Staggered discretizations, pressure corrections schemes and all speed flows

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Continuous problem

- Euler (Navier-Stokes) equations:

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

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

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

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

- For regular functions, taking the inner product of the momentum balance equation by $\boldsymbol{u}$ and using the mass balance equation yields the kinetic energy balance equation:

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

  Subtracting to the total energy balance yields the internal energy balance:

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

  and, from this equation, we get $e \geq 0$.

- Estimates satisfied by the solution: $\varrho \geq 0$, $e \geq 0$, $\displaystyle\int_\Omega \varrho = \int_\Omega \varrho_0$, $\displaystyle\int_\Omega \varrho E = \int_\Omega \varrho_0 E_0$.

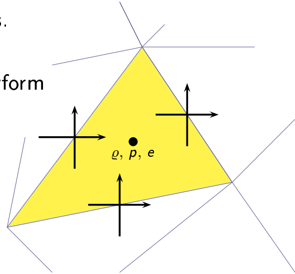
Objectives (1/2)

Derive a scheme for Euler (or Navier-Stokes) equations:

(*i*) unconditionnally stable (*i.e.* same estimates as in the continuous case),

(*ii*) accurate at all Mach numbers,

(*iii*) which converges to the correct weak (discontinuous) solutions.

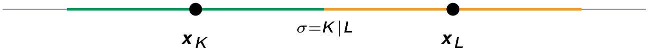


- (*ii*) suggests to use a staggered discretization (*iv*), and to perform upwinding (if any) with respect to the material velocity.
- (*i*) and (*iv*) suggest to solve the internal energy balance:
  - keep e positive,
  - e and $\frac{1}{2}|\boldsymbol{u}|^2$ are not discretized at the same place.
- (*i*) will be a constraint for the choice of the time-stepping algorithm: implicit scheme or pressure correction method.

So a staggered scheme, solving the internal energy balance, upwind/$\boldsymbol{u}$.

ISIS: https://gforge.irsn.fr/gf/project/isis
PELICANS: https://gforge.irsn.fr/gf/project/pelicans

Objectives (2/2)



- Let us consider the equation:

$$\cdots + \partial_x u = \ldots$$

The centered scheme reads:

$$\forall K, \qquad \cdots + \sum_{\sigma = K|L} \frac{1}{2} (u_K + u_L) \cdot \boldsymbol{n}_\sigma = \ldots$$

Let $\varphi \in \mathrm{C}^\infty$, $\varphi_K = \varphi(\boldsymbol{x}_K)$, multiply each equation by φ_K and sum over K. This yields:

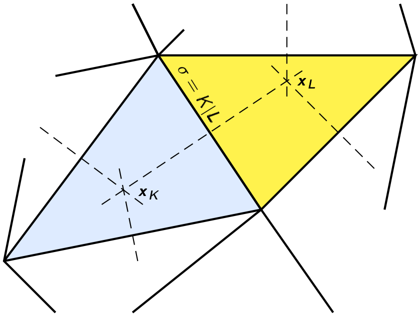
$$\cdots + \sum_{\sigma = K|L} \frac{|K|}{2} u_K \frac{\varphi_L - \varphi_K}{||\boldsymbol{x}_L - \boldsymbol{x}_K||} + \frac{|L|}{2} u_L \frac{\varphi_L - \varphi_K}{||\boldsymbol{x}_L - \boldsymbol{x}_K||} = \ldots$$

i.e.:

$$\ldots \int_\Omega u \, \boldsymbol{\nabla}_h \varphi \, \mathrm{d}\boldsymbol{x} = \ldots$$

- *Morality: "Consider a conservative scheme. Suppose that a sequence of discrete solutions converges. Then the limit is a weak solution."*
- So how to obtain the correct weak solutions of Euler equations while solving the internal energy balance ?

