Staggered schemes for compressible flows

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Outline

Context and objectives

Long time collaboration with IRSN (Institut de Radioprotection et Sûreté Nucléaire)

- **General context: nuclear safety**
  $\rightsquigarrow$ Numerical simulation of incompressible and compressible flows

- Derive a scheme for the compressible Euler (or Navier-Stokes) equations that is
  - stable and precise for all Mach number
  - computationally efficient
    CALIF^{3}S: `https://gforge.irsn.fr/gf/project/califs`

- **Theoretical proofs** of stability, weak consistency... if available

Main features of the schemes

- All Mach scheme ?
  $\rightsquigarrow$ Implicit or semi-implicit (rather than completely segregated) schemes
  $\rightsquigarrow$ staggered (rather than colocated) grids

- Internal energy balance formulation (rather than total energy formulation) even in the presence of shocks
  - easier to deal with on staggered grids
  - $\rightsquigarrow e > 0$

- 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.

The Euler equations: total energy vs. internal energy

- Compressible Euler equations:

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

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

$$\partial_t(\varrho E) + \mathrm{div}\big[(\varrho E + p)\boldsymbol{u}\big] = 0, \qquad \text{(tot.en)}$$

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

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

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

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

$$\partial_t(\varrho e) + \mathrm{div}(\varrho e \boldsymbol{u}) + p\,\mathrm{div}\boldsymbol{u} = 0, \qquad \text{(int.en)}$$

  which implies $e \geq 0$.

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

Importance of 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

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

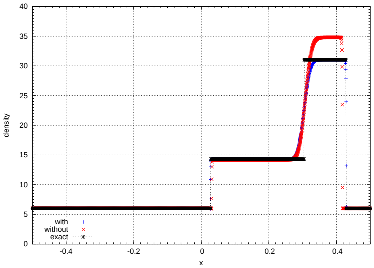
  is discontinuous along a line $x = \sigma t$ then

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

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

The internal energy equation is not conservative

- Dealing with the internal energy:
  - ♯ positive internal energy
  - ♯ convenient for incompressible problems
  - ♭ ρe is not a conservative variable – conservative 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...

Outline

Right and wrong shock speed for Burgers

Burgers equation: for regular positive solutions

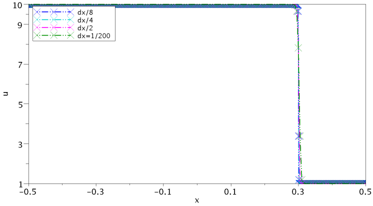
$$(\mathrm{B}) : \partial_t u + \partial_x (u^2) = 0 \iff (\mathrm{BS}) : \partial_t u^2 + \frac{4}{3}\partial_x u^3 = 0.$$

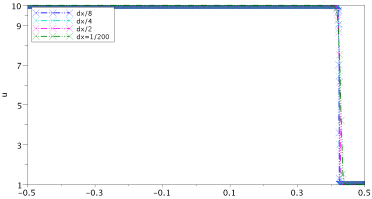
No longer true with irregular solutions:

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) (top) and (BS) (bottom) 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:

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

- Multiply by $2u$:

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

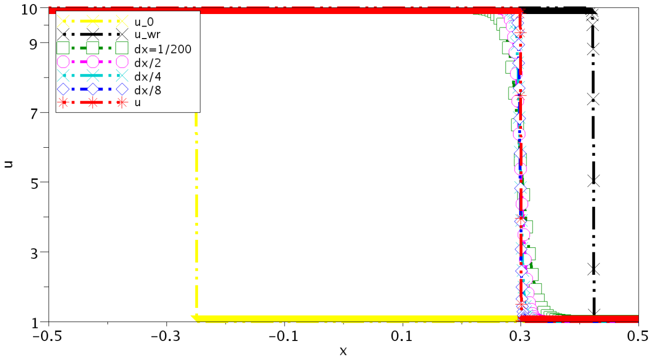
- Discretize $(\text{BS})_\varepsilon$ instead of (BS):

$$\partial_t(u^2) + \frac{4}{3}\partial_x(u^3) - h\varepsilon_0 u\partial_{xx} u = 0, \quad (\text{BS})_\varepsilon \text{ with } 2\varepsilon = h\varepsilon_0.$$

