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DE LA RECHERCHE À L'INDUSTRIE

ON A SHOCK CAPTURING FINITE VOLUME METHOD THAT CAN SOLVE FULLY INCOMPRESSIBLE FLOWS

28 June 2023

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DES/ISAS/DM2S/STMF/LMEC

Commissariat à l'énergie atomique et aux énergies alternatives - www.cea.fr

Context

Low Mach precision vs checkerboard modes

Numerical diffusion of classical schemes

A new class of staggered schemes

Numerical results

Conclusion and perspectives

Context

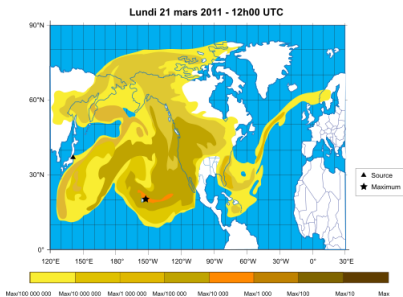
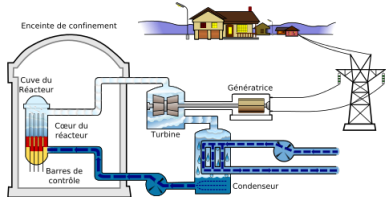
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- ▶ Multicomponent flow : liquid, vapor, solid obstacles
- ▶ Stiff source terms (heat source, boiling, pressure losses)
- ▶ Flow in a wide range of regimes (Ma , Re , Pe)
- ▶ Specifics of two phase flows
 - non conservative models (e.g. two-fluid models)
 - 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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$$\left\{ \begin{array}{l} \frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \mu \Delta \mathbf{u} \\ \frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho H \mathbf{u}) = \lambda \Delta T \end{array} \right. \quad (1)$$

- ▶ ρ, \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 colocated methods (Godunov, Roe, ...)
 - do not satisfy the low Mach asymptotics ✗
- ▶ Centered FV colocated methods
 - satisfy the low Mach asymptotics... ✓
 - but generate spurious checkerboard oscillations ✗

Lid driven cavity test :

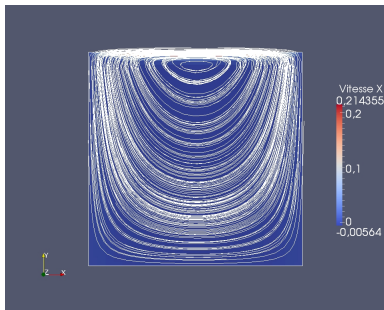


Figure: Implicit upwind scheme

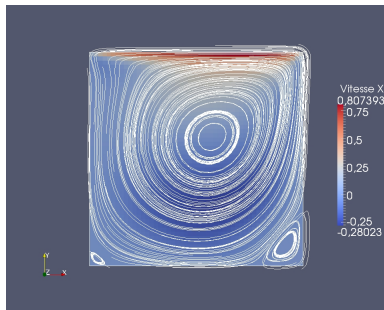
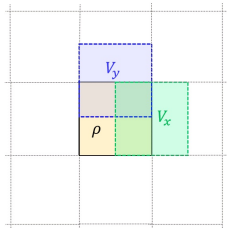


Figure: Implicit centered scheme

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



Staggered shelf	Colocated shelf
no sound speed involved	conservation form
OK for incompressible fluids	linear stability
no checkerboard modes	general meshes

Table: Our shopping list

Roadmap :

- ▶ find a theoretical framework for the design and analysis of staggered schemes
- ▶ rethink the (vectorial) upwinding of colocated schemes
- ▶ give up the geometric intuition behind staggered schemes
- ▶ family of schemes instead of a single one

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Most schemes have a numerical diffusion operator

e.g. a 1D first order non linear PDE

$$\partial_t U + A(U)\partial_x U = 0. \quad (3)$$

yields as $\Delta x \rightarrow 0$:

$$\partial_t U + A\partial_x U = -\Delta x \partial_x D_{disc} \partial_x U + o(\Delta x). \quad (4)$$

- ▶ D_{disc} is connected to stability and precision of the scheme
- ▶ One can derive the numerical diffusion of the scheme
- ▶ Exercise : Compute D_{disc} for colocated and staggered schemes

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

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

Centered discretisation :

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

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

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

Upwind discretisation

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

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

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

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

Staggered discretisation (simple version)

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

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

- ▶ most of the numerical diffusion is on the second equation
- ▶ D_{stag} is not diagonalisable on \mathbb{R}
- ▶ usually based on non conservative forms.

