Schémas implicites ou explicites sur mailles décalées pour Euler et Navier-Stokes compressible

R. Herbin[⋆],

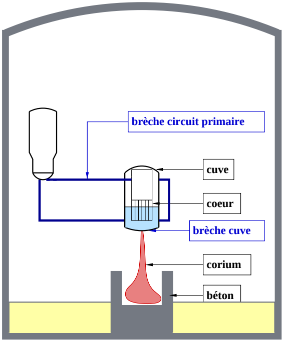
with

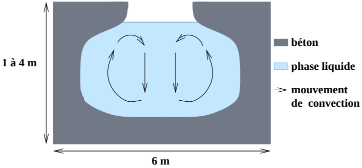
T. Gallouët[⋆], L. Gastaldo[†], W. Kheriji[⋆†], J.-C. Latché[†], T.T. Nguyen[⋆†]

⋆ Université de Provence

† Institut de Radioprotection et de Sûreté Nucléaire (IRSN)

Context





▷ **General context: nuclear safety**
Examples: Accident in a nuclear reactor, following loss of coolant.
Interaction corium–concrete $\rightarrow$ two phase flow

Numerical simulation of compressible flows
numerical code: ISIS, developed at IRSN

▷ **Aim : obtain efficient schemes**

- stable and precise for all Mach number
- sufficiently decoupled so that the numerical solution is not too difficult.

▷ **Theoretical proof** of stability, confirmed by numerical tests. Proof of convergence for “toy problem” (Stokes with EOS $p = \rho^{\gamma}$)

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- **Equations, objectives**

  Space discretization of the fully implicit scheme for NS

  A detour by Burgers... to deal with the internal energy for Euler

  An explicit scheme

  Perspectives

Navier-Stokes and Euler equations...and "derived" forms

- Euler (Navier-Stokes) equations:

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

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

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

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

$\boldsymbol{\tau}$: stress tensor

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

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

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

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

which implies $e \geq 0$.

Fractional time–stepping scheme

- Decoupled scheme: $\rightsquigarrow$ fractional time step methods.
  - Classical for incompressible flows (pressure correction, Chorin 68, Temam 69), (Guermond 06) for a synthesis.
  - Also developed for compressible flows, with either colocated or staggered unknowns..
- Incompressible NS equations

$$\begin{aligned} &\mathrm{div}(\boldsymbol{u}) = 0, && \text{(mass)} \\ &\partial_t \boldsymbol{u} + \mathrm{div}(\boldsymbol{u} \otimes \boldsymbol{u}) - \mathrm{div}\boldsymbol{\tau} + \boldsymbol{\nabla} p = 0, && \text{(mom)} \end{aligned}$$

  - Pressure correction scheme

Prediction step: $$\frac{1}{\delta t}(\boldsymbol{u}^{n+\frac{1}{2}} - \boldsymbol{u}^n) + \mathrm{div}(\boldsymbol{u}^{n+\frac{1}{2}} \otimes \boldsymbol{u}^n) - \mathrm{div}\boldsymbol{\tau}(\boldsymbol{u}^{n+\frac{1}{2}}) + \boldsymbol{\nabla} p^n = 0,$$

Correction step: $$\left| \begin{aligned} &\frac{1}{\delta t}(\boldsymbol{u}^{n+1} - \boldsymbol{u}^{n+\frac{1}{2}}) + \boldsymbol{\nabla}(p^{n+1} - p^n) = 0, \\ &\mathrm{div}(\boldsymbol{u}^{n+1}) = 0, \end{aligned} \right.$$