- Centered finite volume with non conservative diffusion

$$(u_i^{(n)})^2 = (u_i^{(n-1)})^2 + \frac{4\delta t}{3h}\left[\left(\frac{u_{i-1}^{(n-1)} + u_i^{(n-1)}}{2}\right)^3 - \left(\frac{u_i^{(n-1)} + u_{i+1}^{(n-1)}}{2}\right)^3\right]$$
$$+ \frac{\delta t}{h^2}\,\varepsilon_0 h\, u_i^{(n-1)}\left[2u_i^{(n-1)} - u_{i-1}^{(n-1)} - u_{i+1}^{(n-1)}\right].$$

Non conservative numerical diffusion on (BS)



Centered Scheme for $(BS)_{\varepsilon_0 h}$

yellow:	initial condition
black:	upwind scheme on (BS)
other colors:	centered scheme with non conservative diffusion on (BS)

Outline

From Burgers to Euler

For regular solutions,

Burgers:

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

Euler:

$$\left\{\begin{aligned} &\partial_t \varrho + \mathrm{div}(\varrho \boldsymbol{u}) = 0, \\ &\partial_t(\varrho \boldsymbol{u}) + \mathrm{div}(\varrho \boldsymbol{u} \otimes \boldsymbol{u}) + \boldsymbol{\nabla} p = 0, \\ &\partial_t(\varrho E) + \mathrm{div}\big[(\varrho E + p)\boldsymbol{u}\big] = 0. \end{aligned}\right. \iff \left\{\begin{aligned} &\partial_t \varrho + \mathrm{div}(\varrho \boldsymbol{u}) = 0, \\ &\partial_t(\varrho \boldsymbol{u}) + \mathrm{div}(\varrho \boldsymbol{u} \otimes \boldsymbol{u}) + \boldsymbol{\nabla} p = 0, \\ &\partial_t(\varrho e) + \mathrm{div}(\varrho e \boldsymbol{u}) + p\,\mathrm{div}\boldsymbol{u} = 0. \end{aligned}\right.$$

- we had an equation, we now have a system...
- Idea: add a non conservative corrective term to the internal energy equation.
- Which term ? Inspiration comes from copying the formal derivation of the internal energy equation at the discrete level.

Euler equations: total energy = kinetic energy + internal energy

- kinetic energy equation: From mass balance, for "regular" z:

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

$$\Longrightarrow \frac{1}{2}\partial_t(\rho u_i^2) + \frac{1}{2}\operatorname{div}(\rho u_i^2 \boldsymbol{u}) = \rho \partial_t(u_i^2) + \rho \boldsymbol{u} \cdot \nabla(u_i^2)$$

$$= \rho u_i \partial_t u_i + \rho u_i \boldsymbol{u} \cdot \nabla u_i$$

$$= u_i \left[\rho \partial_t u_i + \rho \boldsymbol{u} \cdot \nabla u_i\right] + u_i \underbrace{(\partial_t \varrho + \operatorname{div}(\varrho \boldsymbol{u}))}_{=0}$$

$$= \partial_t(\rho u_i) + \operatorname{div}(\rho u_i \boldsymbol{u}) = -u_i\, \partial_i p, \text{ from momentum balance.}$$

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

- Total energy (Euler):

