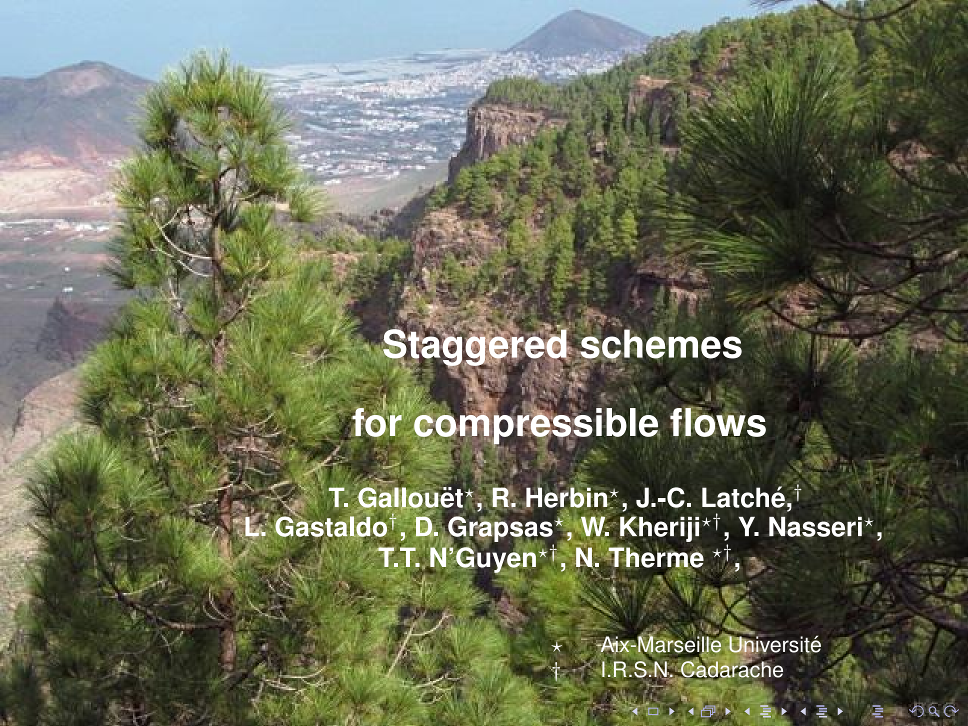

Staggered schemes

for compressible flows

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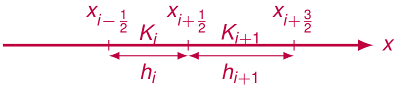
Context and objectives:

- Nuclear safety, IRSN, Calif3S
  `https://gforge.irsn.fr/gf/project/calif3s/`
- Internal energy balance formulation (rather than total energy formulation) even in the presence of shocks
- Upwinding with respect to the material velocity
- Consistency in the Lax-Wendroff sense "*if a conservative numerical scheme for a hyperbolic system of conservation laws converges, then it converges towards a weak solution.*"
- Lax-Wendroff consistency for an *entropy weak* solution.
- All Mach scheme ?
  $\rightsquigarrow$ Implicit or semi-implicit (rather than completely segregated) schemes
  $\rightsquigarrow$ staggered (rather than colocated) grids

Conservative numerical scheme: conservative (and consistent) fluxes

- $f \in C^2(\mathbb{R})$, $\quad \partial_t u + \partial_x(f(u)) = 0$ + IC $\quad (\star)$



- $\displaystyle\int_{K_i} \partial_t u \, dx + (f(u))(x_{i+\frac{1}{2}}, t) - (f(u))(x_{i-\frac{1}{2}}, t) = 0, \quad u(x,0) = u_0(x)$
- Conservative flux: $\displaystyle h_i \frac{u_i^{n+1} - u_i^n}{\delta t} + g_{i+\frac{1}{2}}(u_i^n, u_{i+1}^n) - g_{i-\frac{1}{2}}(u_{i-1}^n, u_i^n) = 0 \qquad (\star\star)$
- Consistent flux: $g(u,u) = f(u)$

- Lax-Wendroff theorem: if $u_{h,\delta t} \to \bar{u}$ a.e. as $h, \delta t \to 0$ and $\|u_{h,\delta t}\|_\infty \leq C$ then $\bar{u}$ is a weak solution to $(\star)$, i.e., $\forall \varphi \in C_c^1(\mathbb{R} \times \mathbb{R}_+, \mathbb{R})$,

$$\int_0^T \int_{\mathbb{R}} \bar{u}(x,t) \partial_t \varphi(x,t) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t + \int_0^T \int_{\mathbb{R}} f(\bar{u}(x,t)) \partial_x \varphi(x,t) \, dx \, dt + \int_{\mathbb{R}} u_0(x) \varphi(x,0) \, dx = 0$$

- Sketch of proof $\varphi \in C_c^\infty$, multiply $(\star\star)$ by φ_i^n, sum over i, sum over n:

$$\sum_n \sum_i \varphi_i^n (g_{i+\frac{1}{2}}^n - g_{i-\frac{1}{2}}^n) = \sum_i g_{i+\frac{1}{2}}^n (u_i^n, u_{i+1}^n) h \frac{\varphi_{i+1}^n - \varphi_i^n}{h} = \int_{\mathbb{R}_+} \int_{\mathbb{R}} f(u_{h,\delta t}) \eth_x \varphi_{h,\delta t} \, dx \, dt$$

$$\to \int_{\mathbb{R}_+} \int_{\mathbb{R}} f(\bar{u}) \partial_x \varphi(x) \, dx \, dt$$

Conservative numerical scheme: conservative variables

- Toro, 1999 *"Formulations based on variables other than the conserved variables (non-conservative variables) fail at shock waves. They give the wrong jump conditions; consequently they give the wrong shock strength, the wrong shock speed and thus the wrong shock position. ... Therefore it appears that there is no choice but to work with conservative methods if shock waves are part of the solution."*

- Shock speed given by Rankine Hugoniot conditions:
  If u, weak solution of

$$\partial_t u + \partial_x(f(u)) = 0 + \text{IC} \qquad (\star)$$

  is discontinuous along a line $x = \sigma t$ then

$$[f(u)] = f(u_\ell) - f(u_r) = \sigma\,(u_\ell - u_r) = \sigma\,[u]$$

So if Lax-consistency is proven, shock speeds are correct.