Fractional time–stepping scheme

- Compressible NS equations

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

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

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

$$p = \wp(\varrho, e) = (\gamma - 1)\, \varrho e,$$

Fractional time stepping scheme

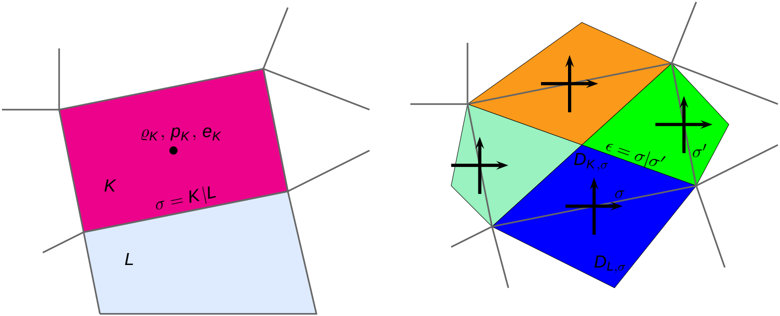
Prediction step:

$$\frac{1}{\delta t}(\varrho^n \boldsymbol{u}^{n+\frac{1}{2}} - \varrho^{n-1}\boldsymbol{u}^n) + \mathrm{div}(\varrho^n \boldsymbol{u}^{n+\frac{1}{2}} \otimes \boldsymbol{u}^n) - \mathrm{div}\boldsymbol{\tau}(\boldsymbol{u}^{n+\frac{1}{2}}) + \boldsymbol{\nabla} p^n = 0,$$

Correction step:

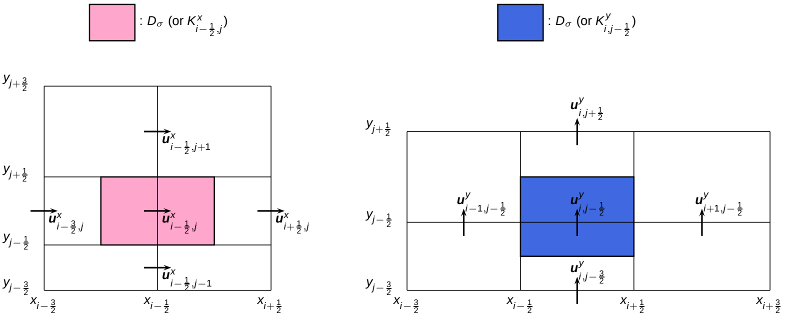
$$\left|\begin{array}{l}
\dfrac{\varrho^n}{\delta t}(\boldsymbol{u}^{n+1} - \boldsymbol{u}^{n+\frac{1}{2}}) + \boldsymbol{\nabla}(p^{n+1} - p^n) = 0, \\
\dfrac{1}{\delta t}(\varrho^{n+1} - \varrho^n) + \mathrm{div}(\varrho^{n+1}\boldsymbol{u}^{n+1}) = 0, \\
\dfrac{1}{\delta t}(\varrho^{n+1}e^{n+1} - \varrho^n e^n) + \mathrm{div}(\varrho e^{n+1}\boldsymbol{u}^{n+1}) + p^{n+1}\, \mathrm{div}\boldsymbol{u}^{n+1} = \\
\qquad\qquad \boldsymbol{\tau}(\tilde{\boldsymbol{u}}) : \boldsymbol{\nabla}\tilde{\boldsymbol{u}} + \mathcal{S}, \\
p^{n+1} = \wp(\varrho^{n+1}, e^{n+1}) = (\gamma - 1)\, \varrho^{n+1} e^{n+1}.
\end{array}\right.$$

Staggered discretization



- Primal mesh : $\mathcal{M}$ = { set of control volumes $K, L, M\ldots$ }.
  Scalar variables defined at cell centers: $(p_K)_{K\in\mathcal{M}}, (\varrho_K)_{K\in\mathcal{M}}, (e_K)_{K\in\mathcal{M}}, \ldots$
- Velocity components defined at the edges : $(v_\sigma)_{\sigma\in\mathcal{F}}$.
  Dual mesh(es) : $\mathcal{M}^* = (D_\sigma)_{\sigma\in\mathcal{F}}$.
  Normal velocity to the face σ denoted by $\boldsymbol{v}_\sigma \cdot \boldsymbol{n}_\sigma$.

The MAC mesh



The dual mesh for the MAC scheme, x and y-component of the velocity.

