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An efficient, second-order, positivity-preserving finite volume scheme for Viscous Euler equations on staggered meshes.

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Context and objectives

Context: staggered Finite Volume (FV) scheme with Runge-Kutta (RK) time-stepping.
Staggered FV type of schemes have been extensively studied by the LIE team at ASNR, but a lot of questions remain regarding the coupling with RK methods.

Goal: Build a second order, positivity preserving and efficient scheme for Navier-Stokes equations.
Efficient in the sense that the Euler part of the equations in computed explicitly, and the diffusive / viscous terms are not taken into account at every time-step.

Main issues:

- Heavy machinery for staggered: dual mass fluxes, dual mass balance equation, internal energy formulation...
- Explicit pressure have been shown to lead to non-entropic schemes

ODE: $\Omega = (x_L, x_R)$ 1D domain, $T > 0$ final time, $f : \Omega \to \mathbb{R}$

$$y'(t) = f(y(t)), \qquad \forall t \in (0, T) \tag{1}$$
$$y(0) = y_0 \tag{2}$$

Time discretization: $(t^n)_{0 \leq n \leq N}$, with $\delta t^n = t^{n+1} - t^n$ the time-step.

RK method: a s-stage RK method is described by a Butcher tableau:

$$\begin{array}{c|cccc} c_1 & a_{1,1} & \dots & \dots & a_{1,s} \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ c_s & a_{s,1} & \dots & \dots & a_{s,s-1} \\ \hline & a_{s+1,1} & \dots & \dots & a_{s+1,s} \end{array}, \qquad \text{with } c_k \text{ pairwise distincts} \tag{3}$$

Runge-Kutta (RK) methods II

The RK method reads (in incremental form): $y^0 = y_0$ and for all $0 \leq n \leq N-1$,

$$\begin{aligned} y^{n,1} &= y^n, \\ \forall 1 \leq k \leq s, \qquad y^{n,k+1} &= y^{n,k} + \delta t^{n,k} \sum_{j=1}^{k} b_{k+1,j} f(y^{n,j}), \\ y^{n+1} &= y^{n,s+1}, \end{aligned} \tag{4}$$

with

$$\delta t^{n,k} = c_k \delta t^{n,k} \quad \text{fractional time-step}, \qquad b_{k+1,j} = \frac{a_{k+1,j} - a_{k,j}}{c_{k+1} - c_k} \quad \text{incremental RK coefficients} \tag{5}$$

Context and objectives

Discretization of a linear convection operator

Viscous Euler equations

Conclusion

Linear convection equation

Ω open bounded subset of $\mathbb{R}^d$, d the space dimension, $T > 0$ final time

$$\rho : (0, T) \times \Omega \to \mathbb{R} \text{ scalar unknown}, \qquad \boldsymbol{u} : (0; T) \times \Omega \to \mathbb{R}^d \text{ velocity}$$

PDE:

$$\partial_t \rho + \mathrm{div}(\rho \boldsymbol{u}) = 0 \tag{6}$$

Here, the velocity is not an unknown.

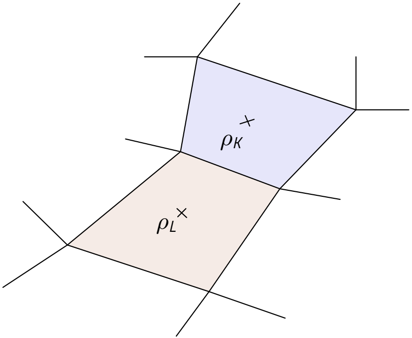
Initial condition: $\rho_0 > 0$

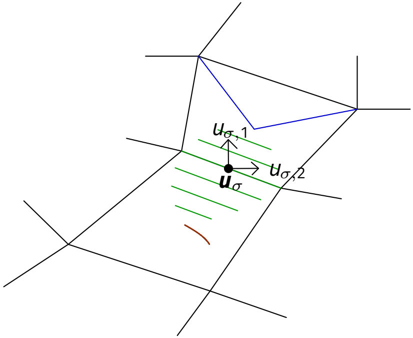
Boundary conditions: $\boldsymbol{u} = 0$ on $\partial\Omega$

Goal: Build second-order positivity-preserving staggered finite volume scheme.