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

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

- Internal energy

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

- Discrete Euler equations solving the internal energy balance

$$\begin{aligned} &\eth_t \varrho + \mathrm{div}_d(\varrho \boldsymbol{u}) = 0, && (\mathrm{mass})_d \\ &\eth_t(\varrho \boldsymbol{u}) + \mathrm{div}_d(\varrho \boldsymbol{u} \otimes \boldsymbol{u}) + \boldsymbol{\nabla}_d p = 0, && (\mathrm{mom})_d \\ &\eth_t(\varrho e) + \mathrm{div}_d(\varrho e \boldsymbol{u}) + p\, \mathrm{div}_d \boldsymbol{u} = {\color{red}?}, && (\mathrm{int.en})_d \\ &p = (\gamma - 1)\, \varrho e. \end{aligned}$$

- Mimick the continuous computation for the kinetic energy

- Discrete kinetic energy

  $(\mathrm{mom})_d$ and $(\mathrm{mass})_d \rightsquigarrow (\mathrm{kin})_d$ equation

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

${\color{red}R}$: non conservative residual term, ${\color{red}R \geq 0}$.

- Correct the discrete internal energy equation: $\eth_t(\rho e) + \mathrm{div}_d(e\boldsymbol{u}) + p\mathrm{div}_d \boldsymbol{u} = {\color{red}R}$

${\color{blue}(\mathrm{int.en})_d}$ + ${\color{green}(\mathrm{kin.en})_d}$ = $(\mathrm{tot.en})_d$? not exactly... (because of staggered grids)

But

- $\int_\Omega {\color{blue}(\mathrm{int.en})_d} + \int_\Omega {\color{green}(\mathrm{kin.en})_d} = (\mathrm{tot.en})_d$

- at the limit $\delta t \to 0$, $h \to 0$, the weak form of the total energy equation is recovered (under strong compactness.

Outline

Required discrete properties

- 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).

- Several possible schemes, segregated explicit, implicit, semi-implicit
- AP scheme : implicit or semi-implicit choice.

Time discretization: implicit or semi-implicit choice

Implicit

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

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

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

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

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 $\tilde{\boldsymbol{u}}^{n+1}$:

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

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

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

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

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

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

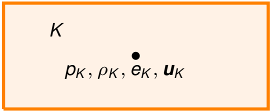
Meshes

Colocated

- Advantages

  Easier Data structure, easily refined

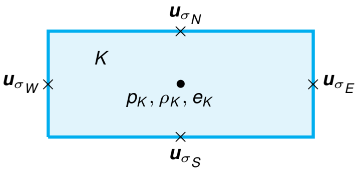
  Total energy easy to define
- Pressure correction scheme studied for the Euler equations (C. Zaza's thesis).
- Drawback: No native inf-sup condition



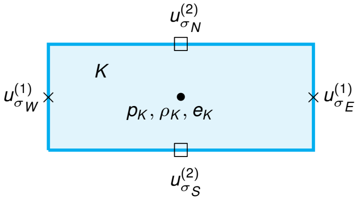
Staggered:

- 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 $\forall p \in P, \int p = 0, \exists \boldsymbol{v} \in V \; : \int p \,\mathrm{div}\boldsymbol{v} \geq \beta \|p\|_{L^2} \|\boldsymbol{v}|_{H^1_d}$
- Drawback: Total energy difficult to compute



Rannacher-Turek unknowns



MAC unknowns, Arakawa C-grid

Space discretization: Finite volume discretization of the mass equation

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

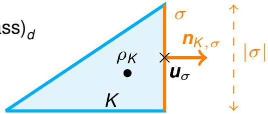
- $\displaystyle\int_K$ (mass) $\rightsquigarrow$

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

- discretization of the fluxes:

$$\frac{|K|}{\delta t}\,(\rho_K^{n+1} - \rho_K^n) + \sum_{\sigma \in \mathcal{E}(K)} F_{K,\sigma}^{n+1} = 0, \qquad (\text{mass})_d$$

$F_{K,\sigma}^{n+1} = |\sigma|\ \rho_\sigma^{n+1}\, \boldsymbol{u}_\sigma^{n+1} \cdot \mathbf{n}_{K,\sigma}$,
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)

