/2}^n U_{i-1/2}^\star + \sigma_{i+1/2}^n U_{i+1/2}^\star \right).$$

- *Step c*. Pseudo-random sampling (projection on the fixed mesh)

$$U_i^{n+1} = \begin{cases} \bar{U}_{i-1}^{n+1} & \text{if} \quad \theta^n \in \left[0, \dfrac{\Delta t}{\Delta x} \max(\sigma_{i-1/2}, 0)\right], \\ \bar{U}_i^{n+1} & \text{if} \quad \theta^n \in \left[\dfrac{\Delta t}{\Delta x} \max(\sigma_{i-1/2}, 0), 1 + \dfrac{\Delta t}{\Delta x} \min(\sigma_{i+1/2}, 0)\right], \\ \bar{U}_{i+1}^{n+1} & \text{if} \quad \theta^n \in \left[1 + \dfrac{\Delta t}{\Delta x} \min(\sigma_{i+1/2}, 0), 1\right]. \end{cases}$$

↪ No average through the shock (shocks localised at the interface of the virtual mesh).

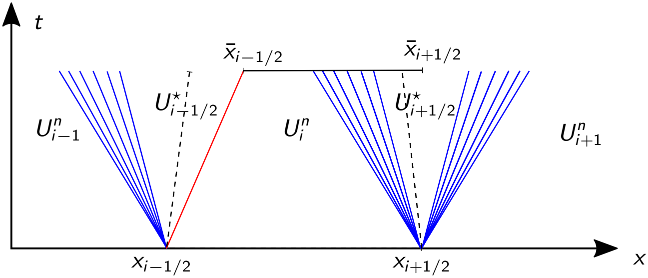
↪ No numerical diffusion added in the process.

↪ More robust than RCM but still stability issues when dealing with strong shock waves (Noh test case).

Anti-diffusive and conservative ALE-Godunov (ACA)

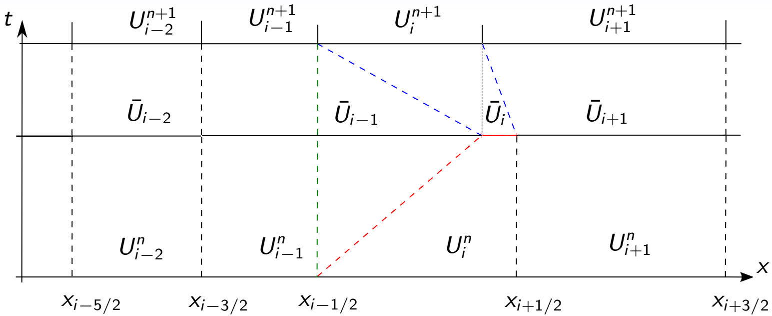
$\hookrightarrow$ RCM and RCM-Godunov not perfectly conservative (conservation in a statistical sense) and stability issues.

- Step a (unchanged). Approximate Riemann solver exact for isolated shock waves (HLL with Roe velocities).
- Step b. (unchanged) Average step on a new mesh defined to follow the shock wave.
- Step c. No pseudo-random sampling (no projection)! Keep working with the moving mesh (not virtual anymore)!



Working with a moving mesh

↪ When a cell becomes too small, a remesh procedure is performed keeping the shock positions (anti-diffusive)



↪ Conservative projection: no average through the shock waves!

↪ Anti-diffusive, conservative and robust!

Two weak shock waves: regular mesh

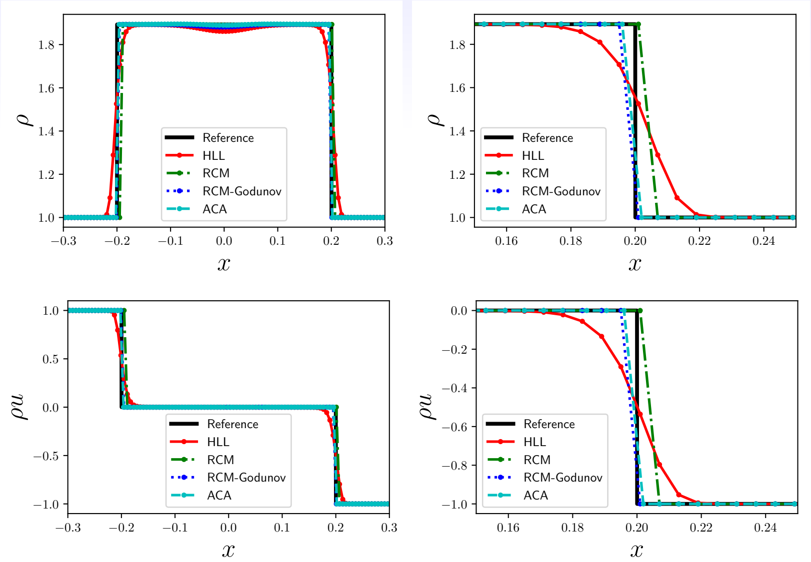


Figure: Density (top), momentum (bottom) with 100 cells. Zoom (right).