A colocated scheme (1/7)



- Mass balance $(\partial_t(\varrho) + \mathrm{div}(\varrho \boldsymbol{u}) = 0)$:
  - Velocity at the face $\sigma = K|L$:

$$\boldsymbol{u}_\sigma = \frac{d_{L,\sigma}}{d_\sigma} \boldsymbol{u}_K + \frac{d_{K,\sigma}}{d_\sigma} \boldsymbol{u}_L, \qquad d_{K,\sigma} = d(\boldsymbol{x}_K, \sigma),\ d_{L,\sigma} = d(\boldsymbol{x}_L, \sigma),\ d_\sigma = d(\boldsymbol{x}_K, \boldsymbol{x}_L).$$

  - Mass flux : $F_{K,\sigma} = |\sigma|\ \varrho_\sigma\ \boldsymbol{u}_\sigma \cdot \boldsymbol{n}_{K,\sigma}$, with ϱ_σ the upwind value of the density at the face.
  - Mass balance: $$\frac{|K|}{\delta t}\,(\varrho_K - \varrho_K^*) + \sum_{\sigma = K|L} F_{K,\sigma} = 0.$$

A colocated scheme (2/7)

- Building convection operators $z \mapsto \partial_t(\varrho z) + \mathrm{div}(\varrho z \boldsymbol{u})$ from the mass balance:
  - Let:
$$\frac{|K|}{\delta t}\,(\varrho_K - \varrho_K^*) + \sum_{\sigma=K|L} F_{K,\sigma} = 0.$$
  - Then (1) the centered operator:
$$(C\boldsymbol{u})_K = \frac{1}{\delta t}\,(\varrho_K\,\boldsymbol{u}_K - \varrho_K^*\,\boldsymbol{u}_K^*) + \frac{1}{|K|}\sum_{\sigma=K|L} F_{K,\sigma}\,\boldsymbol{u}_\sigma, \qquad \boldsymbol{u}_{K|L} = \frac{1}{2}\,(\boldsymbol{u}_K + \boldsymbol{u}_L)$$
    satisfies:
$$(C\boldsymbol{u})_K\cdot\boldsymbol{u}_K = \frac{|K|}{2\delta t}\,(\varrho_K|\boldsymbol{u}_K|^2 - \varrho_K^*|\boldsymbol{u}_K^*|^2) + \frac{1}{2}\sum_{\sigma=K|L} F_{K,\sigma}\,\boldsymbol{u}_K\,\boldsymbol{u}_L + \frac{|K|}{2\delta t}\,\varrho_K^*\,|\boldsymbol{u}_K - \boldsymbol{u}_K^*|^2.$$
  - Then (2) the upwind operator:
$$(Ce)_K = \frac{1}{\delta t}\,(\varrho_K\,e_K - \varrho_K^*\,e_K^*) + \frac{1}{|K|}\sum_{\sigma=K|L} F_{K,\sigma}\,e_\sigma,$$
    with an upwind choice for e_σ satisfies a discrete maximum principle.

A colocated scheme (3/7)

- Momentum balance $(\partial_t(\varrho \boldsymbol{u}) + \mathrm{div}(\varrho \boldsymbol{u} \otimes \boldsymbol{u}) + \boldsymbol{\nabla} p = 0)$:

$$|K| \Big[(C\boldsymbol{u})_K + (\boldsymbol{\nabla} p)_K - (\varepsilon \Delta \boldsymbol{u})_K \Big] = 0.$$

  - Centered convection term.
  - Pressure gradient designed to be the dual operator of the divergence:

$$(\boldsymbol{\nabla} p)_K = \frac{1}{|K|} \sum_{\sigma=K|L} |\sigma| \; p_\sigma \, \boldsymbol{n}_{K,\sigma}, \qquad p_{K|L} = \frac{d_{K,\sigma}}{d_\sigma} p_K + \frac{d_{L,\sigma}}{d_\sigma} p_L.$$

  - A diffusion term is added for stabilisation:

$$-(\varepsilon \Delta \boldsymbol{u})_K = \frac{1}{|K|} \sum_{\sigma=K|L} \varepsilon_\sigma \; \frac{|\sigma|}{d_\sigma} \; (\boldsymbol{u}_K - \boldsymbol{u}_L).$$

Upwind discretization of the convection term: $\varepsilon_\sigma = \dfrac{d_\sigma}{2} \, |\boldsymbol{u}_\sigma \cdot \boldsymbol{n}_{K,\sigma}|$.

A colocated scheme (4/7)

- Internal energy balance $(\partial_t(\varrho e) + \mathrm{div}(\varrho e \boldsymbol{u}) + p\, \mathrm{div} \boldsymbol{u} = 0)$:

$$|K|\ (Ce)_K + (\gamma - 1) \varrho_K\, e_K^+ \sum_{\sigma=K|L} |\sigma|\ \boldsymbol{u}_\sigma \cdot \boldsymbol{n}_{K,\sigma} = S_K,$$

with $e_K^+ = \max(e_K, 0)$ and S_K is a numerical source term.