Right and wrong shock speed for Burgers

Burgers equation: for regular positive solutions

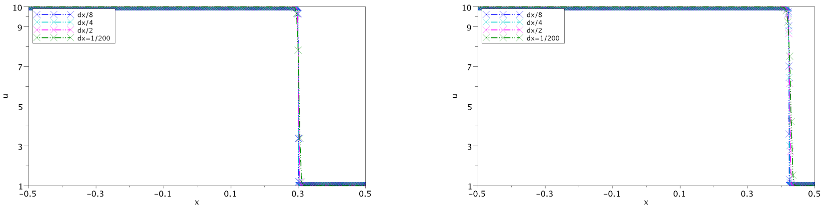
$$(\mathrm{B}) : \partial_t u + \partial_x (u^2) = 0 \iff (\mathrm{BS}) : \partial_t u^2 + \frac{4}{3}\, \partial_x u^3 = 0.$$

No longer true with irregular solutions:

Rankine-Hugoniot gives

$$\sigma = \frac{u_\ell^2 - u_r^2}{u_\ell - u_r} = u_\ell + u_r \text{ and } \sigma = \frac{4}{3}\frac{u_\ell^3 - u_r^3}{u_\ell^2 - u_r^2} = \frac{4}{3}(u_\ell + u_r).$$

Weak solutions of (B) $\neq$ weak solutions of (BS).



Explicit upwind Scheme for (B) (left) and (BS) (right) with different mesh sizes, $CFL = 1$.

Burgers, numerical diffusion

- Burgers (B): upwinding " formarly similar" to add a numerical diffusion.

$$\partial_t u + \partial_x(u^2) - \partial_x((hu - 2\delta t\ u^2)\partial_x u) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

  CFL condition: $hu - 2\delta t\ u^2 \geq 0$

- Burgers "square" (BS): assume $u > 0$, upwinding also " formarly similar" to add a numerical diffusion

$$\partial_t(u^2) + \frac{4}{3}\partial_x(u^3) - \partial_x((2hu^2 - 4\delta t\ u^3)\partial_x u) = 0,$$

- divide by $2u \rightsquigarrow$ (formally)

$$\partial_t u + \partial_x(u^2) - \frac{1}{u}\partial_x((hu^2 - 2\delta t\ u^3)\partial_x u) = 0,\ x \in \mathbb{R},\ t \in \mathbb{R}_+$$

  Non conservative diffusion $\rightsquigarrow$ wrong shock speed for (B)

Benefit from a non conservative numerical diffusion ?

$$\partial_t u + \partial_x(u^2) = 0 + \text{IC} \quad (\text{B}) \qquad \partial_t(u^2) + \frac{4}{3}\,\partial_x(u^3) = 0 + \text{IC} \quad (\text{BS})$$

Explicit upwind scheme on (BS) formally equivalent to:

$$\partial_t u + \partial_x(u^2) \underbrace{- \frac{1}{u}\partial_x((hu^2 - 2\delta t\ u^3)\partial_x u)}_{\text{non conservative numerical diffusion.}} = 0.$$

- Negative result for a non conservative diffusion
  - ☹ Non conservative numerical diffusion on (B) yields
    - wrong shock velocity for (B)
    - correct shock velocity for (BS)
- Positive result for a non conservative diffusion ?
  - ☺ Non conservative numerical diffusion on (BS) yields
    - wrong shock velocity for (BS)
    - correct shock velocity for (B) ?
- How do we choose the non conservative numerical diffusion ?

Non conservative numerical diffusion on (BS)

- Start from viscous Burgers:

$$\partial_t u + \partial_x(u^2) - \varepsilon\partial_{xx} u = 0. \qquad (\mathrm{B})_\varepsilon$$

- Multiply by $2u$:

$$\partial_t(u^2) + \frac{4}{3}\,\partial_x(u^3) - 2u\varepsilon\partial_{xx} u = 0. \qquad (\mathrm{BS})_\varepsilon$$

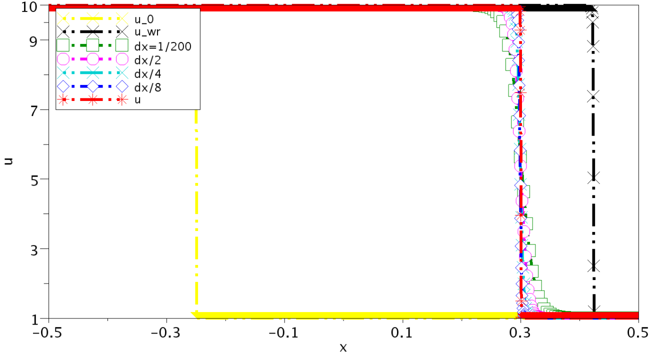
- Discretize $(\mathrm{BS})_\varepsilon$ instead of (BS):

$$\partial_t(u^2) + \frac{4}{3}\partial_x(u^3) - uh\partial_{xx} u = 0, \quad (\mathrm{BS})_h \text{ with } h = 2\varepsilon.$$

- Centered finite volume with non conservative diffusion

$$(u_i^{(n)})^2 = (u_i^{(n-1)})^2 + \frac{4\delta t}{3h}\left[\left(\frac{u_{i-1}^{(n-1)} + u_i^{(n-1)}}{2}\right)^3 - \left(\frac{u_i^{(n-1)} + u_{i+1}^{(n-1)}}{2}\right)^3\right] + \frac{\delta t}{h^2}\, h\, u_i^{(n-1)}\left[2u_i^{(n-1)} - u_{i-1}^{(n-1)} - u_{i+1}^{(n-1)}\right].$$

Non conservative numerical diffusion on (BS)



Centered Scheme for $(BS)_h$,

The Euler (NS) equations: total energy vs. internal energy

- Euler (Navier-Stokes) equations:

$$\partial_t \varrho + \operatorname{div}(\varrho \boldsymbol{u}) = 0, \qquad \text{(mass)}$$

$$\partial_t(\varrho \boldsymbol{u}) + \operatorname{div}(\varrho \boldsymbol{u} \otimes \boldsymbol{u}) - \operatorname{div} \boldsymbol{\tau} + \boldsymbol{\nabla} p = 0, \qquad \text{(mom)}$$

$$\partial_t(\varrho E) + \operatorname{div}\big[(\varrho E + p)\boldsymbol{u}\big] = \operatorname{div}(\boldsymbol{\tau} \boldsymbol{u}), \qquad \text{(tot.en)}$$

$$p = (\gamma - 1)\, \varrho e, \quad E = \frac{1}{2}\, |\boldsymbol{u}|^2 + e.$$

- For regular functions, (mom) $\cdot \boldsymbol{u}$ & (mass) $\rightsquigarrow$ (kin.en):

$$\frac{1}{2}\partial_t(\varrho |\boldsymbol{u}|^2) + \frac{1}{2}\operatorname{div}(\varrho |\boldsymbol{u}|^2 \boldsymbol{u}) + \boldsymbol{\nabla} p \cdot \boldsymbol{u} = \operatorname{div}(\boldsymbol{\tau}) \cdot \boldsymbol{u}. \qquad \text{(kin.en)}$$

Subtracting from (tot.en) yields the internal energy balance:

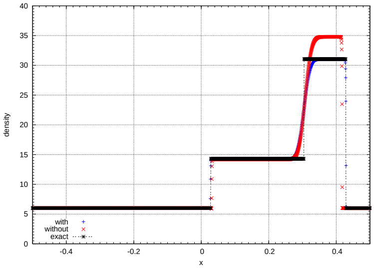
$$\partial_t(\varrho e) + \operatorname{div}(\varrho e \boldsymbol{u}) + p \operatorname{div} \boldsymbol{u} = \boldsymbol{\tau} : \boldsymbol{\nabla} \boldsymbol{u}, \qquad \text{(int.en)}$$

which implies $e \geq 0$.