Two weak shock waves: regular mesh

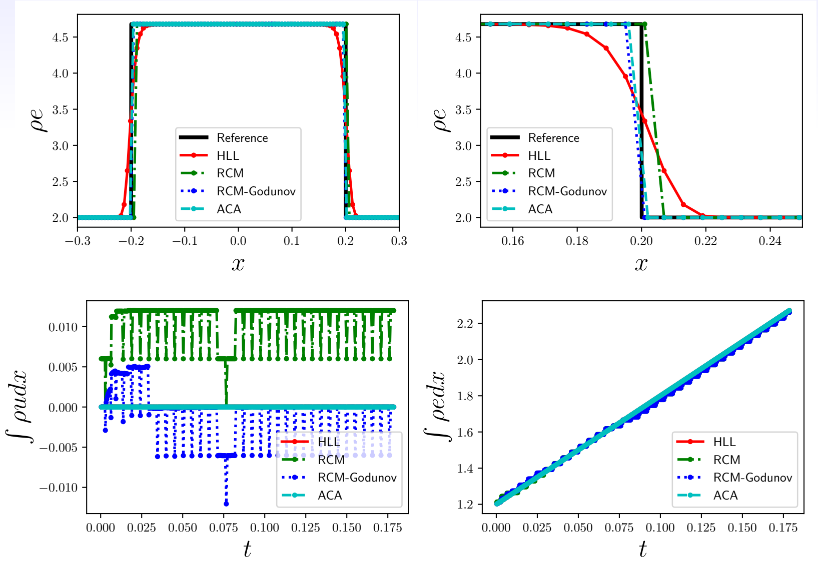


Figure: Energy profiles (top). Momentum and energy conservations (bottom).

Two weak shock waves: Irregular mesh $r = 0.9$

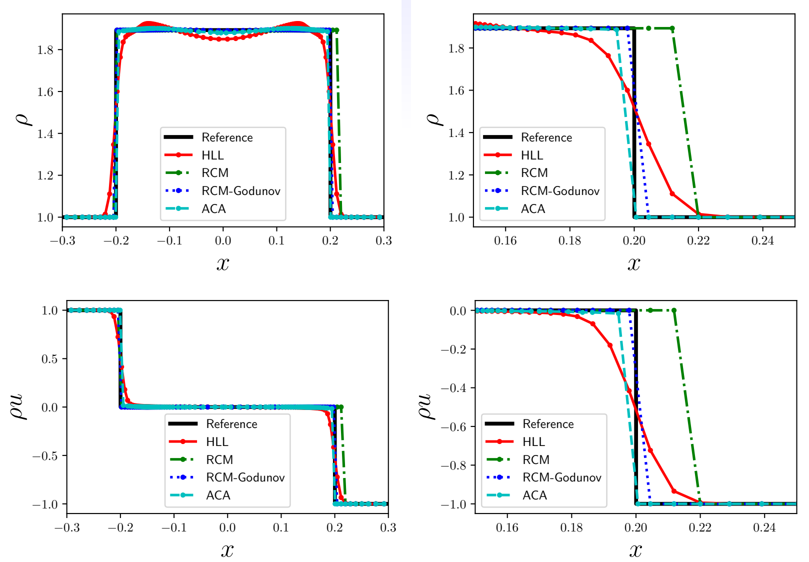


Figure: Density (top), momentum (bottom) with 100 cells. Zoom (right).