Mesh and unknowns

Unstructured meshes, mix of quadrangles and triangles (2D) or hexaedra and simplices (3D), staggered.





Primal mesh

Cells : K, L, M

Scalar unknowns: ρ_K

Dual mesh

Cells : D_σ

Velocity unknowns: $\boldsymbol{u}_\sigma = (u_{\sigma,1}, \dots, u_{\sigma,d})$

2-stage second-order ERK method:

$$\begin{array}{c|cc} 0 & 0 & \\ c_2 & a_{2,1} & 0 \\ \hline & a_{3,1} & a_{3,2} \end{array} = \begin{array}{c|cc} 0 & 0 & \\ \beta & \beta & 0 \\ \hline & 1-\frac{1}{2\beta} & \frac{1}{2\beta} \end{array} \tag{7}$$

with $0 < \beta < 1$.

A-MUSCL approximation

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Not the standard geometrical MUSCL reconstruction !

Notations: Discrete convection equation

$$v_K^{n+1} = v_K^n - \frac{\delta t^n}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| u_{K,\sigma}^n v_\sigma^n = 0, \qquad \text{with } v_K^n > 0. \tag{8}$$

Goal: Compute quasi-second order face approximation v_σ^n such that $v_K^{n+1} > 0$.

Notation: $v_\sigma^n = \text{A-MUSCL}(\check{v}_\sigma^n; u_{K,\sigma}^n, v^n)$, $\check{v}_\sigma^n$ any second order face approximation of v^n.
Under the CFL-like condition:

$$\frac{\delta t^n}{|K|} \leq \frac{1}{2 \displaystyle\sum_{\sigma \in \mathcal{E}(K)} |\sigma| |u_{K,\sigma}^n|}, \tag{9}$$

if $v^n > 0$, then $v^{n+1} > 0$.

Libuse Piar, Fabrice Babik, Raphaele Herbin, and Jean-Claude Latché. A formally second order cell centered scheme for convection-diffusion equations on unstructured non-conforming grids. *International Journal for Numerical Methods in Fluids*

Incremental 2-stage RK method with centered face approximations:

$$\rho^{n,1} = \rho^{n} \tag{10a}$$

$$\rho_K^{n,2} = \rho_K^{n,1} - \frac{\delta t^{n,1}}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| u_{K,\sigma}^{n,1} \check{\rho}_\sigma^{n,1}, \tag{10b}$$

$$\rho^{n+1} = \rho_K^{n,2} - \frac{\delta t^{n,2}}{|K|} \sum_{\sigma \in \mathcal{E}(K)} |\sigma| \underbrace{\left[b_{3,1} u_{K,\sigma}^{n,1} \check{\rho}_\sigma^{n,1} + b_{3,2} u_{K,\sigma}^{n,2} \check{\rho}_\sigma^{n,2} \right]}_{= u_{K,\sigma}^{n,2} \check{\rho}_\sigma^{n,*,\sigma}}, . \tag{10c}$$

Make the first update (10b) **PP:** apply A-MUSCL limiter: $\rho_\sigma^{n,1} = \text{A-MUSCL}(\check{\rho}_\sigma^{n,1}, u_{K,\sigma}^{n,1}, \rho^{n,1})$

Make the second update (10c) **PP:** In the spirit of in [EG], apply a limiter to $\check{\rho}_\sigma^{n,*,\sigma}$.

[EG] : Alexandre Ern, Jean-Luc Guermond. Invariant-domain-preserving high-order time stepping: I. Explicit Runge-Kutta schemes. SIAM Journal on Scientific Computing, 2022, 44 (5), pp.A3366–A3392. ⟨10.1137/21M145793X⟩. ⟨hal-03425367v2⟩