Discretization of the momentum equation

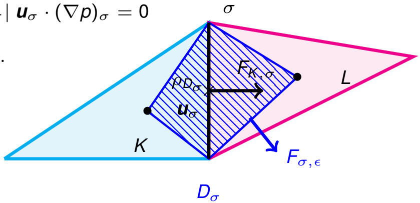
Implicit scheme

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

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

$$\underbrace{\frac{|D_\sigma|}{\delta t}(\rho_{D_\sigma}^{n+1}\,\boldsymbol{u}_\sigma^{n+1} - \rho_{D_\sigma}^{n}\,\boldsymbol{u}_\sigma^{n}) + \sum_{\epsilon\in\mathcal{E}(D_\sigma)} F_{\sigma,\epsilon}^{n+1}\,\boldsymbol{u}_\epsilon^{n+1}}_{\mathcal{C}_d^{n+1}(\rho,\boldsymbol{u})} + |D_\sigma|(\nabla p^{n+1})_\sigma = 0.$$

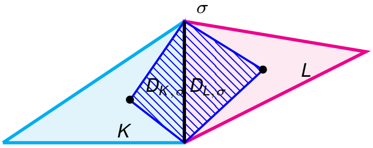
- Grad-div duality : $\sum_{K\in\mathcal{T}} |K|\, p_K\, (\mathrm{div}\boldsymbol{u})_K + \sum_{\sigma\in\mathcal{E}} |D_\sigma|\, \boldsymbol{u}_\sigma \cdot (\nabla p)_\sigma = 0$
  $\rightsquigarrow |D_\sigma|(\nabla p^n)_\sigma = |\sigma|\,(p_L^n - p_K^n)\,\boldsymbol{n}_{K,\sigma}, \sigma = K|L.$



- $\rho_{D_\sigma}^{n+1}$? $F_{\sigma,\epsilon}^{n+1}$?

Discretization of the convection operator

- Choose $\rho^n_{D_\sigma}$, $\rho^{n+1}_{D_\sigma}$ and $F^{n+1}_{\sigma,\epsilon}$ in $\mathcal{C}^{n+1}_d(\rho, \boldsymbol{u})$ so as to obtain a discrete kinetic energy balance.
- Copy the continuous kinetic energy balance: (mom) $\cdot\boldsymbol{u}$ & (mass) $\rightsquigarrow$ (kin.en)
- Same at the discrete level requires compatible mass and momentum equations



$D_\sigma = D_{K,\sigma} \cup D_{L,\sigma}$

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

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

Choose

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

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

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

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

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 $\boldsymbol{u}_\sigma^{n+1}$:

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

... with some algebra, using $\dfrac{|D_\sigma|}{\delta t}\, (\rho_{D_\sigma}^{n+1} - \rho_\sigma^n) + \displaystyle\sum_{\epsilon \in \mathcal{E}(D_\sigma)} F_{\sigma,\epsilon}^{n+1} = 0.$

$\rightsquigarrow$ discrete kinetic energy balance:

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

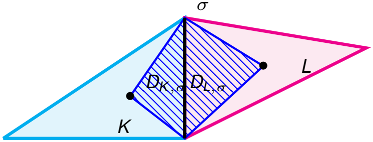
$$+\, |D_\sigma|\, (\boldsymbol{\nabla} p^{n+1})_\sigma \cdot \boldsymbol{u}_\sigma^{n+1} + R_\sigma^{n+1} = 0 \text{ with } R_\sigma^{n+1} \geq 0, \qquad \text{(kin.en)}_\sigma$$

From R_σ to R_K

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

Redistribution of R_σ on the primal cells.

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



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

$$\rightsquigarrow R_K^{n+1} = \frac{1}{2} \sum_{\sigma \in \mathcal{E}(K)} \frac{|D_{K,\sigma}|}{\delta t} \rho_K^n \, |\boldsymbol{u}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2$$

$$\Rightarrow \sum_{K \in \mathcal{T}} R_K^{n+1} - \sum_{\sigma \in \mathcal{E}} R_\sigma^{n+1} = 0$$

Discrete internal energy equation and E.O.S.