Summary of the objectives

Derive a scheme for Euler (or Navier-Stokes) equations which is a natural extension of an existing scheme for incompressible flows:

- staggered discretization $\rightsquigarrow$ inf-sup or LBB condition,
- upwinding with respect to the material velocity $\rightsquigarrow$ positivity of the density,
- solution of the internal energy balance :
  - easier to discretize that total energy (because of staggered grid)
  - $\rightsquigarrow$ positivity of the internal energy,
- pressure correction scheme
  - $\rightsquigarrow$ industrial scheme.
    ISIS: `https://gforge.irsn.fr/gf/project/isis`
    PELICANS: `https://gforge.irsn.fr/gf/project/pelicans`
  - implicit scheme for the (relative) simplicity of exposition
  - explicit variant for the Euler equations

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Finite volume discretization of the mass equation

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

- $\displaystyle\int_K$ (mass) $\rightsquigarrow$ + implicit time discretization $\rightsquigarrow$

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

- discretization of the fluxes:

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

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

FV-FE discretization of the momentum equation

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

- $\displaystyle\int_{D_\sigma}$ (mom) + implicit time discretization $\rightsquigarrow$

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

- Space discretization

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

- $\displaystyle |D_\sigma|(\boldsymbol{\nabla} p^{n+1})_\sigma = -\sum_{M\in\mathcal{M}}\int_M p^{n+1}\,\mathrm{div}\boldsymbol{\varphi}_\sigma\,\mathrm{d}\boldsymbol{x} = |\sigma|\,(p^{n+1}_L-p^{n+1}_K)\,\boldsymbol{n}_{K,\sigma},$
- $\displaystyle |D_\sigma|(\mathrm{div}\tau(\boldsymbol{u}^{n+1}))_\sigma = -\mu\sum_{K\in\mathcal{M}}\int_K\nabla\boldsymbol{u}^{n+1}\cdot\nabla\boldsymbol{\varphi}_\sigma-\frac{\mu}{3}\sum_{K\in\mathcal{M}}\int_K\mathrm{div}\,\boldsymbol{u}^{n+1}\,\mathrm{div}\,\boldsymbol{\varphi}_\sigma.$
- $\boldsymbol{\varphi}_\sigma$ finite element shape function associated to the edge σ..

Discretization of the convection operator

- Choice of ${\rho D_\sigma}^{n+1}$ and $F_{\sigma,\epsilon}^{n+1}$ in $\mathcal{C}_d(\rho^{n+1}, \boldsymbol{u}^{n+1})$?
- Discretize $\mathcal{C}_d(\rho^{n+1}, \boldsymbol{u}^{n+1})$ 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 $\partial_t \rho + \operatorname{div}(\rho\, \boldsymbol{u}) = 0$.

- 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***

Choosing

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

we get

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

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

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

Continuous and discrete kinetic energy balance

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

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

$\rightsquigarrow$ continuous kinetic energy balance:

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

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

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

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

$\rightsquigarrow$ discrete kinetic energy balance:

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

$$- |D_\sigma|(\mathrm{div}\tau(\boldsymbol{u}^{n+1}))_\sigma\,\boldsymbol{u}_\sigma^{n+1} + R_\sigma^{n+1} = 0 \text{ with } R_\sigma^{n+1} \geq 0, \qquad \text{(kin.en)}_\sigma$$

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

Discrete internal energy equation and E.O.S.

- Discretization by upwind finite volume of the discrete internal energy

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

$$+ |K| p_K^{n+1} (\operatorname{div}(\boldsymbol{u}^{n+1}))_K = |K| \left(\boldsymbol{\tau}(\boldsymbol{u}^{n+1}) : \boldsymbol{\nabla} \boldsymbol{u}^{n+1}\right)_K, \qquad (\text{int.en})_d$$

with e_σ^{n+1} upwind choice $\rightsquigarrow$ positivty of e.
$K|\,(\operatorname{div}\boldsymbol{u})_K = \sum_{\sigma \in \mathcal{E}(K)} |\sigma|\, u_\sigma \cdot \boldsymbol{n}_{K,\sigma}$

- grad-div duality

$$\sum_{K \in \mathcal{M}} |K|\, p_K\, (\operatorname{div}\boldsymbol{u})_K + \sum_{\sigma \in \mathcal{E}} |D_\sigma|\, \boldsymbol{u}_\sigma \cdot (\nabla p)_\sigma = 0.$$

