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DE LA RECHERCHE À L'INDUSTRIE

# A CLASS OF CONSERVATIVE $L^2$ -STABLE SCHEMES FOR MULTIPHASE FLOWS ON STAGGERED GRIDS

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Context

Low Mach vs checkerboard modes

Numerical diffusion of classical schemes

A new class of staggered schemes

Nnumerical results

Conclusion and perspectives

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- ▶ Multicomponent flow : liquid, vapor, solid obstacles
- ▶ Stiff source terms (heat source, boiling, pressure losses)
- ▶ Flow in a wide range of regimes ( $Ma$ ,  $Re$ ,  $Pe$ )
- ▶ Specifics of two phase flows
  - non conservative models (e.g. two-fluid models)
  - not always admit entropies (e.g. models with drift)
  - characteristic fields neither GNL neither LD (e.g. models with drift)
  - characteristic speeds are not ordered
  - sonic points are very common (e.g. counter-current flows)

⇒ The mathematical structure and the numerical behaviour are very DIFFERENT between single and multiphase flows

⇒ We need generic and flexible solvers that can adapt to the flow regime

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$$\left\{ \begin{array}{l} \frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \mu \Delta \mathbf{u} \\ \frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho H \mathbf{u}) = \lambda \Delta T \end{array} \right. \quad (1)$$

- ▶  $\rho$ ,  $\mathbf{u}$ ,  $p$  may have very different magnitudes
- ▶ Use reference length  $L_{ref}$ , velocity  $u_{ref}$ , pressure  $p_{ref}$  to scale the equations
- ▶ Dimensionless numbers characterise the flow regimes
- ▶ Recover the low Mach asymptotic



New variables  $\rho := \frac{\rho}{\rho_{ref}}$ ,  $p := \frac{p}{p_{ref}}$ ,  $\mathbf{u} := \frac{\mathbf{u}}{u_{ref}}$

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \frac{1}{M^2} \nabla p = \frac{1}{\text{Re}} \Delta \mathbf{u} \\ \frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho H \mathbf{u}) = \frac{1}{\text{Pe}} \Delta T \end{array} \right. \quad (2)$$

$$M = \frac{u_{ref}}{c_{ref}}, \quad \text{Re} = \frac{L_{ref} u_{ref}}{\frac{\mu}{\rho_{ref}}}, \quad \text{Pe} = \frac{L_{ref} u_{ref}}{\frac{\lambda}{\rho_{ref} c_p}}$$

- ▶ In a nuclear reactor,  $\text{Re} \gg 1$ ,  $\text{Pe} \gg 1$ ,  $M \ll 1$  ( $\|\mathbf{u}\| \ll c$ )
- ▶ We need more precision on  $p$  than on other variables

For well prepared initial data ( $M \ll 1$  initially)

$$\begin{cases} \rho(\vec{x}, t = 0) = \rho_* + O(M)(\vec{x}) \\ p(\vec{x}, t = 0) = p_* + O(M^2)(\vec{x}) \\ \mathbf{u}(\vec{x}, t = 0) = \mathbf{u}_*(\vec{x}) + O(M)(\vec{x}) \end{cases}$$

the solution  $(\rho, p, \mathbf{u})(t, \vec{x})$  to the **compressible Euler equations** takes the form

$$\begin{cases} \rho(\vec{x}, t) = \rho_* + O(M)(\vec{x}, t) \\ p(\vec{x}, t) = p_* + O(M^2)(\vec{x}, t) \\ \mathbf{u}(\vec{x}, t) = \tilde{\mathbf{u}}(\vec{x}, t) + O(M)(\vec{x}, t) \end{cases}$$

where  $\tilde{\mathbf{u}}$  is the solution of the **incompressible Euler equations** with initial data  $\tilde{\mathbf{u}}(\vec{x}, 0) = \mathbf{u}_*(\vec{x})$

- Numerical schemes should preserve this asymptotics

- ▶ Upwind based FV collocated methods (Godunov, Roe, ...)
  - do not satisfy the low Mach asymptotics ✗
- ▶ Centered FV collocated methods
  - satisfy the low Mach asymptotics... ✓

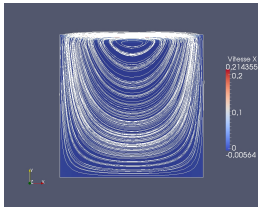


Figure: Implicit **upwind** scheme (Lid driven cavity)