"Incompressible" schemes use the internal energy (or temperature) equation.

Internal energy

- Dealing with the internal energy:
  - ♯ positive internal energy
  - ♯ convenient for incompressible problems
  - ♭ ρe is not a conserved variable – conserved variables : ρ, ρu, ρE



Test 5 of [Toro chapter 4] - Density at $t = 0.035$, $n = 2000$ cells, with and without corrective source terms, and analytical solution.

- Find a way to correct the internal energy equation in order to recover the consistency of the total energy...

Strategy for a numerical scheme for Euler

How to get correct weak solutions of Euler equations while solving the internal energy balance ?

General idea: $(\text{int.en})_d$ + $(\text{kin.en})_d \rightsquigarrow$ "$(\text{tot.en})_d$"

More precisely:

- $(\text{mom})_d$ and $(\text{mass})_d \rightsquigarrow$ discrete kinetic energy $(\frac{1}{2}\rho|\boldsymbol{u}|^2)$ equation

$$\eth_t(\frac{1}{2}\rho|\boldsymbol{u}|^2) + \mathrm{div}_d(\frac{1}{2}\rho|\boldsymbol{u}|^2\boldsymbol{u}) + \boldsymbol{u}\cdot\nabla_d p + R = 0$$

R : non conservative residual term, $R \geq 0$.

- $(\text{int.en})_d$: $\eth_t(\rho e) + \mathrm{div}_d(e\boldsymbol{u}) + p\,\mathrm{div}_d\boldsymbol{u} = R$

- Perform Lax-Wendroff consistency analysis of the scheme:
  (a) Suppose bounds and convergence for a sequence of discrete solutions
    - control in BV and L^∞,
    - convergence in L^p, for $p \geq 1$.

  (b) Let φ be a regular function,
    - interpolate,
    - test the kinetic energy balance,
    - test the internal energy balance,
    - and pass to the limit in the scheme.

The corrective term in the internal energy balance is such that, at the limit, the weak form of the total energy equation is recovered.

Euler equations: total energy = kinetic energy + internal energy

Total energy (Euler):

$$\partial_t(\varrho E) + \mathrm{div}\left[(\varrho E + p)\boldsymbol{u}\right] = 0, \quad E = e + \frac{1}{2}|u|^2$$

$$\Longrightarrow \partial_t(\rho e) + \mathrm{div}(\rho e \boldsymbol{u}) + p\,\mathrm{div}\boldsymbol{u} + \frac{1}{2}\partial_t(\rho\,|\boldsymbol{u}|^2) + \frac{1}{2}\mathrm{div}(\rho\,|\boldsymbol{u}|^2\,\boldsymbol{u}) + \boldsymbol{u}\cdot\nabla p = 0.$$

From mass balance, for "regular" z:

$$\partial_t(\rho z) + \mathrm{div}(\rho z \boldsymbol{u}) = \underbrace{(\partial_t \varrho + \mathrm{div}(\varrho \boldsymbol{u}))}_{=0.} z + \rho\,\partial_t z + \rho \boldsymbol{u}\cdot\nabla z,$$

$$\begin{aligned}\Longrightarrow \frac{1}{2}\partial_t(\rho u_i^2) + \frac{1}{2}\mathrm{div}(\rho u_i^2 \boldsymbol{u}) &= \rho\partial_t(u_i^2) + \rho\boldsymbol{u}\cdot\nabla(u_i^2) = \rho u_i \partial_t u_i + \rho u_i \boldsymbol{u}\cdot\nabla u_i \\ &= u_i\,\left[\rho\partial_t u_i + \rho\boldsymbol{u}\cdot\nabla u_i\right] = u_i[\partial_t(\rho u_i) + \mathrm{div}(\rho u_i \boldsymbol{u})] \\ &= -u_i\,\partial_i p, \ \text{from momentum balance.}\end{aligned}$$

$$\Longrightarrow \frac{1}{2}\partial_t(\rho\,|\boldsymbol{u}|^2) + \frac{1}{2}\mathrm{div}(\rho\,|\boldsymbol{u}|^2\,\boldsymbol{u}) = \boldsymbol{u}\cdot\left[\partial_t(\rho\boldsymbol{u}) + \mathrm{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u})\right] = -\boldsymbol{u}\cdot\nabla p.$$

and $\partial_t(\rho e) + \mathrm{div}(\rho e \boldsymbol{u}) + p\,\mathrm{div}(\boldsymbol{u}) = 0.$

Required discrete properties

Aim: compute discrete kinetic balance from discrete mass and discrete momentum by copying the continuous computation.

- Discrete transport property, i.e. discrete equivalent of
  $\partial_t(\rho z) + \mathrm{div}(\rho z \boldsymbol{u}) = \rho\, \partial_t z + \rho \boldsymbol{u} \cdot \nabla z, \qquad z = u_i.$

  $\Longrightarrow$ Compatible discretization of mass and momentum balance equation

- Discrete duality
  i.e. discrete equivalent of $\mathrm{div}(p\boldsymbol{u}) = p\,\mathrm{div}\boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} p.$

- Positivity of the residual $R \geq 0$ in the discrete kinetic energy balance equation (to ensure the positivity of the internal energy).

$\rightsquigarrow$ Points to be taken care of when designing the scheme(s).