- discrete E.O.S.

$$p_K^{n+1} = (\gamma - 1)\rho_K^{n+1}\, e_K^{n+1}. \qquad (\text{eos})_d$$

The implicit scheme for Navier-Stokes

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

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

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

$$p_K^{n+1} = (\gamma - 1)\rho_K^{n+1}\, e_K^{n+1}.$$

Existence, stability

- Kinetic energy conservation + internal energy conservation $\rightsquigarrow$ stability estimate :

$$\sum_{K \in \mathcal{M}} |K|\, \rho_K^n e_K^n + \frac{1}{2} \sum_{\sigma \in \mathcal{E}_{\rm int}} |D_\sigma|\, \rho_\sigma^n\, |u_\sigma^n|^2 \leq \sum_{K \in \mathcal{M}} |K|\, \rho_K^0 e_K^0 + \frac{1}{2} \sum_{\sigma \in \mathcal{E}_{\rm int}} |D_\sigma|\, \rho_\sigma^0\, |u_\sigma^0|^2.$$

- $\exists$ at least a solution to the scheme (topological degree argument), and $e_K \geq 0$.
- $\rho > 0$ and $p > 0$.

Summary: main features of the implicit staggered scheme for NS

- Staggered discretization (ρ, p, e) in cell and $\boldsymbol{u}$ on faces
- Upwind choice for $\rho \rightsquigarrow$ 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 (kin.en) & upwind choice for e_K
  $\rightsquigarrow$ positivity of e
- Conservation of total mass, Estimate on the total energy
- Existence to a solution to the scheme
- Similar results for the fractional time stepping scheme
- Extends to drift-diffusion model of two phase flows.

What about Euler ?

- Euler equations:

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

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

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

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

- 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:

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

- What about discontinous solutions ?
  - Numerical results show that the speed of shocks is not correct.
  - A “blunt” discretization of internal energy equation yields wrong shock speed.

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Right and wrong shock speeds for Burgers

Burgers equation: for regular positive solutions

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

No longer true with irregular solutions:

Rankine Hugoniot gives

$$\sigma = u_\ell + u_r \text{ and } \sigma = \tfrac{4}{3}(u_\ell + u_r).$$

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

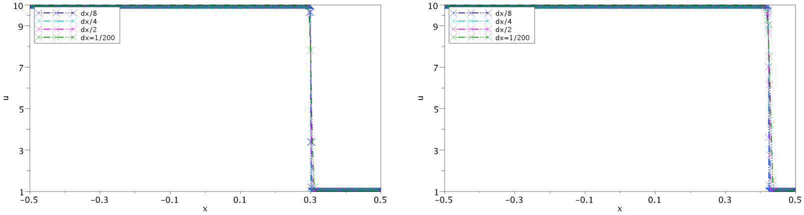


Figure: Upwind Scheme for (B) (left) and (BS) (right) with different mesh sizes, $CFL = 1$.

Non conservative numerical diffusion

- $$\partial_t u + \partial_x (u^2) = 0, \text{ + initial condition} \quad \text{(B)}$$

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

- Explicit upwind scheme on (BS) formally equivalent to:

$$\partial_t u^2 + (4/3)\partial_x (u^3) - \partial_x ((2hu^2 - 4ku^3)\partial_x u) = 0,$$

$$\text{or: } \partial_t u + \partial_x (u^2) \underbrace{- \frac{1}{u}\partial_x ((hu^2 - 2ku^3)\partial_x u)} = 0.$$

D : non conservative numerical diffusion.

☹ Non conservative numerical diffusion on (B) yields $\begin{cases} \text{wrong shock velocity for (B)} \\ \text{correct shock velocity for (BS)} \end{cases}$

but

☺ Non conservative numerical diffusion on (BS) yields $\begin{cases} \text{wrong shock velocity for (BS)} \\ \text{correct shock velocity for (B)} \end{cases}$?