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

- Discretization by upwind finite volume of the discrete internal energy

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

  - e_σ^{n+1} upwind choice $\rightsquigarrow$ positivity of e (since $R_K^{n+1} \geq 0$ and $p_K = 0$ if $e_K \leq 0$.)
  - $|K|\,(\mathrm{div}\boldsymbol{u})_K = \sum_{\sigma\in\mathcal{E}(K)} |\sigma|\; u_\sigma \cdot \mathbf{n}_{K,\sigma}$.

- discrete E.O.S.

$$p_K^{n+1} = \begin{cases} (\gamma-1)\rho_K^{n+1}\, e_K^{n+1}. \text{ if } e_K > 0 \\ 0 \text{ otherwise.} \end{cases} \qquad (\mathrm{eos})_d$$

Outline

Discrete entropy inequality

- Derivation of a discrete entropy inequality

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

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

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

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

- 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

Outline

Weak consistency theorems

- **[Godunov, Math. Sbornik 1959]**
  Godunov's scheme for barotropic Euler equations on a uniform 1D mesh:

  If with the diminishing mesh size the difference solution converges,

  then it converges to the generalized solution of the differential equation.

- **[Lax and Wendroff, Comm. pure appl. math. 1960]** Consider a numerical scheme for a system of nonlinear (hyperbolic) conservation laws on a uniform 1D mesh ;

  if the scheme is conservative, with consistent fluxes, and converges boundedly almost everywhere towards a limit as δt and h tend to 0,

  then this limit is necessarily a weak solution of the system.

- 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., $\forall \varphi \in C_c^1(\mathbb{R} \times \mathbb{R}_+, \mathbb{R})$,

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

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

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

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

Lax Wendroff analysis: total energy recovered

▷ Kinetic energy

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

▷ Internal energy

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

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

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

$$-\int_0^T\!\!\int_\Omega\left[\rho\,E\,\partial_t\varphi + (\rho\,E + p)\,u\,\nabla\varphi\right] - \int_\Omega \rho_0(x)\,E_0(x)\,\varphi(x,0) \quad = \quad 0$$

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

Same kind of computation on the discrete entropy inequality $\rightsquigarrow$ weak entropy solution.

Outline

A limited centered scheme

Higher order on the convective fluxes: modification of the semi-implicit scheme

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

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

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

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

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

Upwind choice:
$\mathrm{div}_K(\rho^n\,\boldsymbol{u}^{n+1}) = \sum_{\sigma\in\mathcal{E}(K)} F^n_{K,\sigma}$ with $F^n_{K,\sigma} = |\sigma|(\rho^n_K(\boldsymbol{u}_\sigma \cdot \boldsymbol{n}_{K,\sigma})^+ - \rho^n_L(\boldsymbol{u}_\sigma \cdot \boldsymbol{n}_{K,\sigma})^-)$.

$$\rho_K^{n+1} = \left(1 - \frac{\delta t}{|K|}\sum_{\sigma\in\mathcal{E}(K)} |\sigma|\, u^+_{K,\sigma}\right)\rho_K + \frac{\delta t}{|K|}\sum_{\sigma\in\mathcal{E}(K)} |\sigma|\, u^-_{K,\sigma}(\rho^n_L);$$

$$\rightsquigarrow \min \rho^n_K \leq \rho^{n+1}_K \leq \max \rho^n_K.$$

A limited centered scheme

Start from a centered scheme: $\widetilde{\rho}^n_\sigma$ second order approximation of ρ on σ

$$\mathrm{div}_d(\rho^n\, \boldsymbol{u}^{n+1}) = \sum_K F^n_{K,\sigma} \text{ with } F^n_{K,\sigma} = |\sigma|(\widetilde{\rho}^n_\sigma \underbrace{(\boldsymbol{u}_\sigma \cdot \boldsymbol{n}_{K,\sigma})}_{u_{K,\sigma}}{}^+ - \widetilde{\rho}^n_\sigma (\boldsymbol{u}_\sigma \cdot \boldsymbol{n}_{K,\sigma})^-).$$