  - Upwind convection term.
  - If the solutions exists, and if $S_K \geq 0$, $e > 0$.
  - $\exists$ at least a solution (topological degree argument), and, for this solution, $e^+ = e$ (the scheme is consistent).

A colocated scheme (5/7)

S_K ?

- Strategy: try to build a (conservative) discrete total energy balance equation.
- Kinetic energy balance, without diffusion ($\varepsilon = 0$):
  $(\partial_t(\varrho E_c) + \mathrm{div}(\varrho E_c \boldsymbol{u}) + \boldsymbol{u} \cdot \boldsymbol{\nabla} p = 0,\ E_c = \frac{1}{2}|\boldsymbol{u}|^2)$
  - Multiply the momentum balance equation by $\boldsymbol{u}_K$ and use the mass balance:

$$\frac{|K|}{2\delta t}\,(\varrho_K|\boldsymbol{u}_K|^2 - \varrho_K^*|\boldsymbol{u}_K^*|^2) + \frac{1}{2}\sum_{\sigma=K|L} F_{K,\sigma}\boldsymbol{u}_K\boldsymbol{u}_L + (\boldsymbol{\nabla} p)_K \cdot \boldsymbol{u}_K = R_K.$$

  - Then, adding to the internal energy balance yields a total energy balance $(\partial_t(\varrho E) + \mathrm{div}(\varrho E \boldsymbol{u}) + \mathrm{div}(p\boldsymbol{u}) = 0)$:

$$\frac{|K|}{\delta t}\,(\varrho_K E_K - \varrho_K^* E_K^*) + \sum_{\sigma=K|L} F_{K,\sigma} E_\sigma + \sum_{\sigma=K|L} |\sigma|\ (p\boldsymbol{u})_\sigma \cdot \boldsymbol{n}_{K,\sigma} = R_K + S_K,$$

with:

$$E_K = e_K + \frac{1}{2}\,|\boldsymbol{u}_K|^2,$$

$$E_\sigma = e_\sigma + \frac{1}{2}\,\boldsymbol{u}_K \cdot \boldsymbol{u}_L,$$

$$(p\boldsymbol{u})_{K|L} = \frac{d_{K,\sigma}}{d_\sigma} p_K\,\boldsymbol{u}_L + \frac{d_{L,\sigma}}{d_\sigma} p_L\,\boldsymbol{u}_K.$$

A colocated scheme (6/7)

- S_K and total energy balance, without diffusion (continued):
  - Rest term:

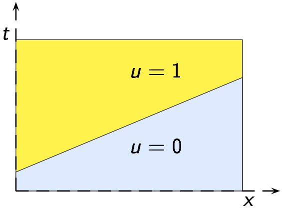
$$R_K = -\frac{|K|}{2\delta t}\ \varrho_K^*\ |\boldsymbol{u}_K - \boldsymbol{u}_K^*|^2.$$

For a regular function ($|\boldsymbol{u}_K - \boldsymbol{u}_K^*| \leq C\,\delta t$):

$$\sum_n \sum_{K\in\mathcal{M}} \delta t |R_K| \leq C\delta t$$

...but for a discontinuous function:

$$\sum_n \sum_{K\in\mathcal{M}} \delta t |R_K| \simeq |\Omega|.$$



=> choose $S_K = -R_K$.

A colocated scheme (7/7)

- Kinetic energy balance, S_K and total energy balance, with diffusion ($\varepsilon \neq 0$):
  - With a dissipation term:

$$R_K += \quad -\Big[\sum_{\sigma=K|L} \varepsilon_\sigma \, \frac{|\sigma|}{d_\sigma} \, (\boldsymbol{u}_K - \boldsymbol{u}_L)\Big] \cdot \boldsymbol{u}_K,$$

$$S_K += \quad \frac{1}{2} \sum_{\sigma=K|L} \varepsilon_\sigma \, \frac{|\sigma|}{d_\sigma} \, |\boldsymbol{u}_K - \boldsymbol{u}_L|^2.$$

  - Then:

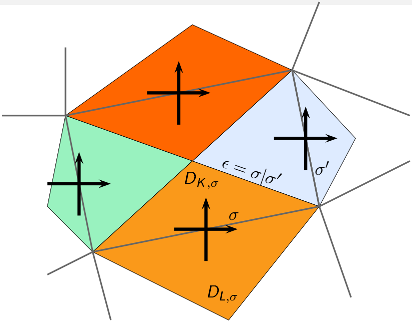
$$R_K + S_K = \frac{1}{2} \sum_{\sigma=K|L} \varepsilon_\sigma \, \frac{|\sigma|}{d_\sigma} \, (\boldsymbol{u}_K - \boldsymbol{u}_L) \cdot (\boldsymbol{u}_K + \boldsymbol{u}_L).$$

    At the continuous level, the viscous term at the right-hand side of the total energy balance reads $\mathrm{div}(\varepsilon \boldsymbol{\nabla}^t \boldsymbol{u} \; \boldsymbol{u})$, so we need an approximation on the face of $(\boldsymbol{\nabla}^t \boldsymbol{u} \; \boldsymbol{u}) \cdot \boldsymbol{n} = (\boldsymbol{\nabla} \boldsymbol{u} \; \boldsymbol{n}) \cdot \boldsymbol{u} = \sum_{i=1}^3 \boldsymbol{u}_i \; \boldsymbol{\nabla} \boldsymbol{u}_i \cdot \boldsymbol{n} \ldots$ which is what we get.
  - $R_K + S_K$ is conservative: conservation of $\displaystyle\int_\Omega \varrho E$.
  - Let $\varphi \in \mathrm{C}_c^\infty(\Omega \times (0,T))$, and φ_K be an approximation of φ on K at the current time step. Then :

$$\sum_n \sum_{K \in \mathcal{M}} \delta t \; (R_K + S_K) \; \varphi_K \quad = \frac{1}{2} \sum_{\sigma=K|L} \varepsilon_\sigma \, \frac{|\sigma|}{d_\sigma} \, (\boldsymbol{u}_K - \boldsymbol{u}_L) \cdot (\boldsymbol{u}_K + \boldsymbol{u}_L)(\varphi_K - \varphi_L)$$

$$\leq C_\varphi \; \|\varepsilon\|_{\mathrm{L}^\infty} \; \|\boldsymbol{u}\|_{\mathrm{L}^\infty} \; \|\boldsymbol{u}\|_{BV}.$$

A staggered scheme (1/2)



- The velocity is now defined at the center of the faces.
- The approximation of $\boldsymbol{u}_\sigma$ becomes natural.
- Up to this change, the mass mass balance and the left-hand side of the internal energy balance are left unchanged.
- Build mass fluxes at the dual faces in such a way that the mass balance is ensured on the diamond cells†, and write the momentum balance equation on the diamond cells, following the same guidelines⋆ as for the colocated scheme.

†: L. Gastaldo, R. Herbin, W. Kheriji, JCL, FVCA 6.

⋆: convection term buit from the mass balance, pressure gradient built by duality.

A staggered scheme (2/2)

- A kinetic energy balance is still available, but is associated to faces, and can no more be combined to the internal energy equation (defined on primal meshes) to obtain a total energy balance equation.

- Strategy:

  1- Suppose bounds and convergence for a sequence of discrete solutions, compatible with the regularity of the sought continuous solutions: control in BV and L^∞, convergence in L^p, for $p \geq 1$.

  3- Let φ a regular function, (φ_σ) an interpolate on the faces and (φ_K) an interpolate on the cells, at the current time step. Multiply the kinetic energy balance by φ_σ, the internal energy balance by φ_K, sum over the time steps, i, σ and K and pass to the limit in the scheme.

  S_K is chosen in such a way to recover, at the limit, the weak form of the total energy equation.

- S_K:

$$S_K = \sum_{\sigma \in \mathcal{E}(K)} \frac{|D_{K,\sigma}|}{\delta t}\ \varrho^*_K\ |\boldsymbol{u}_\sigma - \boldsymbol{u}^*_\sigma|^2 + \sum_{\epsilon \subset K,\ \epsilon=\sigma|\sigma'} \varepsilon_\epsilon\ \frac{|\epsilon|}{d_\epsilon}\ |\boldsymbol{u}_\sigma - \boldsymbol{u}_{\sigma'}|^2.$$