Non conservative numerical diffusion on (BS)

Viscous Burger:

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

Multiplying by $2u$:

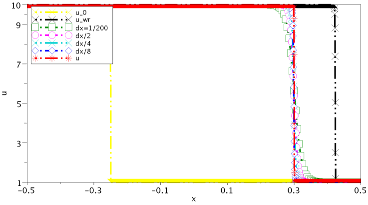
$$\partial_t u^2 + \frac{4}{3}\, \partial_x u^3 - 2u\varepsilon \partial_{xx} u = 0. \qquad \text{(BS)}_\varepsilon$$

Discretize (BS)_ε instead of (BS):

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

Centered finite volume

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



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:

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

Additional difficulty

- we had an equation, we now have a system...

Inspiration comes from copying the formal derivation of the internal energy equation at the discrete level.
Idea: add a corrective term to the internal energy equation.

An implicit scheme for Euler

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

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

$$\frac{|K|}{\delta t}(\rho_K^{n+1} e_K^{n+1} - \rho_K^n e_K^n) + \sum_{\sigma \in \mathcal{E}(K)} F_{K,\sigma}^{n+1} e_\sigma^{n+1} + |K| \, p_K^{n+1} \left(\mathrm{div}\left(\boldsymbol{u}^{n+1}\right)\right)_K = S_K^{n+1}, \qquad (\text{int.en})_d$$

$$p_K^{n+1} = (\gamma - 1)\rho_K^{n+1} \, e_K^{n+1}.$$

Existence, stability

- If the solutions exists, and if $S_K \geq 0$, $e \geq 0$.
- Kinetic energy conservation + internal energy conservation $\rightsquigarrow$ stability estimate (provided that S_K may be absorbed).
- $\exists$ at least a solution (topological degree argument), and $e \geq 0$.
- $\rho > 0$ and $p > 0$.

Strategy for Euler

Check that the correct weak solutions of Euler equations while solving the internal energy balance ?

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

More precisely:

1- Obtain discrete kinetic energy balance (with residual term) from $(\text{mom})_d$ and $(\text{mass})_d$.

2- Perform 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.

Choice of S_K

▷ Kinetic energy

$$\frac{|D_\sigma|}{2\delta t}\big(\varrho_\sigma^{n+1}|\boldsymbol{u}_\sigma^{n+1}|^2 - \varrho_\sigma^n|\boldsymbol{u}_\sigma^n|^2\big) + \frac{1}{2}\sum_{\epsilon=\sigma|\sigma'} F_{\sigma'}^{n+1}\boldsymbol{u}_\sigma^{n+1}\boldsymbol{u}_{\sigma'}^{n+1} + (\boldsymbol{\nabla} p)_\sigma^{n+1}\cdot \boldsymbol{u}_\sigma^{n+1} = -R_\sigma^{n+1}, \text{(kin.en)}_\sigma$$

▷ Internal energy

$$\frac{|K|}{\delta t}(\rho_K^{n+1}e_K^{n+1} - \rho_K^n e_K^n) + \sum_{\sigma\in\mathcal{E}(K)} F_{K,\sigma}^{n+1}e_\sigma^{n+1} + |K|\, p_K^{n+1}\,(\mathrm{div}(\boldsymbol{u}^{n+1}))_K = S_K^{n+1}, \quad \text{(int.en)}_d$$

▷ Multiply kinetic egergy balance and internal energy balance by interpolates φ_σ and φ_K

$$\underbrace{\sum_n\sum_{\sigma\in\mathcal{E}}(\text{kinetic})_\sigma\varphi_\sigma + \sum_n\sum_{K\in\mathcal{M}}(\text{energy })_K\varphi_K}_{\downarrow} = \underbrace{\sum_n\sum_{K\in\mathcal{M}}\delta t S_K\varphi_K + \sum_n\sum_{\sigma\in\mathcal{E}}\delta t R_\sigma\varphi_\sigma}_{\downarrow}.$$

$$-\int_{\Omega\times(0,T)}\Big[\rho E\,\partial_t\varphi + (\rho E + p)\,u\,\nabla\varphi\Big]\,\mathrm{d}\boldsymbol{x} - \int_\Omega \rho_0(x)\,E_0(x)\,\varphi(x,0)\,\mathrm{d}x \qquad\qquad 0$$