Noh problem (strong shock): regular mesh

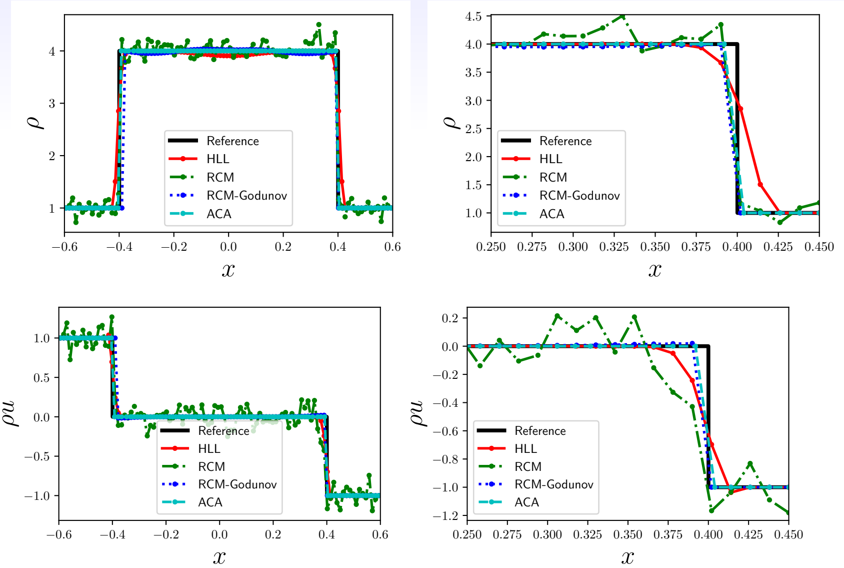


Figure: Density (top) and momentum (bottom) with 100 cells. Zoom (right).

Noh problem (strong shock): Irregular mesh $r = 0.9$

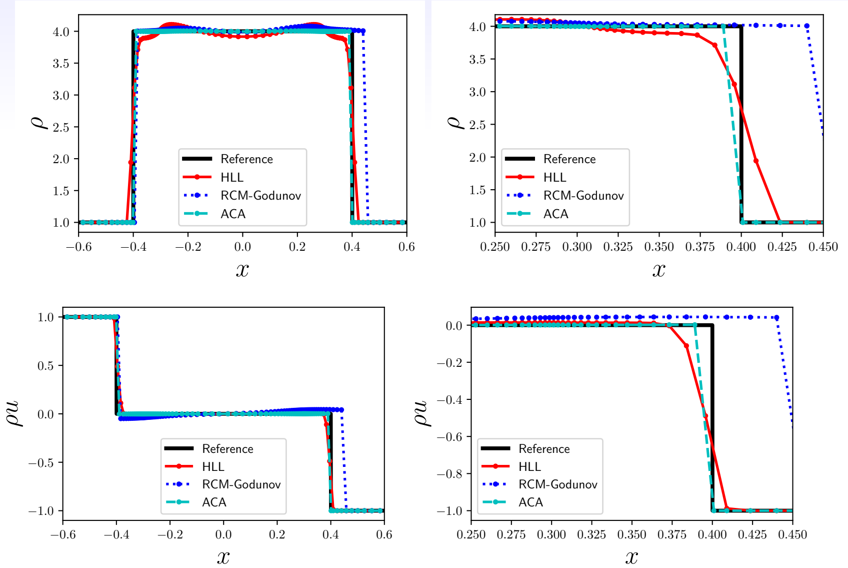


Figure: Density (top) and momentum (bottom) with 100 cells. Zoom (right).

Noh problem: Irregular mesh

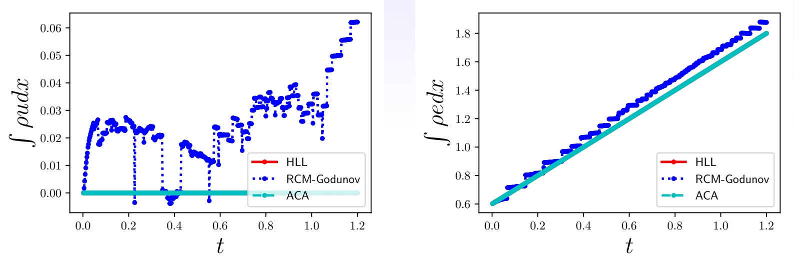


Figure: Momentum and energy conservations.

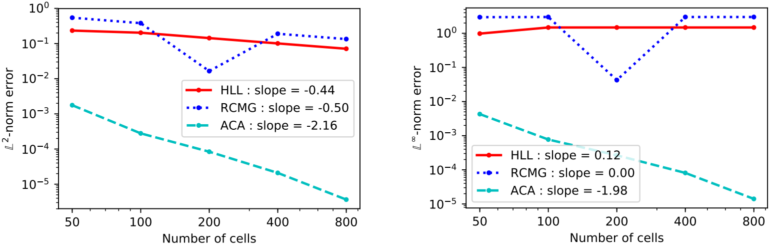


Figure: L^2 and L^∞ convergence (regular mesh).