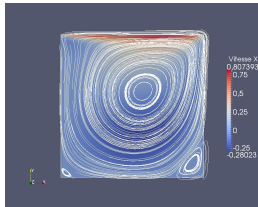


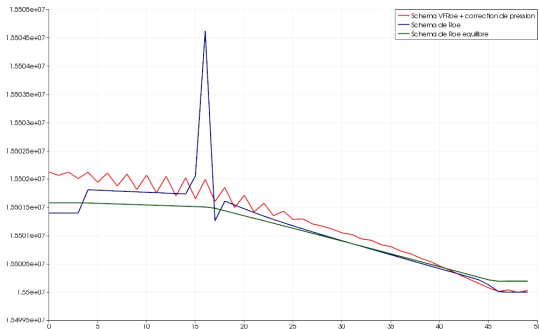
Figure: Implicit **centered** scheme (Lid driven cavity)

⇒ It is tempting to reduce the numerical diffusion ...

- ▶ but generate spurious **checkerboard** oscillations ✗

- ▶ 4 equations two phase model
- ▶ 1D heated channel
- ▶ Stiff source terms : heat power, phase change
- ▶ Compare upwind and centered schemes

$$\left\{ \begin{array}{l} \frac{\partial(\phi\rho)}{\partial t} + \nabla \cdot (\phi\rho\vec{V}) = 0, \\ \frac{\partial(\phi\rho C)}{\partial t} + \nabla \cdot (\phi\rho C\vec{V} + \phi\rho C(1-C)\vec{V}_r) = \nabla \cdot (\phi K_{cv} \nabla C) + \phi\Gamma_v, \\ \frac{\partial(\phi\rho\vec{V})}{\partial t} + \nabla \cdot (\phi\rho\vec{V} \otimes \vec{V} + \phi\rho C(1-C)\vec{V}_r \otimes \vec{V}_r + \phi P\mathbb{I}_d) = P\nabla\phi + \nabla \cdot (\phi\vec{\sigma}) + \phi\vec{\tau} + \phi\rho\vec{g} \\ \frac{\partial(\phi\rho E)}{\partial t} + \nabla \cdot (\phi\rho H\vec{V} + \phi\rho C(1-C)(H_v - H_l)\vec{V}_r) = \phi\rho\vec{g} \cdot \vec{V} + \phi Q + \nabla \cdot (\phi\vec{q}) \end{array} \right. \quad (3)$$



- ▶ The **exact stationary pressure** (green) is **decreasing**
- ▶ Upwind schemes (blue) → Spurious oscillations ✗
- ▶ Centered schemes (red) → Spurious oscillations ✗
- ▶ **Staggered schemes** capture the correct dynamics ✓

Empirical numerical observations :

- ▶ **Colocated FV** → lack robustness
  - “Corrected” Riemann solvers based on the theory of hyperbolic systems of conservation law
  - Predictor-corrector solvers inspired by the incompressible regime (projection methods)
- ▶ **Staggered FV** → more robust wrt source terms but
  - Often based on non conservative formulations
  - Extension to general meshes is delicate

Why such different behaviours ?

- ▶ nothing to do with nonlinearities
- ▶ linked to the coupling between the variables

⇒ need a theoretical framework for the design and analysis of staggered schemes

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Consider a 1D first order non linear PDE

$$\partial_t U + A(U)\partial_x U = 0. \quad (4)$$

and a first order semi-discretisation *disc*

$$\partial_t U_i + A_{disc}^+ \frac{U_i - U_{i-1}}{\Delta x} + A_{disc}^- \frac{U_{i+1} - U_i}{\Delta x} = 0. \quad (5)$$

The equivalent equation of the scheme is  $\Delta x \rightarrow 0$  :

$$\partial_t U + A\partial_x U = \mathcal{D}(U, \Delta x) + o(\Delta x) \quad (6)$$

$$= -\Delta x D_{disc} \partial_{xx} U + o(\Delta x). \quad (7)$$

- ▶  $A = A_{disc}^+ + A_{disc}^-$  (consistency of (5) with (4))
- ▶  $D = A_{disc}^+ - A_{disc}^-$  represents the numerical diffusion

→  $D$  is connected to stability and precision of the scheme.

→ Compute  $D$  for the linear wave equation



Neglect inertia  $\frac{q^2}{\rho} = \rho u^2$  in the Euler equations :

$$\text{(Wave system)} \quad \begin{cases} \partial_t \rho + \partial_x q = 0 \\ \partial_t q + c^2 \partial_x \rho = 0 \end{cases}$$

→ linear hyperbolic system with eigenvalues  $\pm c$ .