Time discretization : I - Decoupled (explicit) choice

- Decoupled 1: natural ordering, bad idea..., $\rho \to \boldsymbol{u} \to e \to p$

$$\frac{1}{\delta t}(\varrho^{n+1} - \varrho^n) + \mathrm{div}(\varrho^n \boldsymbol{u}^n) = 0, \qquad (\text{mass})_d \quad \rightsquigarrow \quad \varrho^{n+1}$$

$$\frac{1}{\delta t}(\varrho^{n+1}\boldsymbol{u}^{n+1} - \varrho^n \boldsymbol{u}^n) + \mathrm{div}(\varrho^n \boldsymbol{u}^n \otimes \boldsymbol{u}^n) + \boldsymbol{\nabla} p^n = 0, \qquad (\text{mom})_d \quad \rightsquigarrow \quad \boldsymbol{u}^{n+1}.$$

$$\frac{1}{\delta t}(\varrho^{n+1} e^{n+1} - \varrho^n e^n) + \mathrm{div}(\varrho^n e^n \boldsymbol{u}^n) + p^n \,\mathrm{div} \boldsymbol{u}^{n+1} = R^n, \qquad (\text{int.en})_d \quad \rightsquigarrow \quad e^{n+1}$$

$$p^{n+1} = \wp(\varrho^{n+1}, e^{n+1}) = (\gamma - 1)\, \varrho^{n+1} e^{n+1}, \qquad (\text{eos})_d \quad \rightsquigarrow \quad p^{n+1}$$

- Decoupled 2: better idea..., $\rho \to e \to p \to \boldsymbol{u}$

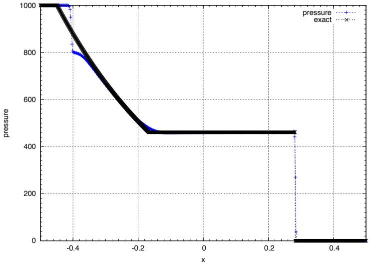
$$\frac{1}{\delta t}(\varrho^{n+1} - \varrho^n) + \mathrm{div}(\varrho^n \boldsymbol{u}^n) = 0, \qquad (\text{mass})_d \quad \rightsquigarrow \quad \varrho^{n+1}$$

$$\frac{1}{\delta t}(\varrho^{n+1} e^{n+1} - \varrho^n e^n) + \mathrm{div}(\varrho^n e^n \boldsymbol{u}^n) + p^n \,\mathrm{div} \boldsymbol{u}^{n} = R^n, \qquad (\text{int.en})_d \quad \rightsquigarrow \quad e^{n+1}$$

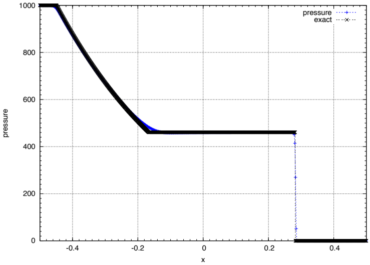
$$p^{n+1} = \wp(\varrho^{n+1}, e^{n+1}) = (\gamma - 1)\, \varrho^{n+1} e^{n+1}, \qquad (\text{eos})_d \quad \rightsquigarrow \quad p^{n+1}$$

$$\frac{1}{\delta t}(\varrho^{n+1}\boldsymbol{u}^{n+1} - \varrho^n \boldsymbol{u}^n) + \mathrm{div}(\varrho^n \boldsymbol{u}^n \otimes \boldsymbol{u}^n) + \boldsymbol{\nabla} p^{n+1} = 0, \qquad (\text{mom})_d \quad \rightsquigarrow \quad \boldsymbol{u}^{n+1}.$$

Time discretization : I -Decoupled choice



$\rho \to \boldsymbol{u} \to e \to p$



$\rho \to e \to p \to \boldsymbol{u}$

[E. Toro, *Riemann solvers and numerical methods for fluid dynamics*, third edition, test 3 of chapter 4].

Decoupled scheme : Why choose $\rho \to e \to p \to \boldsymbol{u}$?

- Formal derivation of the entropy balance for regular functions

$$\partial_t(\rho s) + \mathrm{div}(\rho \boldsymbol{u} s) = 0$$

For Euler perfect gas $s = \ln\left(\frac{p}{\rho^\gamma}\right) = \phi(\rho) + \rho\psi(e)$, $\phi(\rho) = \rho \ln(\rho)$, $\psi(e) = -\frac{1}{\gamma-1}\ln e$.

$$\left|\begin{array}{ll} \partial_t \varrho + \mathrm{div}(\rho \boldsymbol{u}) = 0 & \times\ \phi'(\rho) = 1 + \ln\varrho,\ \phi'' \geq 0 \\ \partial_t(\varrho e) + \mathrm{div}(\varrho \boldsymbol{u} e) + p\,\mathrm{div}\boldsymbol{u} = 0 & \times\ \psi'(e) = -\dfrac{1}{(\gamma-1)e},\ \psi'' \geq 0 \end{array}\right.$$

$$\rightsquigarrow \left|\begin{array}{l} \partial_t(\phi(\varrho)) + \mathrm{div}(\phi(\varrho)\boldsymbol{u}) + \underbrace{(\varrho\,\phi'(\varrho) - \phi(\varrho))}_{=\varrho}\mathrm{div}\boldsymbol{u} = 0 \\ \partial_t(\varrho\psi(e)) + \mathrm{div}(\varrho\boldsymbol{u}\psi(e)) + \underbrace{\psi'(e)p}_{=-\varrho}\ \mathrm{div}\boldsymbol{u} = 0 \\ \hline \partial_t(\varrho s) + \mathrm{div}(\varrho \boldsymbol{u} s) + \underbrace{\left[\varrho\,\phi'(\varrho) - \phi(\varrho) + \psi'(e)p\right]}_{=0}\ \mathrm{div}\boldsymbol{u} = 0. \end{array}\right.$$

- We need $\mathrm{div}(\varrho\boldsymbol{u})$ and $p\,\mathrm{div}\boldsymbol{u}$ at the same time level to mimick this computation at the discrete level.
  - Choice 1 $\rho \to \boldsymbol{u} \to e \to p \rightsquigarrow \mathrm{div}(\varrho^n \boldsymbol{u}^n)$ and $p^n\,\mathrm{div}\boldsymbol{u}^{n+1}$
  - Choice 2 $\rho \to e \to p \to \boldsymbol{u} \rightsquigarrow \mathrm{div}(\varrho^n \boldsymbol{u}^n)$ and $p^n\,\mathrm{div}\boldsymbol{u}^n$

Time discretization : II - Implicit or semi-implicit choice

Implicit

$$\frac{\rho^{n+1}-\rho^{n}}{\delta t}+\operatorname{div}(\rho^{n+1}\,\boldsymbol{u}^{n+1})=0, \qquad (\text{mass})_d$$

$$\frac{1}{\delta t}(\varrho^{n+1}\boldsymbol{u}^{n+1}-\varrho^{n}\boldsymbol{u}^{n})+\operatorname{div}(\varrho^{n+1}\boldsymbol{u}^{n+1}\otimes\boldsymbol{u}^{n+1})+\boldsymbol{\nabla}p^{n+1}=0, \qquad (\text{mom})_d$$

$$\frac{1}{\delta t}(\varrho^{n+1}e^{n+1}-\varrho^{n}e^{n})+\operatorname{div}(\varrho^{n+1}e^{n+1}\boldsymbol{u}^{n+1})+p^{n+1}\operatorname{div}\boldsymbol{u}^{n+1}=R^{n+1}, \qquad (\text{int.en})_d$$

$$p^{n+1}=\wp(\varrho^{n+1},e^{n+1})=(\gamma-1)\,\varrho^{n+1}e^{n+1}, \qquad (\text{eos})_d$$