$\rightsquigarrow$ physical bounds may be not respected

Find ρ^n_σ, limitation of $\widetilde{\rho}^n_\sigma$ so as to keep the bounds on ρ;
For $\sigma = K|L$, $\rho^n_\sigma = \rho^n_K + \rho^n_\sigma - \rho^n_K$ and $\rho^n_\sigma = \rho^n_L + \rho^n_\sigma - \rho^n_L \rightsquigarrow$

$$\mathrm{div}_d(\rho^n\, \boldsymbol{u}^{n+1}) = \sum_K F^n_{K,\sigma} \text{ with } F^n_{K,\sigma} = |\sigma|(\rho^n_K + \rho^n_\sigma - \rho^n_K)(u_{K,\sigma})^+ - (\rho^n_L + \rho^n_\sigma - \rho^n_L)(u_{K,\sigma})^-).$$

$$\rho^{n+1}_K = \left(1 - \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| u^+_{K,\sigma}\right) \rho_K - \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| u^+_{K,\sigma} (\rho^n_\sigma - \rho^n_K)$$
$$+ \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| u^-_{K,\sigma} \rho^n_L + \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| u^-_{K,\sigma} (\rho^n_\sigma - \rho^n_L);$$

Conditions for physical bounds

For a given σ, K^+, (K^-): upwind (downwind) cell to σ, $u_{K^+,\sigma} \geq 0$, $(u_{K^-,\sigma} \leq 0)$
suppose $\exists \alpha_\sigma, \beta_\sigma \in [0,1]$ and $M_\sigma^n \neq K^+$, neighbour of K ;

$$\rho_\sigma^n - \rho_{K^+}^n = \alpha_\sigma^\rho(\rho_{K^+}^n - \rho_{M_\sigma^n}^n), \qquad \text{limit-M}$$

$$\rho_\sigma^n - \rho_{K^-}^n = \beta_\sigma^\rho(\rho_{K^-}^n - \rho_{K^-}^n). \qquad \text{limit-L}$$

$\rightsquigarrow$

$$\rho_K^{n+1} = \underbrace{\left(1 - \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| u_{K,\sigma}^+ (1+\alpha_\sigma^\rho)\right)}_{\geq 0 \text{ under CFL}} \rho_K^n + \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} \underbrace{|\sigma| u_{K,\sigma}^+ \alpha_\sigma^\rho}_{\geq 0} \rho_{M_\sigma}^n$$

$$+ \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} \underbrace{|\sigma| u_{K,\sigma}^- (1-\beta_\sigma^\rho)}_{\geq 0} \rho_L^n + \frac{\delta t}{|K|} \sum_{\sigma \in \mathcal{E}(K)} \underbrace{|\sigma| u_{K,\sigma}^- \beta_\sigma^\rho}_{\geq 0} \rho_L^n.$$

$$\forall K \in \mathcal{T}, \qquad \delta t \leq \frac{|K|}{2 \sum_{\sigma \in \mathcal{E}(K)} |\sigma| |u_{K,\sigma}^{n+1}|}. \qquad \text{CFL}$$

Algorithm for the limitation

For $\sigma = K|L \in \mathcal{E}$, $\tilde{\rho}_\sigma$: second order approximation by linear combination of ρ_K, ρ_L and neighbours of K and L.

- Limit $\tilde{\rho}_\sigma$ to enforce the condition (limit-M).