Centered discretisation :

$$\begin{cases} \partial_t \rho_i + \frac{q_{i+1} - q_{i-1}}{2\Delta x} = 0 \\ \partial_t q_i + c^2 \frac{\rho_{i+1} - \rho_{i-1}}{2\Delta x} = 0 \end{cases}$$

- ▶  $D_{centre} = 0$  (scheme is order 2)
- ▶  $D_{centre}$  is diagonalisable
- ▶ odd/even decoupling ( $Ker(D)$  is too rich)

## Upwind discretisation

$$\begin{cases} \partial_t \rho_i + \frac{q_{i+1} - q_{i-1}}{2\Delta x} = c \frac{\rho_{i+1} - 2\rho_i + \rho_{i-1}}{\Delta x} \\ \partial_t q_i + c^2 \frac{\rho_{i+1} - \rho_{i-1}}{2\Delta x} = c \frac{q_{i+1} - 2q_i + q_{i-1}}{\Delta x} \end{cases}$$

$$D_{upwind} = |A_{wave}| = \begin{pmatrix} c & 0 \\ 0 & c \end{pmatrix}, \quad A_{wave} = \begin{pmatrix} 0 & 1 \\ c^2 & 0 \end{pmatrix}.$$

- ▶ same diffusion rate on each equation
- ▶  $D_{upwind}$  is diagonalisable on  $\mathbb{R}$

## Staggered discrétisation “simple”

$$\left\{ \begin{array}{l} \partial_t \rho_i + \frac{q_{i+1/2} - q_{i-1/2}}{\Delta x} = 0 \\ \partial_t q_{i+1/2} + c^2 \frac{\rho_{i+1} - \rho_i}{\Delta x} = 0 \end{array} \right., \quad U_i = \begin{pmatrix} \rho_i \\ q_{i+1/2} \end{pmatrix}.$$

$$D_{stag} = \begin{pmatrix} 0 & 1 \\ -c^2 & 0 \end{pmatrix}, \quad A_{wave} = \begin{pmatrix} 0 & 1 \\ c^2 & 0 \end{pmatrix}.$$

- ▶ most of the numerical diffusion is on the second equation.
- ▶  $D_{stag}$  is not diagonalisable on  $\mathbb{R}$

Most staggered are however based on non conservative forms.

Staggered discrétisation from the literature (more complex)

$$\begin{cases} \partial_t \rho_i + \frac{1}{\Delta x} (\rho_{i+\frac{1}{2}}^{up} u_{i+\frac{1}{2}} - \rho_{i-\frac{1}{2}}^{up} u_{i-\frac{1}{2}}) = 0 \\ \partial_t \left( \bar{\rho}_{i+\frac{1}{2}} u_{i+\frac{1}{2}} \right) + c^2 \frac{1}{\Delta x} (\rho_{i+1} - \rho_i) = 0, \end{cases} \quad (8)$$

avec

$$\begin{cases} \rho_{i+\frac{1}{2}}^{up} = \frac{\rho_i + \rho_{i+1}}{2} + \mathit{sign}(u_{i+\frac{1}{2}}) \frac{\rho_i - \rho_{i+1}}{2}, \\ \bar{\rho}_{i+\frac{1}{2}} = \frac{1}{2} (\rho_i + \rho_{i+1}). \end{cases} \quad (9)$$

$$\mathcal{D}(U, \Delta x) = \Delta x \begin{pmatrix} \mathit{sign}(u) & 0 \\ 0 & 1 \end{pmatrix} \partial_x \left[ \begin{pmatrix} u & 0 \\ c^2 & 0 \end{pmatrix} \partial_x \begin{pmatrix} \rho \\ q \end{pmatrix} \right]. \quad (10)$$

- ▶ If  $\mathit{sign}(u)$  the scheme is linearisable and stable
- ▶ If  $\mathit{sign}(u)$  the scheme is not linéarisable

- For a given matrix  $D$ , there exists a conservative scheme with diffusion operator  $D$

Justification : Consider a **conservative system**

$$\partial_t U + \partial_x F(U) = 0 \quad \text{forme conservative}$$

a **conservative scheme**

$$\partial_t U_i + \frac{F_{i,i+1} - F_{i-1,i}}{\Delta x} = 0 \quad (11)$$

with **numerical fluxes**  $F_{ij}$

$$F_{i,j} = \frac{F(U_i) + F(U_j)}{2} + D \frac{U_i - U_j}{2}, \quad (12)$$

has numerical diffusion  $D$ .

Indeed when  $\Delta x \rightarrow 0$ , (11) yields

$$\partial_t U + \partial_x F(U) = \Delta x D \partial_{xx} U + \mathcal{O}((\Delta x)^2).$$

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We need to symmetrise the system in order to bound the solution.