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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 $\bar{U} = PU$:

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

- ▶ after symetrisation, **the energy is constant in time**

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

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

$$\|\bar{U}(\cdot, t)\|_{L^2} = \|\bar{U}_0\|_{L^2}.$$

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

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

$$\Rightarrow \|\bar{U}_h(\cdot, t)\|_{L^2} \leq \|\bar{U}_{h0}\|_{L^2}. \quad (5)$$

- 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 $c \gg \|\mathbf{u}\|$ ✗

► **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 ✓

- 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)
- 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 scheme is conservative
- ▶ The scheme can be colocated or staggered
- ▶ 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 :

$$\partial_t \rho + \nabla \cdot (\rho \vec{u}) = 0 \quad (6)$$

$$\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \vec{\nabla} p = 0 \quad (7)$$

$$\partial_t (\rho (\mathbf{e} + \frac{1}{2} \|\vec{u}\|^2)) + \nabla \cdot ((\rho \mathbf{e} + \frac{1}{2} \rho \|\vec{u}\|^2 + p) \vec{u}) = 0 \quad (8)$$

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 :

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

In the physical basis :

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

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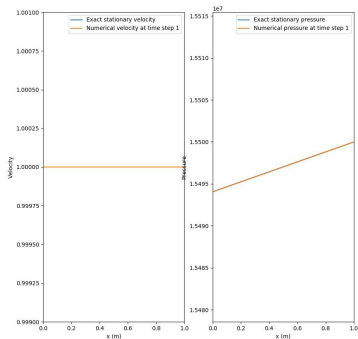
Incompressible flow correspond to $c \rightarrow \infty$

- ▶ Choose a staggered type upwinding (complex eigenvalues)
- ▶ use primitive variables (p, u) instead of $(\rho, q = \rho u)$
- ▶ check that there is no blow-up when $c \rightarrow \infty$
- ▶ note that the scheme should be implicit if $c = \infty$

$$\mathcal{D} = \text{sign}(\vec{u}_{ij} \cdot \vec{n}) \begin{pmatrix} \frac{\vec{u}_{ij} \cdot \vec{n}}{c_{ij}^2} & \rho(p)^t \vec{n} \\ -\vec{n} - \frac{(\vec{u}_{ij} \cdot \vec{n})}{c_{ij}^2} \vec{u}_{ij} & \rho(p)(\vec{u}_{ij} \otimes \vec{n} + (\vec{u}_{i,j} \cdot \vec{n}) \mathbb{I}_d) \end{pmatrix}$$

Numerical tests description :

- ▶ incompressible flow
- ▶ external force $\vec{f} = \rho \vec{g}$ the gravity
- ▶ reach stationary state
- ▶ exact velocity is constant
- ▶ exact pressure is constant

Implicit p-staggered scheme for isothermal Euler equations
1D channel under gravity

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	ρ_L	u_L	p_L	ρ_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)

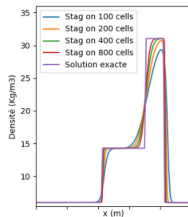
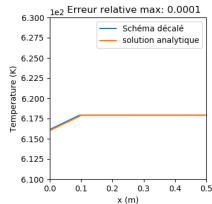
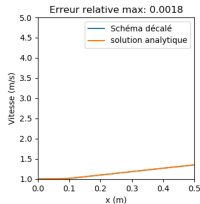
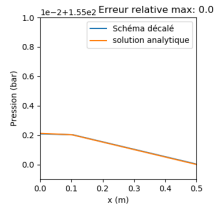
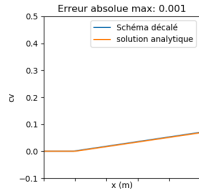
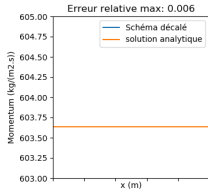
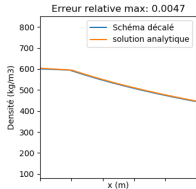


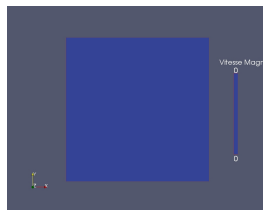
Figure: Densité du test Toro4

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



- ▶ fluide au repos $\vec{v} = \vec{0}$
- ▶ 3 parois fixes
- ▶ 1 paroi mobile
- ▶ Grille rectangulaire 50x50



Nombre de Mach : $1e - 3$

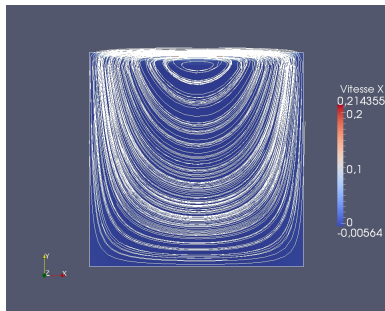


Figure: Colocalisé conservatif
(schéma de Roe implicite)

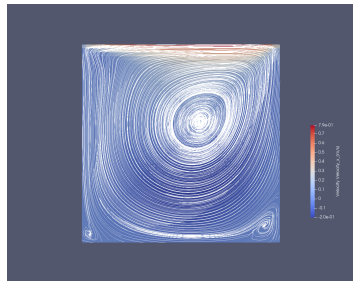


Figure: Décalé conservatif

Schéma décalé conservatif :

- ▶ Prise en compte de la viscosité
- ▶ Bonne précision à faible nombre de Mach
- ▶ Pas de modes en échiquiers

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With the new “staggered” class

- ▶ Simulation of shock waves
- ▶ Simulation of boiling flows
- ▶ Simulation of low Mach flows
- ▶ Simulation of incompressible flows

Convergence to the analytical solution (except near void).

Checkerboard analysis : formalised TVD analysis (FVCA10).

We can now study

- ▶ More complex models (6 equations)
- ▶ Entropy balance
- ▶ 'porosity' jumps
- ▶ general meshes
- ▶ saddle point issue



Thanks! Any questions?