Semi-implicit

Pressure gradient scaling step: $(\overline{\boldsymbol{\nabla}p})^{n+1}=\left(\frac{\rho^{n}}{\rho^{n-1}}\right)^{\frac{1}{2}}(\boldsymbol{\nabla}p^{n})$

Prediction step – Solve for $\tilde{\boldsymbol{u}}^{n+1}$:

$$\frac{1}{\delta t}\left(\rho^{n}\tilde{\boldsymbol{u}}^{n+1}-\rho^{n-1}\boldsymbol{u}^{n}\right)+\operatorname{div}(\rho^{n}\tilde{\boldsymbol{u}}^{n+1}\otimes\boldsymbol{u}^{n})+(\overline{\boldsymbol{\nabla}p})^{n+1}=0, \qquad (\text{mom})_d$$

Correction step – Solve for p^{n+1}, e^{n+1}, ρ^{n+1} and $\boldsymbol{u}^{n+1}$:

$$\frac{1}{\delta t}\rho^{n}\left(\boldsymbol{u}^{n+1}-\tilde{\boldsymbol{u}}^{n+1}\right)+(\boldsymbol{\nabla}p^{n+1})-(\overline{\boldsymbol{\nabla}p})^{n+1}=0,$$

$$\frac{\rho^{n+1}-\rho^{n}}{\delta t}+\operatorname{div}(\rho^{n+1}\,\boldsymbol{u}^{n+1})=0, \qquad (\text{mass})_d$$

$$\frac{1}{\delta t}(\rho^{n+1}e^{n+1}-\rho^{n}e^{n})+\operatorname{div}(\rho^{n+1}e^{n+1}\boldsymbol{u}^{n+1})+p^{n+1}(\operatorname{div}(\boldsymbol{u}^{n+1}))=R^{n+1}, \qquad (\text{int.en})_d$$

$$\rho^{n+1}=\varrho(e^{n+1},p^{n+1}). \qquad (\text{eos})_d$$

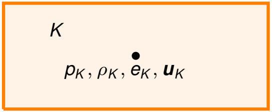
Meshes

Colocated

- Advantages

  Easier Data structure, easily refined

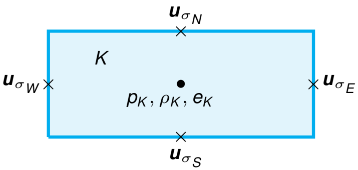
  Total energy easy to define
- Pressure correction scheme studied for the Euler equations (C. Zaza's thesis).
- Drawback: No native inf-sup condition



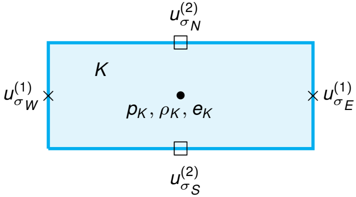
Staggered:

- Crouzeix-Raviart (on simplices) / Rannacher-Turek (on quadrangles) $\rightsquigarrow$ full velocities on the edges (faces)

  MAC: $\rightsquigarrow$ normal velocities on the edges (faces)
- Inf-sup condition $\forall p \in P, \int p = 0, \exists \boldsymbol{v} \in V \ : \int p \operatorname{div} \boldsymbol{v} \geq \beta \|p\|_{L^2} \|\boldsymbol{v}|_{H^1_d}$
- Drawback: Total energy difficult to compute



Rannacher-Turek unknowns



MAC unknowns, Arakawa C-grid

Space discretization: Finite volume discretization of the mass equation

$$\frac{\rho^{n+1} - \rho^n}{\delta t} + \operatorname{div}(\rho^{n+1}\,\boldsymbol{u}^{n+1}) = 0, \qquad \text{(mass)}$$

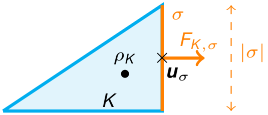
- $\int_K$ (mass) $\rightsquigarrow$

$$\int_K \frac{\rho^{n+1} - \rho^n}{\delta t} + \int_{\partial K} (\rho^{n+1}\,\boldsymbol{u}^{n+1} \cdot \mathbf{n}_K) = 0.$$

- discretization of the fluxes:

$$\frac{|K|}{\delta t}\,(\rho_K^{n+1} - \rho_K^n) + \sum_{\sigma \subset \partial K} F_{K,\sigma}^{n+1} = 0,$$

$F_{K,\sigma}^{n+1} = |\sigma|\ \rho_\sigma^{n+1} \boldsymbol{u}_\sigma^{n+1} \cdot \mathbf{n}_{K,\sigma}$,
numerical flux through σ.



- ρ_σ^{n+1} upwind approximation of ρ^{n+1} at the face σ with respect to $\boldsymbol{u}_\sigma^{n+1} \cdot \boldsymbol{n}_{K,\sigma}$.
- $\rightsquigarrow$ Positive density: $\rho^{n+1} > 0$ if ($\rho^n > 0$ and $\rho > 0$ at inflow boundary)

Discrete internal energy equation and E.O.S.

$$\frac{1}{\delta t}(\rho^{n+1}e^{n+1} - \rho^n e^n) + \mathrm{div}(\rho^{n+1}e^{n+1}\boldsymbol{u}^{n+1}) + p^{n+1}(\mathrm{div}(\boldsymbol{u}^{n+1})) = R^{n+1}$$

- Discretization by upwind finite volume of the discrete internal energy

$$\frac{|K|}{\delta t}(\rho_K^{n+1}e_K^{n+1} - \rho_K^n e_K^n) + \sum_{\sigma\subset\partial K)} F_{K,\sigma}^{n+1} e_\sigma^{n+1} + |K| \; p_K^{n+1}\,(\mathrm{div}\boldsymbol{u}^{n+1})_K = R_K^{n+1},$$

  - e_σ^{n+1} upwind choice $\rightsquigarrow$ positivity of e (if $R_K^{n+1} \geq 0$)
  - $|K|\,(\mathrm{div}\boldsymbol{u})_K = \sum_{\sigma\subset\partial K} |\sigma|\; u_\sigma \cdot \mathbf{n}_{K,\sigma}.$