An explicit time discretization

- Scheme (time semi-discrete setting):

$$
\begin{aligned}
&\frac{1}{\delta t}(\varrho - \varrho^*) + \operatorname{div}(\varrho^* \boldsymbol{u}^*) = 0,\\
&\frac{1}{\delta t}(\varrho \boldsymbol{u} - \varrho^* \boldsymbol{u}^*) + \operatorname{div}(\varrho^* \boldsymbol{u}^* \otimes \boldsymbol{u}^*) - \operatorname{div}\boldsymbol{\tau}(\boldsymbol{u}^*) + \boldsymbol{\nabla} p^* = 0,\\
&\frac{1}{\delta t}(\varrho e - \varrho^* e^*) + \operatorname{div}(\varrho^* e^* \boldsymbol{u}^*) + p^* \operatorname{div}\boldsymbol{u}^* = \boldsymbol{\tau}(\boldsymbol{u}^*) : \boldsymbol{\nabla}\boldsymbol{u}^*,\\
&p = (\gamma - 1)\ \varrho e.
\end{aligned}
$$

- S_K:

$$
S_K = - \sum_{\sigma \in \mathcal{E}(K)} \frac{|D_{K,\sigma}|}{\delta t}\ \varrho_K\ |\boldsymbol{u}_\sigma - \boldsymbol{u}^*_\sigma|^2 + \sum_{\epsilon \subset K,\ \epsilon = \sigma|\sigma'} \varepsilon_\epsilon\ \frac{|\epsilon|}{d_\epsilon}\ |\boldsymbol{u}^*_\sigma - \boldsymbol{u}^*_{\sigma'}|^2.
$$

A pressure correction scheme

- Scheme (time semi-discrete setting):

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

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

- S_K:

$$S_K = \sum_{\sigma \in \mathcal{E}(K)} \frac{|D_{K,\sigma}|}{\delta t}\ \varrho_K^*\ |\tilde{\boldsymbol{u}}_\sigma - \boldsymbol{u}_\sigma^*|^2 + \sum_{\epsilon \subset K,\ \epsilon = \sigma|\sigma'} \varepsilon_\epsilon\ \frac{|\epsilon|}{d_\epsilon}\ |\tilde{\boldsymbol{u}}_\sigma - \tilde{\boldsymbol{u}}_{\sigma'}|^2.$$

- If a pressure renormalization step is added, this scheme is unconditionnally stable ($\varrho > 0$, $e > 0$, ϱ and ϱE controlled in $\mathrm{L}^\infty(0, T; \mathrm{L}^1)$).

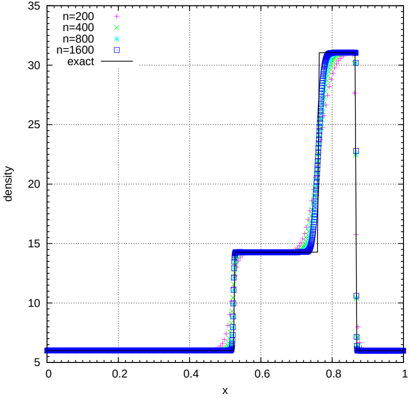
  In addition, the time splitting yields a control on $\delta t\ \boldsymbol{\nabla} p$ in $\mathrm{L}^\infty(0, T; \mathrm{L}^2)$.

A Riemann Problem

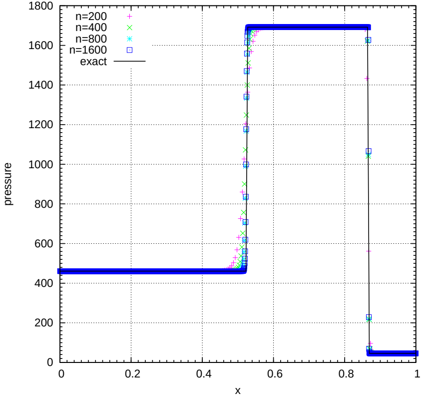
- [P. Woodward, P. Collela, JCP 1984]

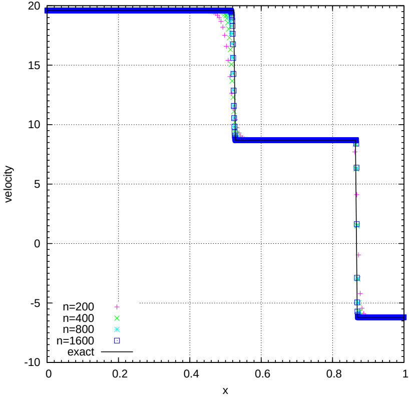
  [E. Toro, *Riemann solvers and numerical methods for fluid dynamics*, third edition, test 5 of chapter 4].