Choice of the source term

- Implicit scheme, with centered choice for u_σ:

$$\forall \sigma \in \mathcal{E},\ R_\sigma^{n+1} = -\frac{1}{2}\ \frac{|D_\sigma|}{\delta t}\ \rho^n_{D_\sigma}\ |\boldsymbol{u}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2$$

$$\forall K \in \mathcal{M},\ S_K^{n+1} = \frac{1}{2} \sum_{\sigma \in \mathcal{E}(K)} \frac{|D_{K,\sigma}|}{\delta t} \rho^n_K\ |\boldsymbol{u}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2$$

With this choice,

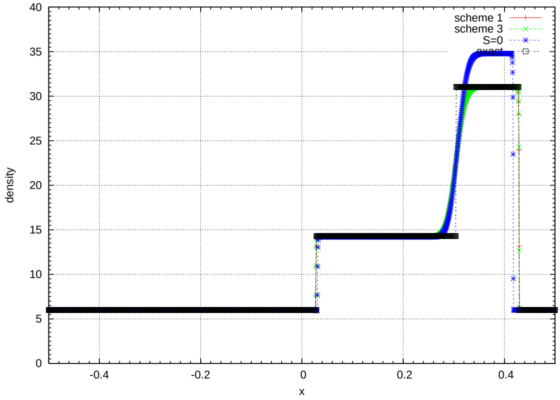
$$\sum_n \sum_{\sigma \in \mathcal{E}} \delta t |R_\sigma| \varphi_\sigma + \sum_n \sum_{K \in \mathcal{M}} \delta t |S_K| \varphi_K \to 0 \text{ as mesh size } \to 0.$$

thanks to the fact that

$$|D_\sigma| \rho_{D_\sigma} = |D_{K,\sigma}|\ \rho_K + |D_{L,\sigma}|\ \rho_L$$

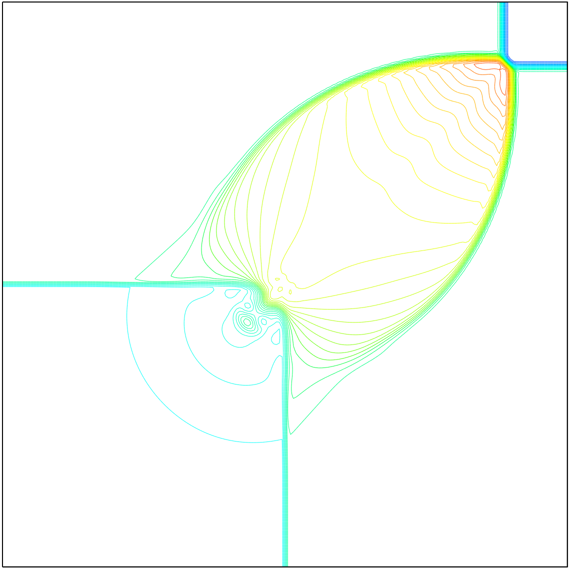
1D Riemann problem

- Scheme 1, scheme 3, and what is obtained without corrective term:



[E. Toro, *Riemann solvers and numerical methods for fluid dynamics*, third edition, test 5 of chapter 4].

2D Riemann problem



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Explicit scheme for the Euler equation: $\rho \to \boldsymbol{u} \to e \to p$

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

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

$$\frac{|K|}{\delta t}(\rho_K^{n+1} e_K^{n+1} - \rho_K^n e_K^n) + \sum_{\sigma \in \mathcal{E}(K)} F_{K,\sigma}^n e_\sigma^n + |K|\, p_K^n \left(\mathrm{div}(\boldsymbol{u}^{n+1})\right)_K = S_K^n, \qquad (\text{int.en})_d$$

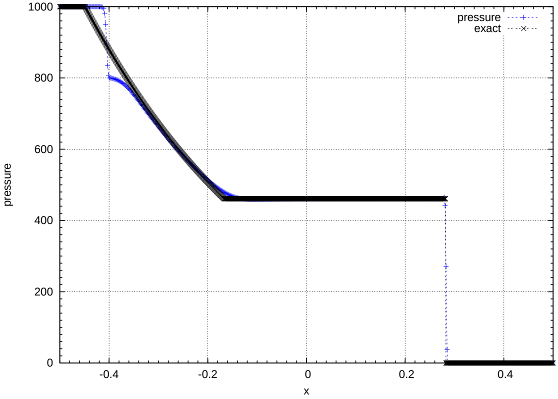
$$p_K^{n+1} = (\gamma - 1)\rho_K^{n+1}\, e_K^{n+1}.$$