Sod problem (regular mesh)

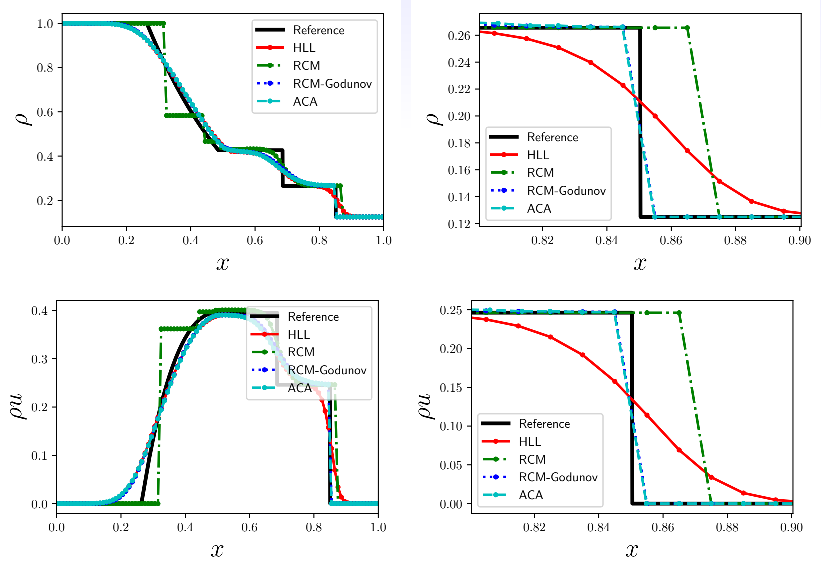


Figure: Density (top) and momentum (bottom) with 100 cells. Zoom (right).

Sedov problem (strong shock) (regular mesh)

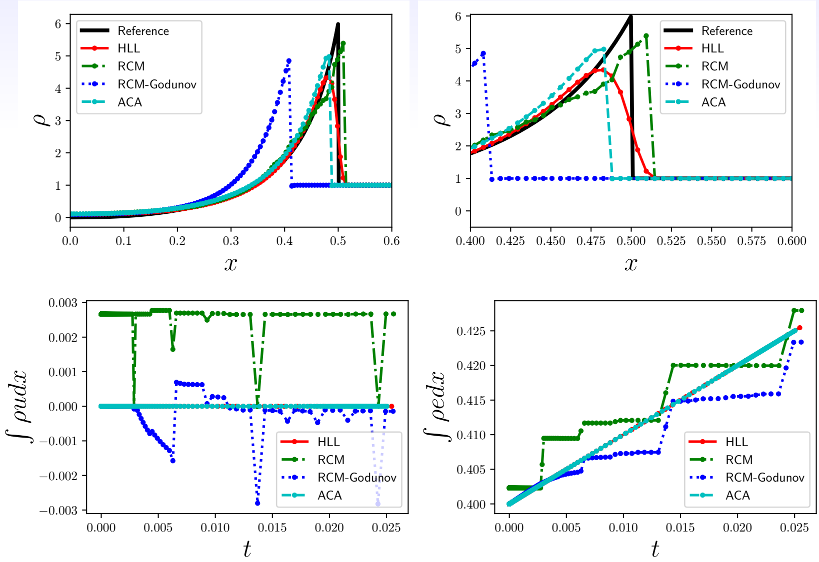


Figure: Energy profiles (top). Momentum and energy conservations (bottom).

Conclusion, perspectives and open questions

- Failure of standard (Godunov) schemes to capture shock waves on meshes with localised refinements.
- Anti-diffusive strategies considered:
  - Random Choice Method (not stable!)
  - Hybrid Random Choice Godunov (good but stability issues for Noh problem)
  - Anti-diffusive and Conservative ALE-Godunov (ACA)
- Perspectives:
  - Keep understanding the second Noh artefact
  - 2D extensions (challenging!)
  - General equation of states
  - Lagrangian formalism
  - Interface reconstruction strategy (collaboration with C. Chalons)[16]
  - ...

[16] B. Després, E. Labourasse, F. Lagoutière. Jacques-Louis Lions Report (2007).