  Two shocks travelling to the right, contact discontinuity.
- Computation performed with the upwind explicit scheme.
- $\delta t = h/50$, so a cfl number close to $1/2$.
- An additional diffusion term is added in the momentum balance equation, in the range of $\varrho \boldsymbol{u} h/2$.

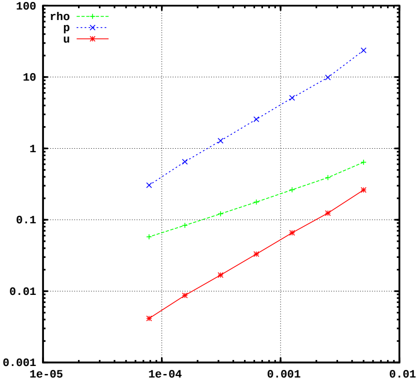


A Riemann Problem





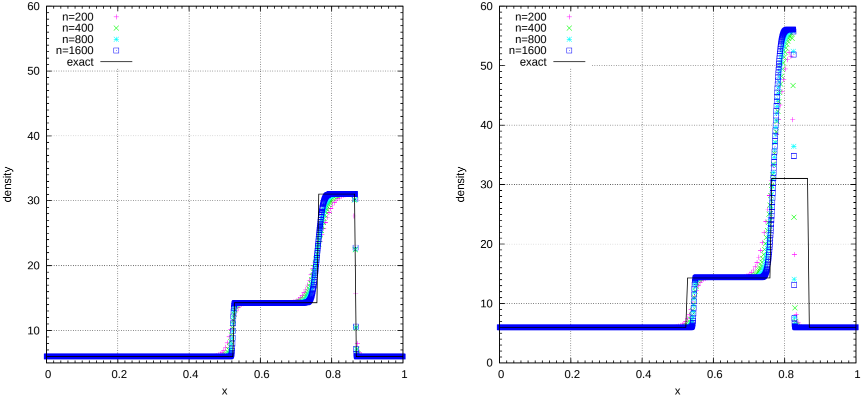
A Riemann Problem



- Difference between the numerical and analytical solution (L^1 norm), as a function of the time and space step (cfl ≈ 0.4).
- First order convergence for the quantities which remain constant through the contact discontinuity ($\boldsymbol{u}$, p).

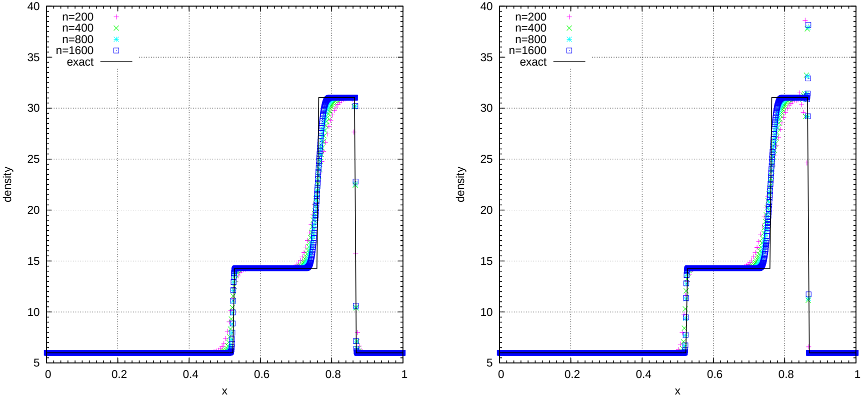
  Convergence as $h^{1/2}$ for ϱ.

A Riemann Problem



Right: $S_K = 0$.

A Riemann Problem



Right: no additional diffusion.

Conclusion

- A class of naive schemes for Euler equations:
  - staggered mesh,
  - upwinding with respect to the (material) velocity, centered approximation of the pressure gradient,
  - total energy equation $\hookrightarrow$ internal energy equation + source term,
  - a reasonably decoupled (?) unconditionally stable time discretization (?).
- Convergence ?
  1. estimates: $\varrho > 0$, $e > 0$, ϱ and ϱE controlled in $\mathrm{L}^\infty(0, T; \mathrm{L}^1)$, entropy ?
  2. Compactness: far from being sufficient !
     (no control on the translations)
  3. Passage to the limit in the scheme: OK.
- Tests under progress.
- Further developments: less diffusive versions (entropy viscosity technique ?)