  $\mathcal{J}_K$: set of neighbours M of K such that $\rho_K - \rho_M \neq 0$ sign($\rho_K - \rho_M$) = sign ($\tilde{\rho}_\sigma - \rho_K$). - If $\mathcal{J}_K = \emptyset$ then $\bar{\rho}_\sigma = \rho_K$ (upwind choice). - Otherwise, choose $M_\sigma \in \mathcal{J}_K$ such that $|\rho_K - \rho_{M_\sigma}| = \max\{|\rho_K - \rho_M|, M \in \mathcal{J}_K\}$, compute $\alpha = \min\left(1, \dfrac{\tilde{\rho}_\sigma - \rho_K}{\rho_K - \rho_{M_\sigma}}\right)$, and set

  $$\bar{\rho}_\sigma = \rho_K + \alpha_{K,\sigma}(\rho_K - \rho_{M_\sigma}).$$

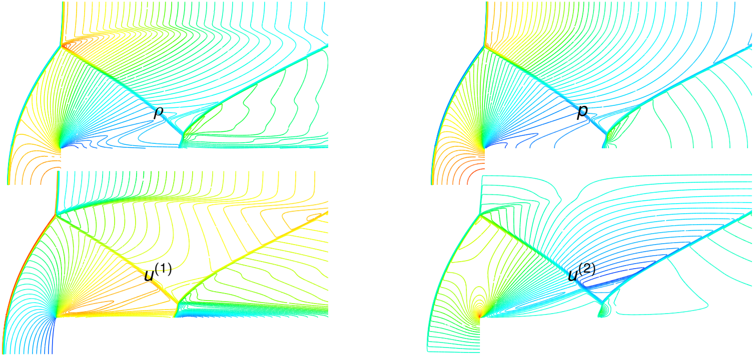
  The value $\bar{\rho}_\sigma$ satisfies the condition (limit-M).

- Limit $\bar{\rho}_\sigma$ to obtain a value ρ_σ satisfying (limit-L) :
  - If $\bar{\rho}_\sigma - \rho_K$ and $\rho_L - \rho_K$ do not have the same sign, set $\rho_\sigma = \rho_K$ (upwind choice).
  - Otherwise,

    - if $|\bar{\rho}_\sigma - \rho_K| \geq |\rho_L - \rho_K|$, we set $\rho_\sigma = \rho_L$,
    - else we set $\rho_\sigma = \bar{\rho}_\sigma$.

Outline

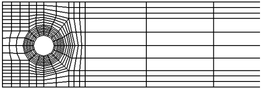
Numerical tests - I Euler, high Mach



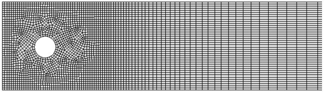
Mach 3 facing step (Woodward Collela)
MAC space discretization, 1200×400 uniform grid, $\delta t = h/4 = 0.001$, $(u_1 + c = 4$ at the inlet boundary).

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



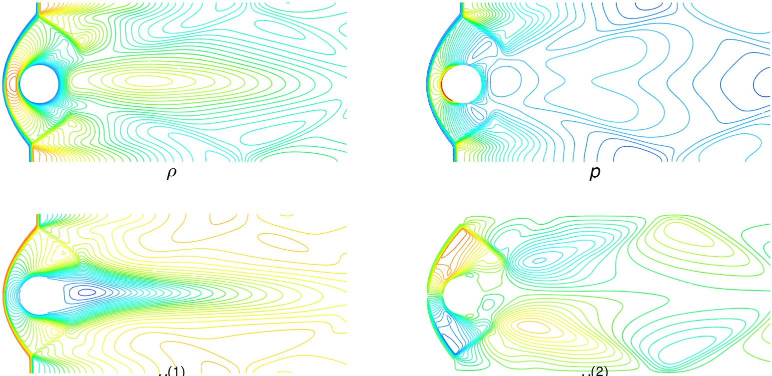
fine mesh

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 $\simeq 3$, $Re \simeq 100$.
$p_{\rm ext} = \gamma/10\,\rho$, $c = 0.1$.
$\text{mes} = 10^{-3}$.
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