Let $\alpha > 0$ and let $C_+^n = \max\{\rho^{n,2}/\rho^{n,1}\}$ and $C_-^n = \min\{\rho^{n,2}/\rho^{n,1}\}$. Let

$$I_\alpha^n = \begin{cases} \left[\frac{1}{b_{3,1}}\left(\frac{1}{\alpha} - b_{3,2}\right) C_+^n, -\frac{b_{3,2}}{b_{3,1}} C_-^n\right] & \text{if } \frac{1}{b_{3,1}}\left(\frac{1}{\alpha} - b_{3,2}\right) C_+^n < -\frac{b_{3,2}}{b_{3,1}} C_-^n, \\ \emptyset & \text{else.} \end{cases} \tag{11}$$

Then set $U_\sigma^n = \dfrac{u_{K,\sigma}^{n,1}}{u_{K,\sigma}^{n,2}}$ and

$$\rho_\sigma^{n,*,\sigma} = \begin{cases} \text{A-MUSCL}(\check{\rho}_\sigma^{n,*,\sigma}; u_{K,\sigma}^{n,2}, \rho^{n,*,\sigma}) & \text{if } U_\sigma^n \in I_\alpha^n \\ \text{A-MUSCL}(\check{\rho}_\sigma^{n,*,\sigma}; u_{K,\sigma}^{n,2}, \rho^{n,2}) & \text{if } U_\sigma^n \notin I_\alpha^n \end{cases} \tag{12}$$

Optimal RK method: midpoint rule, for the largest I_α^n interval (regardless of α)

$$\begin{array}{c|cc} 0 & 0 & \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array} \tag{13}$$

Theorem 1

Let $\alpha > 0$. Under the following CFL-like condition:

$$\frac{\delta t^n}{|K|} < \frac{\alpha}{\sum_{\sigma \in \mathcal{E}(K)} |\sigma| |u_{K,\sigma}^{n,2}|}, \tag{14}$$

if ρ^n is positive, so is ρ^{n+1}.

Remark: this allows to take δt^n up to 2α times larger than with a standard RK method while preserving positivity.

Choice of $\alpha \in (1/2, 1)$: influences the length of I_α^n

- smaller α: better accuracy,
- bigger α: larger time-step.

System of non-linear convection equations:

$$\partial_t \rho + \mathrm{div}(\rho \boldsymbol{u}) = 0, \tag{15a}$$

$$\partial_t(\rho u) + \mathrm{div}(\rho u \boldsymbol{u}) = 0. \tag{15b}$$

Velocity discretization: standard staggered finite volume method, midpoint time-discretization

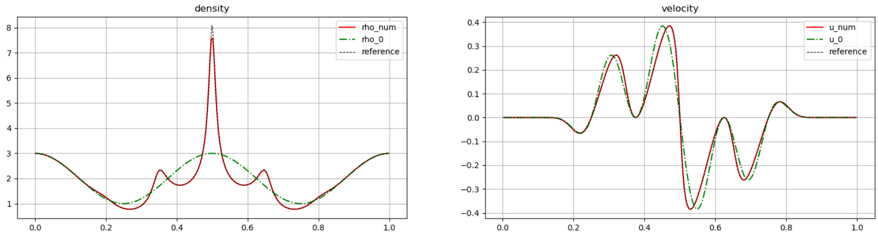


Figure: PP-ERK method, $\alpha = 0.9$, CFL = 1.7, $N_x = 256$

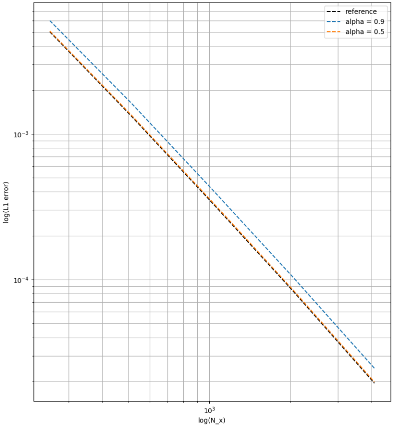


Figure: L^1-error. PP-ERK method. $\alpha = 0.9$, CFL = 1.7 (blue); $\alpha = 0.5$, CFL = 0.95 (orange).

Remark: For convection equations, the accuracy is not influenced a lot by α.

- Discretization of convection operators.
- Positivity-preserving method (under CFL condition).
- Time-steps up to 2α times larger than standard RK methods, with α close to 1.
- Second-order numerical accuracy.