After linearisation, we have the linear hyperbolic system

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

$A$  must be diagonalisable  $\Rightarrow$  symetrisation is possible

$$S = P^{-1}AP, \quad {}^tS = S$$

- ▶ change of variables  $\bar{U} = PU$  :

$$\partial_t \bar{U} + S \partial_x \bar{U} = 0$$

- ▶ Using “symetrisation”, **the energie is constant in time**

$$\partial_t \int_{\mathbb{R}} \|\bar{U}\|^2 dx = 0.$$

- ▶ **Hence the stability** at the continuous level:

Same steps as in the continuous case

- 1 Consider a general numerical diffusion operator  $D$
- 2 Compute the evolution of the norm in the symetrising basis

$$\partial_t \int_{\mathbb{R}} \|\bar{U}_h\|^2 dx = -h \int {}^t(\partial_x \bar{U}_h)(\bar{D} + {}^t\bar{D})(\partial_x \bar{U}_h) + o(h).$$

the dissipation rate is given by the spectrum of  $\bar{D} + {}^t\bar{D}$

- 3 We conclude that
  - the scheme is stable provided

$$\boxed{\bar{D} + {}^t\bar{D} \geq 0}$$

$$\Rightarrow \|\bar{U}_h(\cdot, t)\|_{L^2} \leq \|\bar{U}_{h0}\|_{L^2}. \quad (13)$$

- the scheme is precise provided  $\bar{D} + {}^t\bar{D}$  does not involve the sound speed



► **Upwind scheme :**

$$D_{upwind} = c\mathbb{I}_d, \quad \bar{D}_{upwind} = c\mathbb{I}_d, \quad \bar{D}_{upwind} + {}^t\bar{D}_{upwind} = c\mathbb{I}_d.$$

- Strong coupling between cell ✓
- Numerical dissipation is too strong if  $c \gg \|u\|$  ✗

► **centered scheme :**

$$D_{centered} = 0, \quad \bar{D}_{centered} = 0, \quad \bar{D}_{centered} + {}^t\bar{D}_{centered} = 0.$$

- Numerical dissipation is zero ✓
- Odd/even decoupling ✗

► **staggered scheme :**

$$D_{stag} = \begin{pmatrix} 0 & 1 \\ -c^2 & 0 \end{pmatrix}, \quad \bar{D}_{stag} = \begin{pmatrix} 0 & c \\ -c & 0 \end{pmatrix}, \quad \bar{D}_{stag} + {}^t\bar{D}_{stag} = 0.$$

- Numerical dissipation is zero ✓
- Strong coupling between neighbouring cells ✓

- 1 Choose a matrix  $D$  satisfying the stability and precision criteria
  - $\bar{D} + {}^t\bar{D} \geq 0$  (stability)
  - $\bar{D} + {}^t\bar{D}$  does not involve the sound speed  $c$  (precision)
- 2 compute the fluxes between cells using the expression :

$$F_{i,j} = \frac{F(U_i) + F(U_j)}{2} + D \frac{U_i - U_j}{2}$$

Remarks :

- ▶ The schéme can be colocated or staggered, one step or multistep
- ▶ The scheme is generally implicit if  $Sp(\bar{D}) \subset i\mathbb{R}$
- ▶ One can have zero numerical dissipation  $\|\bar{U}_h(\cdot, t)\|_{L^2} = \|\bar{U}_{h0}\|_{L^2}$  and non zero numerical diffusion  $\bar{D}$

We consider the following Euler equations :

$$\partial_t \rho + \nabla \cdot (\rho \vec{u}) = 0 \quad (14)$$

$$\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \vec{\nabla} p = 0 \quad (15)$$

$$\partial_t (\rho (e + \frac{1}{2} \|\vec{u}\|^2)) + \nabla \cdot ((\rho e + \frac{1}{2} \rho \|\vec{u}\|^2 + p) \vec{u}) = 0 \quad (16)$$

Symmetrisation with  $\left. \frac{\partial p}{\partial \rho} \right|_e$ ,  $\left. \frac{\partial p}{\partial e} \right|_\rho$  not appearing on the diagonal :

$$S = \begin{pmatrix} u & \sqrt{\left. \frac{\partial p}{\partial \rho} \right|_e} & 0 \\ \sqrt{\left. \frac{\partial p}{\partial \rho} \right|_e} & u & \sqrt{\left. \frac{\partial p}{\partial e} \right|_\rho} \frac{p}{\rho^2} \\ 0 & \sqrt{\left. \frac{\partial p}{\partial e} \right|_\rho} \frac{p}{\rho^2} & u \end{pmatrix}.$$