- discrete E.O.S. $\qquad p_K^{n+1} = (\gamma-1)\rho_K^{n+1}\; e_K^{n+1}. \qquad (\mathrm{eos})_d$

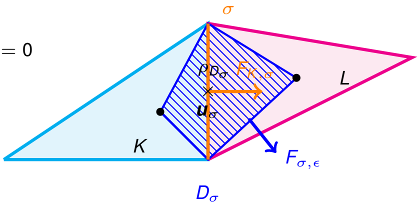
Discretization of the momentum equation

$$\frac{1}{\delta t}\,(\rho^n \tilde{\boldsymbol{u}}^{n+1} - \rho^{n-1}\boldsymbol{u}^n) + \mathrm{div}(\rho^n \tilde{\boldsymbol{u}}^{n+1} \otimes \boldsymbol{u}^n) + (\overline{\nabla p})^{n+1} \qquad (\mathrm{mom})^n$$

- $\displaystyle\int_{D_\sigma} (\mathrm{mom})^n \rightsquigarrow \underbrace{\int_{D_\sigma} \frac{\rho^n \tilde{\boldsymbol{u}}^{n+1} - \rho^{n-1}\boldsymbol{u}^n}{\delta t} + \int_{\partial D_\sigma} \rho^n \tilde{\boldsymbol{u}}^{n+1} \otimes \boldsymbol{u}^n \cdot \boldsymbol{n}_K}_{\mathcal{C}(\rho^n, \boldsymbol{u}^n)} + \int_{D_\sigma} (\overline{\nabla p})^{n+1} = 0.$
- Space discretization

$$\underbrace{\frac{|D_\sigma|}{\delta t}\,(\rho^n_{D_\sigma}\, \tilde{\boldsymbol{u}}^{n+1}_\sigma - \rho^{n-1}_{D_\sigma}\, \boldsymbol{u}^n_\sigma) + \sum_{\epsilon \subset \partial D_\sigma} F^n_{\sigma,\epsilon}\, \tilde{\boldsymbol{u}}^{n+1}_\epsilon}_{\mathcal{C}_d(\rho^n, \boldsymbol{u}^n)} + |D_\sigma| \sqrt{\frac{\rho^n_{D_\sigma}}{\rho^{n-1}_{D_\sigma}}}(\nabla p^n)_\sigma = 0,$$

- Grad-div duality :
  $\displaystyle\sum_{K \in \mathcal{T}} |K|\, p_K\, (\mathrm{div}\boldsymbol{u})_K + \sum_{\sigma \in \mathcal{E}} |D_\sigma|\, \boldsymbol{u}_\sigma \cdot (\nabla p)_\sigma = 0$
  $\rightsquigarrow |D_\sigma| (\nabla p^n)_\sigma = |\sigma|\, (p^n_L - p^n_K)\, \boldsymbol{n}_{K,\sigma}$
  for $\sigma = K|L$.



- $\rho^n_{D_\sigma}$? $F^n_{\sigma,\epsilon}$?

Discretization of the convection operator

- Choice of $\rho^n_{D_\sigma}$, $\rho^{n-1}_{D_\sigma}$ and $F^n_{\sigma,\epsilon}$ in $\mathcal{C}_d(\rho^n, \boldsymbol{u}^n, \tilde{\boldsymbol{u}}^{n+1})$?
- Discretize $\mathcal{C}_d(\rho^n, \boldsymbol{u}^n, \tilde{\boldsymbol{u}}^{n+1})$ so as to obtain a discrete kinetic energy balance.
- Copy the continuous kinetic energy balance:

$$\text{(mom)} \cdot \boldsymbol{u} \;\&\; \text{(mass)} \rightsquigarrow \text{(kin.en)}$$

with some formal algebra... using $\partial_t \rho + \mathrm{div}(\rho\, \boldsymbol{u}) = 0$.

- Do the same at the discrete level ?

♭ Momentum on dual cells, mass on primal cells...

♯ Idea: ***reconstruct a mass balance on the the dual cells***

Choose

- $\rho_{D_\sigma} = \frac{1}{|D_\sigma|} (|D_{K,\sigma}|\, \rho_K + |D_{L,\sigma}|\, \rho_L)$
- $F_{\sigma,\epsilon}$: linear combination of the primal fluxes $(F_{K,\sigma})_{\sigma \subset \partial K}$.

so that a discrete mass balance holds on the dual cells D_σ:

$$\forall \sigma \in \mathcal{E}_{\mathrm{int}}, \qquad \frac{|D_\sigma|}{\delta t} (\rho^{n+1}_{D_\sigma} - \rho^n_{D_\sigma}) + \sum_{\epsilon \subset \partial D_\sigma} F^{n+1}_{\sigma,\epsilon} = 0.$$

Then take $\mathcal{C}_d(\rho^n, \boldsymbol{u}^n, \tilde{\boldsymbol{u}}^{n+1}) = \dfrac{|D_\sigma|}{\delta t} (\rho^n_{D_\sigma}\, \tilde{\boldsymbol{u}}^{n+1}_\sigma - \rho^{n-1}_{D_\sigma}\, \boldsymbol{u}^n_\sigma) + \displaystyle\sum_{\epsilon \subset \partial D_\sigma} F^n_{\sigma,\epsilon}\, \tilde{\boldsymbol{u}}^{n+1}_\epsilon$

with $\boldsymbol{u}^{n+1}_\epsilon = \frac{1}{2} (\boldsymbol{u}^{n+1}_\sigma + \boldsymbol{u}^{n+1}_{\sigma'})$

Discrete kinetic energy balance: computation of R_σ

- Continuous setting: Multiply continuous momentum by $\boldsymbol{u}$:

$$\Big(\partial_t(\rho\,\boldsymbol{u}) + \mathrm{div}(\rho\,\boldsymbol{u}\otimes\boldsymbol{u}) + \nabla p = 0\quad\Big)\cdot\boldsymbol{u}$$

  ... with some formal algebra... using $\partial_t\rho + \mathrm{div}(\rho\,\boldsymbol{u}) = 0$,
  $\rightsquigarrow$ continuous kinetic energy balance:

$$\partial_t(\frac{1}{2}\,\rho\,|\boldsymbol{u}|^2) + \mathrm{div}((\frac{1}{2}\,\rho\,|\boldsymbol{u}|^2)\,\boldsymbol{u}) + \boldsymbol{\nabla} p\cdot\boldsymbol{u} = 0 \qquad \text{(kin.en)}$$