Viscous Euler equations

Ω open bounded connected subset of $\mathbb{R}^d$, d the space dimension, $T > 0$ final time
$\rho : (0,T) \times \Omega \to \mathbb{R}$ density, $\quad \boldsymbol{u} : (0,T) \times \Omega \to \mathbb{R}^d$ velocity, $\quad p : (0,T) \times \Omega \to \mathbb{R}$ pressure,
$E : (0,T) \times \Omega \to \mathbb{R}$ energy, $\quad e : (0,T) \times \Omega \to \mathbb{R}$ internal energy

Viscous Euler equations:

$$\partial_t \rho + \mathrm{div}(\rho \boldsymbol{u}) = 0 \qquad \text{(Mass balance equation)}$$

$$\forall 1 \leq i \leq d, \qquad \partial_t(\rho u_i) + \mathrm{div}(\rho u_i \boldsymbol{u}) + (\nabla p)_i = \mathrm{div}(\lambda_{\boldsymbol{u}} G(\boldsymbol{x}) \nabla u_i) \qquad \text{(Momentum balance equation)}$$

$$\partial_t(\rho E) + \mathrm{div}(\rho E \boldsymbol{u}) + \mathrm{div}(p \boldsymbol{u}) - \mathrm{div}(\lambda_e G(\boldsymbol{x}) \nabla e) = 0 \qquad \text{(Total energy balance equation)}$$

$$p = (\gamma - 1)\rho e \qquad \text{(Equation of state)}$$

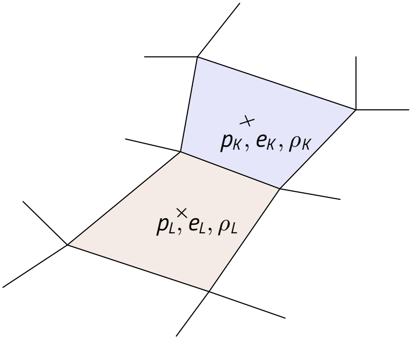
$$E = \frac{1}{2}|\boldsymbol{u}|^2 + e \qquad \text{(Energy)}$$

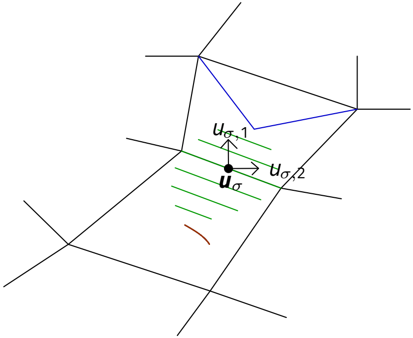
with $\lambda_{\boldsymbol{u}}$ and λ_e constant diffusion coefficients, G smooth function with compact support $\subset \Omega$

Initial conditions: $\rho_0, \boldsymbol{u}_0, e_0$, with $\rho_0 > 0$, $e_0 > 0$.

Boundary conditions: $\boldsymbol{u} = 0$, $\nabla e \cdot \boldsymbol{n} = 0$ on $\partial\Omega$.

Unstructured meshes, mix of quadrangles and triangles (2D) or hexaedra and simplices (3D), staggered.





Primal mesh

Cells : K, L, M

Scalar unknowns: p_K, e_K, ρ_K

Dual mesh

Cells : D_σ

Velocity unknowns: $\boldsymbol{u}_\sigma = (u_{\sigma,1}, \ldots, u_{\sigma,d})$

Inviscid part: 4-stage Segregated-RK (SRK), explicit and implicit midpoint rules

$$\begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{4} & \frac{1}{4} & 0 & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \\ \frac{3}{4} & 0 & \frac{1}{2} & \frac{1}{4} & 0 \\ \hline & 0 & \frac{1}{2} & 0 & \frac{1}{2} \end{array} \qquad \begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{4} & 0 & \frac{1}{4} & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \\ \frac{3}{4} & 0 & \frac{1}{2} & 0 & \frac{1}{4} \\ \hline & 0 & \frac{1}{2} & 0 & \frac{1}{2} \end{array} \tag{17}$$