- $\boldsymbol{u}^{n+1}$: to recover total energy balance, thanks to discrete kinetic energy.
- $\mathcal{S}^n$ obtained by requiring that

$$\sum_n \sum_{\sigma \in \mathcal{E}} \delta t |R_\sigma| \varphi_\sigma + \sum_n \sum_{K \in \mathcal{M}} \delta t |S_K| \varphi_K \to 0 \text{ as mesh size } \to 0.$$

where R_σ is the (positive) remainder in the discrete kinetic energy equation.

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



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

A better explicit scheme for the Euler equations: $\rho \to e \to p \to \boldsymbol{u}$

Same space discretization as the implicit scheme.

Time discretization is now:

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

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

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

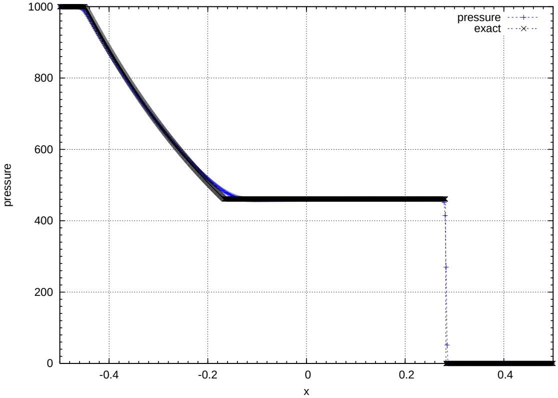
$$\frac{1}{\delta t}(\varrho^{n+1} \boldsymbol{u}^{n+1} - \varrho^{n} \boldsymbol{u}^{n}) + \operatorname{div}(\varrho^{n} \boldsymbol{u}^{n} \otimes \boldsymbol{u}^{n}) + \boldsymbol{\nabla} p^{n+1} = 0, \qquad (\text{mom})_d \quad \rightsquigarrow \quad \boldsymbol{u}^{n+1}.$$

- $\mathcal{S}^n$ obtained by requiring that

$$\sum_{n} \sum_{\sigma \in \mathcal{E}} \delta t |R_\sigma| \varphi_\sigma + \sum_{n} \sum_{K \in \mathcal{M}} \delta t |S_K| \varphi_K \to 0 \text{ as mesh size } \to 0.$$

  where R_σ is the (positive) remainder in the discrete kinetic energy equation.

Explicit scheme: $\rho \to e \to p \to \boldsymbol{u}$



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

Why choose $\rho \rightarrow e \rightarrow p \rightarrow \boldsymbol{u}$?

- Derivation of the entropy balance at the continuous level: $s = \psi(\rho, e)$; $\partial_t s + \boldsymbol{u} \cdot \boldsymbol{\nabla} s$.

$$\left| \begin{array}{ll} \partial_t \varrho + \boldsymbol{u} \cdot \boldsymbol{\nabla} \varrho + \varrho \,\mathrm{div} \boldsymbol{u} = 0 & \times \partial_\varrho \psi(\rho, e) \\ \partial_t e + \boldsymbol{u} \cdot \boldsymbol{\nabla} e + \dfrac{e}{\varrho} \,\mathrm{div} \boldsymbol{u} = 0 & \times \partial_e \psi(\rho, e) \end{array} \right.$$

$$\rightsquigarrow \partial_t s + \boldsymbol{u} \cdot \boldsymbol{\nabla} s + \underbrace{\left[\varrho\, \partial_\varrho s + \frac{e}{\varrho} \partial_e s \right]}_{=0} \mathrm{div} \boldsymbol{u} = 0.$$