- Discrete setting: Similarly, multiply discrete momentum by $\tilde{\boldsymbol{u}}_\sigma^{n+1}$:

$$\Big(\frac{|D_\sigma|}{\delta t}\,(\rho_{D_\sigma}^n\,\tilde{\boldsymbol{u}}_\sigma^{n+1} - \rho_\sigma^{n-1}\,\boldsymbol{u}_\sigma^n) + \sum_{\epsilon\subset\partial D_\sigma} F_{\sigma,\epsilon}^n\,\tilde{\boldsymbol{u}}_\epsilon^{n+1} + |D_\sigma|(\overline{\boldsymbol{\nabla} p}^{n+1})_\sigma = 0\Big)\cdot\tilde{\boldsymbol{u}}_\sigma^{n+1}$$

  ... with some algebra... using
  - Mass on dual cell: $\dfrac{|D_\sigma|}{\delta t}\,(\rho_{D_\sigma}^n - \rho_\sigma^{n-1}) + \displaystyle\sum_{\epsilon\subset\partial D_\sigma} F_{\sigma,\epsilon}^n = 0.$
  - Scaling of the pressure $\rho^{n-1}|(\overline{\boldsymbol{\nabla} p})^{n+1}|^2 = \rho^n|\boldsymbol{\nabla} p^n|^2$.
  - Correction equation $\dfrac{1}{\delta t}\,\rho^n\,\boldsymbol{u}^{n+1} + \boldsymbol{\nabla} p^{n+1} = \dfrac{1}{\delta t}\,\rho^n\tilde{\boldsymbol{u}}^{n+1} + (\overline{\boldsymbol{\nabla} p})^{n+1}$

  $\rightsquigarrow$ discrete kinetic energy balance:

$$\frac{1}{2}\,\frac{|D_\sigma|}{\delta t}\Big[\rho_\sigma^n|\boldsymbol{u}_\sigma^{n+1}|^2 - \rho_{D_\sigma}^{n_1}|\boldsymbol{u}_\sigma^n|^2\Big] + \frac{1}{2}\sum_{\epsilon=D_\sigma|D_{\sigma'}} F_{\sigma,\epsilon}^n\,\tilde{\boldsymbol{u}}_\sigma^{n+1}\cdot\tilde{\boldsymbol{u}}_{\sigma'}^{n+1}$$

$$+\,|D_\sigma|\,(\boldsymbol{\nabla} p^{n+1})_\sigma\cdot\boldsymbol{u}_\sigma^{n+1} + R_\sigma^{n+1} + \mathcal{P}_\sigma^{n+1} = 0 \text{ with } R_\sigma^{n+1}\geq 0, \qquad \text{(kin.en)}_\sigma$$

From R_σ to R_K

$$R_\sigma = \frac{|D_\sigma|}{\delta t} \rho_{D_\sigma}^{n-1} |\widetilde{\boldsymbol{u}}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2 \to 0 \text{ for regular functions, but NOT for discontinuous functions.}$$

By definition of ρ_{D_σ}, for $\sigma = K|L$,

$$R_\sigma = \frac{|D_{K,\sigma}|}{\delta t} \rho_K^{n-1} \, |\widetilde{\boldsymbol{u}}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2 + \frac{|D_{L,\sigma}|}{\delta t} \rho_L^{n-1} \, |\widetilde{\boldsymbol{u}}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2$$

$$\rightsquigarrow R_K = \frac{1}{2} \sum_{\sigma \subset \partial K} \frac{|D_{K,\sigma}|}{\delta t} \rho_K^{n-1} \, |\widetilde{\boldsymbol{u}}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2$$

$$\Rightarrow \sum_{K \in \mathcal{T}} R_K - \sum_{\sigma \in \mathcal{E}} R_\sigma = 0$$

Passage to the limit: total energy recovered

▷ Kinetic energy

$$(\mathrm{kin})^n_\sigma = \frac{|D_\sigma|}{2\delta t}\big(\varrho^{n+1}_\sigma |\boldsymbol{u}^{n+1}_\sigma|^2 - \varrho^n_\sigma |\boldsymbol{u}^n_\sigma|^2\big) + \frac{1}{2}\sum_{\epsilon = D_\sigma | D_{\sigma'}} F^n_{\sigma,\epsilon}\, \tilde{\boldsymbol{u}}^{n+1}_\sigma \cdot \tilde{\boldsymbol{u}}^{n+1}_{\sigma'} + (\boldsymbol{\nabla} p)^{n+1}_\sigma \cdot \boldsymbol{u}^{n+1}_\sigma = -R^{n+1}_\sigma + \mathcal{P}^{n+1}_\sigma,$$

▷ Internal energy

$$(\mathrm{int})^n_K = \frac{|K|}{\delta t}\big(\rho^{n+1}_K e^{n+1}_K - \rho^n_K e^n_K\big) + \sum_{\sigma \subset \partial K} F^n_{K,\sigma}\, e^n_\sigma + |K|\, p^{n+1}_K\, (\mathrm{div}\, \boldsymbol{u}^{n+1})_K = R^{n+1}_K,$$

▷ φ : test function
Multiply $(\mathrm{kin})_\sigma$ by interpolate φ^n_σ and $(\mathrm{int})_K$ by interpolate φ^n_K

$$\underbrace{\sum_n \sum_{\sigma\in\mathcal{E}} (\mathrm{kin})^n_\sigma \varphi^n_\sigma + \sum_n \sum_{K\in\mathcal{T}} (\mathrm{int})^n_K \varphi^n_K}_{\downarrow} = \underbrace{\sum_n \sum_{K\in\mathcal{T}} \delta t R_K \varphi^n_K - \sum_n \sum_{\sigma\in\mathcal{E}} \delta t R_\sigma \varphi^n_\sigma}_{\downarrow} + \underbrace{\sum_n \sum_{\sigma\in\mathcal{E}} \delta t \mathcal{P}_\sigma \varphi^n_\sigma}_{\downarrow}.$$

$$-\int_0^T\!\!\int_\Omega \Big[\rho\, E\, \partial_t \varphi + (\rho\, E + p)\, u\, \nabla\varphi\Big] \qquad\qquad 0 \qquad\qquad 0$$

$$-\int_\Omega \rho_0(x)\, E_0(x)\, \varphi(x,0)$$

In particular, the pressure terms combine themselves to converge to $-p\boldsymbol{u} \cdot \boldsymbol{\nabla}\varphi$.