Diffusive terms: 2-stage Non-standard Diagonally Implicit RK with Explicit first step (NEDIRK):

$$\begin{array}{c|ccc} 0 & 0 & & \\ 1 & 0 & 1 & \\ \hline & \frac{1}{2} & 0 & \frac{1}{2} \end{array} \tag{18}$$

Numerical scheme: for ODE $y'(t) = f(y(t)) + g(y(t)) + h(y(t))$

Stage 1:

$$y^{n,2} - \frac{\delta t^n}{4} g(y^{n,2}) = y^{n,1} + \frac{\delta t^n}{4} f(y^{n,1}), \tag{19}$$

Stage 2:

$$\tilde{y}^{n,3} = y^{n,2} - \frac{\delta t^n}{4} f(y^{n,1}) + \frac{\delta t^n}{2} f(y^{n,2}) + \frac{\delta t^n}{4} g(y^{n,2}), \tag{20}$$

$$y^{n,3} - \delta t^n h(y^{n,3}) = \tilde{y}^{n,2} \tag{21}$$

Stage 3:

$$y^{n,4} - \frac{\delta t^n}{4} g(y^{n,4}) = y^{n,3} + \frac{\delta t^n}{4} f(y^{n,3}), \tag{22}$$

Stage 4:

$$\tilde{y}^{n,5} = y^{n,4} - \frac{\delta t^n}{4} f(y^{n,3}) + \frac{\delta t^n}{2} f(y^{n,4}) + \frac{\delta t^n}{4} g(y^{n,4}), \tag{23}$$

$$y^{n+1} - \delta t^n h(y^{n+1}) = \tilde{y}^{n,5} \tag{24}$$

Internal energy formulation (staggered meshes).

- PP-ERK for convection operators,
- EDIRK staggered finite volume for pressure gradient (dual of discrete finite volume divergence),
- EIDIRK TPFA for diffusion terms.

$$\partial_t \rho + \mathrm{div}(\rho \boldsymbol{u}) = 0, \tag{25a}$$

$$\partial_t(\rho e) + \mathrm{div}(\rho e \boldsymbol{u}) + p\mathrm{div}(\boldsymbol{u}) - \mathrm{div}(\lambda_e G(\boldsymbol{x})\nabla e) = 0, \tag{25b}$$

$$p = (\gamma - 1)\rho e, \tag{25c}$$

$$\forall 1 \leq i \leq d, \qquad \partial_t(\rho u_i) + \mathrm{div}(\rho u_i \boldsymbol{u}) + (\nabla p)_i = \mathrm{div}(\lambda_{\boldsymbol{u}} G(\boldsymbol{x})\nabla u_i), \tag{25d}$$

Under the CFL-like condition:

Theorem 2

$$\frac{\delta t^n}{|K|} \leq \frac{1}{2 \displaystyle\sum_{\sigma \in \mathcal{E}(K)} |\sigma||u_{K,\sigma}^{n,2}|}, \tag{26}$$

if $\rho^n > 0$, then $\rho^{n+1} > 0$.

Comparison with segregated Euler scheme: δt^n_{ref} the maximum time-step of a segregated Euler scheme with implicit diffusion

- **Material CFL:** up to 4α times larger
- **Acoustic CFL:** segregated scheme, not truly implicit so the acoustic CFL is required. Up to 2 times larger.
- **Parabolic CFL:** no parabolic CFL as the RK method for the diffusion is A-stable
- **Time-step:** $2\delta t^n_{ref} \leq \delta t^n \leq 4\delta t^n_{ref}$
- **Efficiency:** 2 convection stage per δt^n_{ref}, 1 diffusion stage per δt^n_{ref}
- **Accuracy:** second-order accurate
- **Positivity preserving:** for ρ, for e under parabolic CFL

For the same number of diffusion stage (same number of systems to solve) as a segregated Euler scheme, the scheme is second-order accurate.