In the symetrising basis :

$$\bar{D}_{Stag} = \begin{pmatrix} |u| & \sqrt{\frac{\partial p}{\partial \rho}}|_e & 0 \\ -\sqrt{\frac{\partial p}{\partial \rho}}|_e & |u| & -\sqrt{\frac{\partial p}{\partial e}}|_\rho \frac{p}{\rho^2} \\ 0 & \sqrt{\frac{\partial p}{\partial e}}|_\rho \frac{p}{\rho^2} & |u| \end{pmatrix}$$

In the physical basis :

$$D_{Stag} = \begin{pmatrix} |u| - u & 1 & 0 \\ -\frac{\partial p}{\partial \rho}|_e - u^2 + \frac{1}{\rho} \frac{\partial p}{\partial e}|_\rho \left(\frac{u^2}{2} - e\right) & u + |u| - \frac{u}{\rho} \frac{\partial p}{\partial e}|_\rho & \frac{1}{\rho} \frac{\partial p}{\partial e}|_\rho \\ -u \left(c^2 + E - \frac{p}{\rho} + \frac{1}{\rho} \left(\frac{u^2}{2} - e\right) \frac{\partial p}{\partial e}|_\rho\right) & E - \frac{p}{\rho} - \frac{u^2}{\rho} \frac{\partial p}{\partial e}|_\rho & \frac{1}{\rho} \left(u \frac{\partial p}{\partial e}|_\rho + |u| \rho\right) \end{pmatrix}$$

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## Problèmes de Riemann difficiles

- ▶ Evaluation de la Tests robustesse de méthodes numériques
- ▶ Solutions exactes disponibles → évaluation de la précision
- ▶ Evaluation des méthodes numériques en présence d'ondes de choc et de contact
- ▶ La loi d'état est celle d'un gaz parfait

| Test  | $\rho_L$ | $u_L$    | $p_L$   | $\rho_R$ | $u_R$     | $p_R$   |
|-------|----------|----------|---------|----------|-----------|---------|
| Toro1 | 1        | 0.75     | 1       | 0.125    | 0         | 0.1     |
| Toro2 | 1        | -2       | 0.4     | 1        | 2         | 0.4     |
| Toro3 | 1        | 0        | 1000    | 1        | 0         | 0.01    |
| Toro4 | 5.99924  | 19.5975  | 460.894 | 5.99242  | -6.19633  | 46.0950 |
| Toro5 | 1        | -19.5975 | 1000    | 1        | -19.59745 | 0.01    |
| Toro6 | 1.4      | 0        | 1       | 1.4      | 0         | 1       |
| Toro7 | 1.4      | 0.1      | 1       | 1        | 0.1       | 1       |

Table: Initial data for the seven tests Toro1, ... , Toro7

- ▶ Convergence de 6 tests sur 7
- ▶ Echec du test Toro2 (densité négative car régime proche du vide)

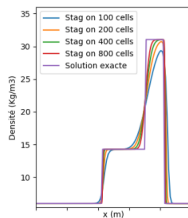
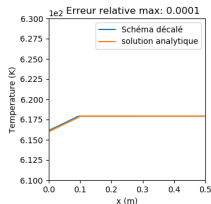
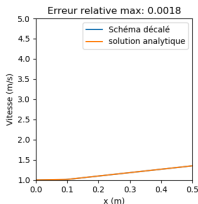
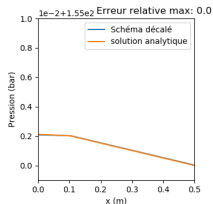
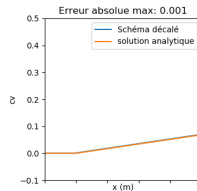
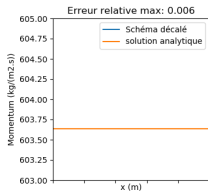
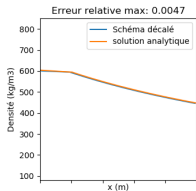


Figure: Densité du test Toro4

Nécessité d'un benchmark similaire diphasique  
Benchmark 2D et/ou avec termes source pour vérification des  
codes de calcul

- ▶ Canal 1D
- ▶ chauffage
- ▶ changement de phase





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With the new “staggered” class

- ▶ Simulation of shock waves
- ▶ Simulation of heated flows
- ▶ Simulation of boiling flows
- ▶ Simulation of singular pressure loss

Convergence to the analytical solution (except near void).

It remains to formalise the TVD analysis.

We can now study

- ▶ More complex models (two phase flows)
- ▶ Entropy balance
- ▶ Extension to general meshes



**Thanks! Any questions?**