Thank you

ACA scheme for an isolated shock wave

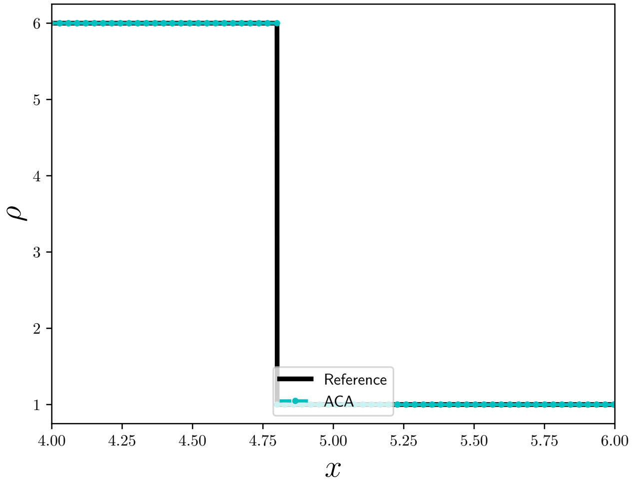


Figure: Density profile

FV representation

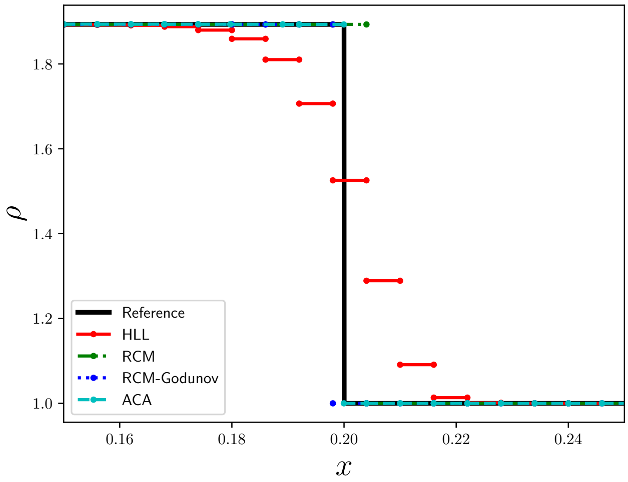


Figure: Density profile for the double shock problem.

Exact capture of isolated shock

Property

The HLL approximate solver with Roe velocities is exact for an isolated shock wave.

Rankine-Hugoniot conditions

$$\sigma(U^L - U^R) = F(U^L) - F(U_R),$$

where σ denotes the shock velocity

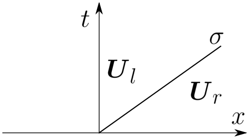


Figure: (x, t)-diagram representing an isolated shock wave

HLL approximate Riemann solver with Roe velocities (case of a 3-shock)

$$\lambda_1 = \tilde{u} - \tilde{c}, \qquad \lambda_3 = \tilde{u} + \tilde{c} = \sigma.$$

Exact capture of isolated shock

The HLL intermediate state rewrites

$$U^{\star} = \frac{(\tilde{u}+\tilde{c})U^R - (\tilde{u}-\tilde{c})U^L - \sigma(U^R - U^L)}{2\tilde{c}},$$
$$= \frac{(\tilde{u}+\tilde{c}-\sigma)U^R + (\sigma-\tilde{u}+\tilde{c})U^L}{2\tilde{c}}.$$

Using $\lambda_3 = \tilde{u}+\tilde{c} = \sigma$

$$U^{\star} = U^L.$$

$\hookrightarrow$ The HLL approximate solver with Roe velocities is then exact for isolated shock wave.

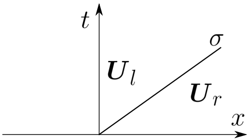
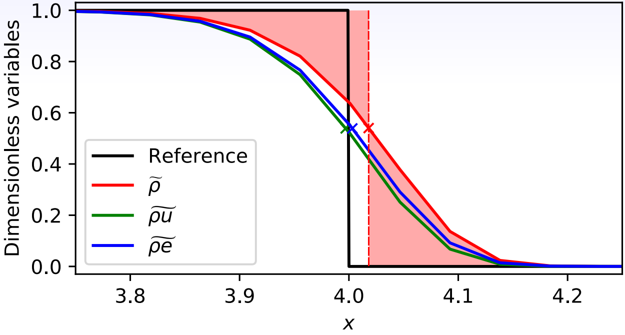


Figure: (x, t)-diagram representing an isolated shock wave

Heaviside



Looking for x_0 (cross) such that

$$\int_{\mathbb{R}} (u^L - u(x))H(x_0 - x)dx = \int_{\mathbb{R}} (u(x) - u^R)H(x - x_0)dx$$

where $H(x_0 - x) = 1 - H(x - x_0)$.