- 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.
  - $\rho \rightarrow \boldsymbol{u} \rightarrow e \rightarrow p \rightsquigarrow \mathrm{div}(\varrho^n \boldsymbol{u}^n)$ and $p^n \,\mathrm{div} \boldsymbol{u}^{n+1}$
  - $\rho \rightarrow e \rightarrow p \rightarrow \boldsymbol{u} \rightsquigarrow \mathrm{div}(\varrho^n \boldsymbol{u}^n)$ and $p^{n+1} \,\mathrm{div} \boldsymbol{u}^{n+1}$

Stability analysis of the explicit scheme

- Kinetic energy identity:

$$\frac{1}{2}\frac{|D_\sigma|}{\delta t}(\rho_\sigma {\mathbf{u}^{\mathbf{n+1}}}_\sigma^2 - \rho_\sigma^n {\mathbf{u}_\sigma^n}^2) + \frac{1}{2}\sum_{\substack{\epsilon\in\mathcal{E}(D_\sigma)\\ \epsilon=D_\sigma|D_{\sigma'}}} F^n_{D_\sigma,\epsilon}\mathbf{u}^n_\sigma\mathbf{u}^n_{\sigma'}$$

$$+ |\sigma|(p_L^{n+1} - p_K^{n+1})\mathbf{n}_{K|L}\cdot {\mathbf{u}^{\mathbf{n+1}}}_\sigma = -R^n_\sigma$$

- Up to a term tending to zero (under L^∞ and BV estimates for $\boldsymbol{u}$),

$$R_\sigma{}^n = \frac{|D_\sigma|}{\delta t}\,\varrho_\sigma^{n+1}\,|\boldsymbol{u}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n|^2 + \sum_{\epsilon=D_\sigma|D'_\sigma} F^n_{\sigma,\epsilon}\,|\boldsymbol{u}^n_\sigma - \boldsymbol{u}^n_{\sigma'}|^2$$

$$+ \sum_{\epsilon=D_\sigma|D'_\sigma} F^n_{\sigma,\epsilon}\,(\boldsymbol{u}_\sigma^{n+1} - \boldsymbol{u}_\sigma^n)\cdot(\boldsymbol{u}^n_\sigma - \boldsymbol{u}^n_{\sigma'}),$$

  which is non-negative under the CFL condition (ans so is S_K is constructed to compensate R_σ.)

- Stability: under the CFL:

$$\delta t \le \min\left(\frac{|K|}{\gamma\sum_{\sigma\in\mathcal{E}(K)}(|\sigma|\mathbf{u}^*_\sigma\cdot\mathbf{n}_{K,\sigma})^+};\ \frac{\xi_K^\sigma|K|\rho_K^*}{(F^*_{K,\sigma})^+ + \sum_{\epsilon\in\mathcal{E}(D_\sigma),\epsilon\subset K}(F^*_{D_\sigma,\epsilon})^+}\right)$$

  $\rho_K^n > 0$, $e_K > 0$.

Summary of the results for the explicit scheme

For the Euler equations, we have an explicit scheme with the following properties:

- Under a CFL condition, $\rho_K^n \geq 0$ and $e_K^n \geq 0$ $\forall n \geq 1$ if $\rho_K^0 \geq 0$ and $e_K^0 \geq 0$.
- Discrete kinetic energy balance holds.
- The scheme is consistent : under compactness assumptions, the discrete solution tends to a weak solution of the Euler systems (proof in 1D).
- Numerical discontinuous solutions have correct shocks.
- Numerical entropy weak solutions (choosing an adequate order when solving the equations).

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Perspectives

- Integration in the home made open source software, ISIS, with a fractional time step method (pressure correction).
  ISIS: `https://gforge.irsn.fr/gf/project/isis`
- Ongoing: extensive tests for problems ranging from hyperbolic to low Mach number flows.
- Do the schemes converge to an entropy weak solution ?
- Theoretical study of the limit of the discrete problem as $Ma \to 0$. Ph. D. K. Mallem (just starting).
- To develop: less diffusive schemes, adavtive mesh refinement procedures.

  Similar scheme for barotropic flows $\rightsquigarrow$ application to (low Mach number) shallow water problems ?
- Extension to reactive flows (deflagration, detonation) Ph.D. N. Therme (starting in November).