Entropy

- Derivation of a discrete entropy inequality

$$\eth_t(\rho s) + \mathrm{div}_d(\rho \boldsymbol{u} s) \leq 0$$

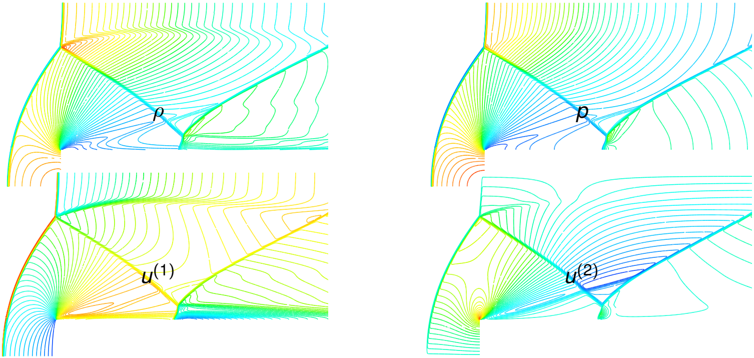
For Euler perfect gas $s = \phi(\rho) + \rho\psi(e)$, $\phi(\rho) = \rho \ln(\rho)$, $\psi(e) = -\frac{1}{\gamma-1}\ln e$.

$$\left| \begin{array}{ll} \eth_t \varrho + \mathrm{div}_d(\rho \boldsymbol{u}) = 0 & \times\ \phi'(\rho) = 1 + \ln \varrho,\ \ \phi'' \geq 0 \\ \eth_t(\varrho e) + \mathrm{div}_d(\varrho \boldsymbol{u} e) + p\, \mathrm{div}_d \boldsymbol{u} = R & \times\ \psi'(e) = -\dfrac{1}{(\gamma-1)e}, \psi'' \geq 0 \end{array} \right.$$

$$\rightsquigarrow \left| \begin{array}{l} \eth_t(\phi(\varrho)) + \mathrm{div}_d(\phi(\varrho)\boldsymbol{u}) + \underbrace{(\varrho\,\phi'(\varrho) - \phi(\varrho))}_{=\varrho} \mathrm{div}_d \boldsymbol{u} + r_\rho = 0 \\ \eth_t(\varrho\psi(e)) + \mathrm{div}_d(\varrho \boldsymbol{u}\psi(e)) + \underbrace{\psi'(e)p}_{=-\varrho}\, \mathrm{div}_d \boldsymbol{u} + r_e = \underbrace{\psi'(e)R}_{\leq 0} \\ \hline \eth_t(\varrho s) + \mathrm{div}_d(\varrho \boldsymbol{u} s) + \underbrace{\Big[\varrho\,\phi'(\varrho) - \phi(\varrho) + \psi'(e)p\Big]}_{=0} \mathrm{div}_d \boldsymbol{u} \leq -r_\rho - r_e. \end{array} \right.$$

- If $r_\rho \geq 0$ and $r_e \geq 0 \rightsquigarrow$ discrete entropy estimates: : implicit upwind scheme
- If $r_\rho + r_e \geq r \to 0 \rightsquigarrow$ limit entropy estimates: explicit upwind scheme

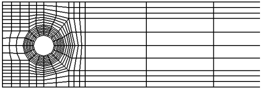
Numerical tests - I Euler, high Mach



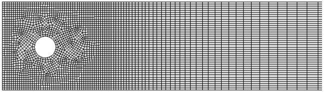
Mach 3 facing step (Woodward Collela)
MAC space discretization, 1200 $\times$ 400 uniform grid, $\delta t = h/4 = 0.001$, ($u_1 + c = 4$ at the inlet boundary).

Numerical tests - II Flow past cylinder, low Mach

Flow past a cylinder, benchmark Schäfer and S. Turek, Mach $\simeq 0.003$, $Re \simeq 100$.
Pressure correction scheme, Rannacher-Turek FE.



coarse mesh



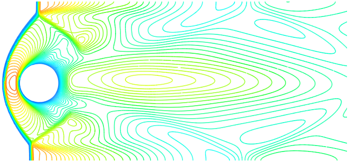
fine mesh

Mesh	Space unks	$c_{d,max}$	$c_{l,max}$	St
m2	64840	3.4937	0.9141	0.2850
m3	215545	3.2887	0.9891	**0.2955**
m4	381119	3.2614	**1.0062**	**0.2972**
m5	531301	**3.2365**	**1.0148**	**0.2976**
Reference range		3.22 − 3.24	0.99 − 1.01	0.295 − 0.305

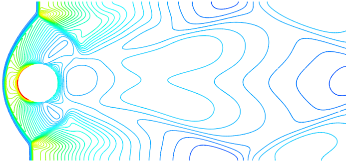
Table: Drag and lift coefficients and Strouhal number.

Numerical tests - II Flow past cylinder, high Mach

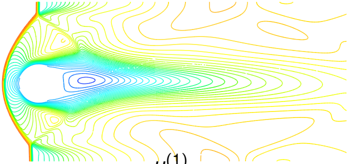
Flow past a cylinder, Mach $\simeq 3$, $Re \simeq 100$.
$p_{\text{ext}} = \gamma/10\,\rho$, $c = 0.1$.
$\text{mes} = 10^{-3}$.
impermeability and and perfect slip condition at the upper and lower boundaries
$\boldsymbol{u} = (1,0)^t$. at inlet.
$\delta t = 10^{-4}$. Rannacher-Turek FE.



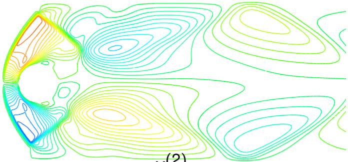
ρ



p



$u^{(1)}$



$u^{(2)}$

$t = 5$, mesh of 10^6

Summary: main features of the class of schemes

- Discretization of the internal equation
- Upwind choice for ρ, $\rightsquigarrow$ positivity of the density,
- Compatible discretization of (mass) and (mom)
  & careful choice of ρ_{D_σ} and fluxes in (mom) to recover a mass conservation on the dual cells
  $\rightsquigarrow$ discrete kinetic energy inequality
- Compatible discretization of (mass) and (int.en) & upwind choice for e_K under CFL
  $\rightsquigarrow$ positivity of e
- Conservation of total mass
- Existence of a solution to the scheme (topological degree argument)
- Velocity and pressure are constant through the contact discontinuity: p^n and $\boldsymbol{u}^n$ constant $\Rightarrow$ p^{n+1} and $\boldsymbol{u}^{n+1}$ constant.
- Lax-consistency : under compactness assumptions, the discrete solution tends to a weak solution of the Euler systems.
- Numerical discontinuous solutions have correct shocks.

Recent and on going work

- Higher order scheme for the MUSCL-type and additional viscosity.

- Low Mach limit for barotropic NS and Euler (with K. Saleh).
- Analysis of the MAC scheme in primitive variables for variable density incompressible flows (with K. Mallem)
- Convergence for barotropic NS ($\gamma \geq 3$) and strong-weak error estimates for barotropic NS (with D. Maltese, and A. Novotny).
- Reactive flows (D. Grapsas).
- Shallow water equations (H.P. Gunawan, Y. Nasseri)