Numerical results I

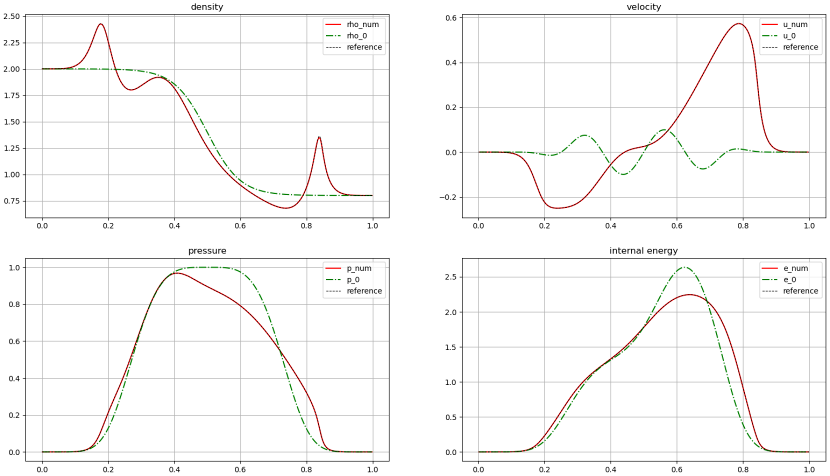


Figure: Test 1: $\lambda_e = 1/40$, $\lambda_{\boldsymbol{u}} = 1/60$. PP-IMEX method. $\alpha = 0.9$, $CFL_{ac} = 1.9$, $CFL_{mat} = 3.5$, $N_x = 256$.

Numerical results II

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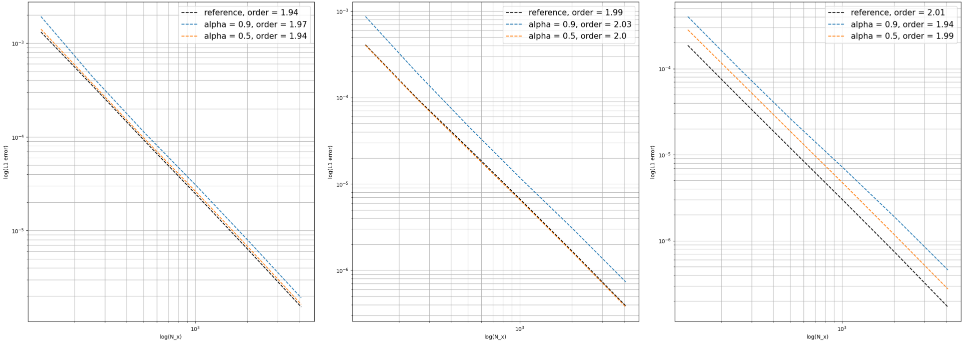

Figure: Test 1, L^1-errors. PP-IMEX method, $CFL_{ac} = 1.9$, $CFL_{mat} = 3.9\alpha$. ρ (left), e (centre), p (centre).

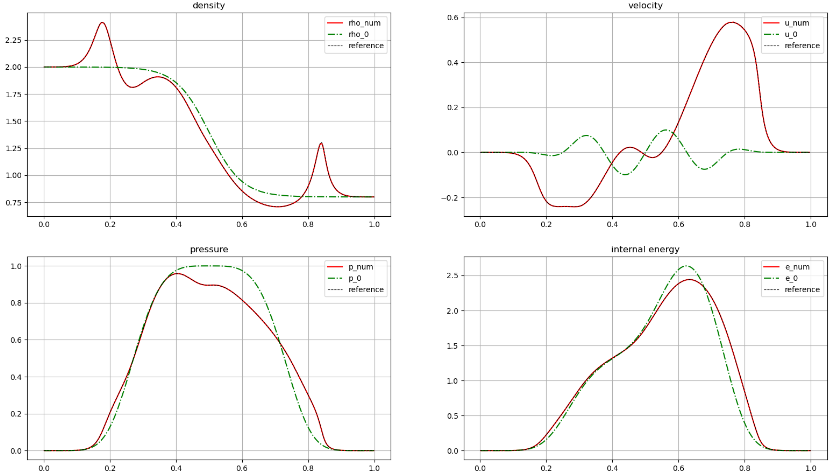

Figure: Test 2: $\lambda_e = 1/400$, $\lambda_{\boldsymbol{u}} = 1/600$. PP-IMEX method. $\alpha = 0.9$, $CFL_{ac} = 1.9$, $CFL_{mat} = 3.5$, $N_x = 256$.

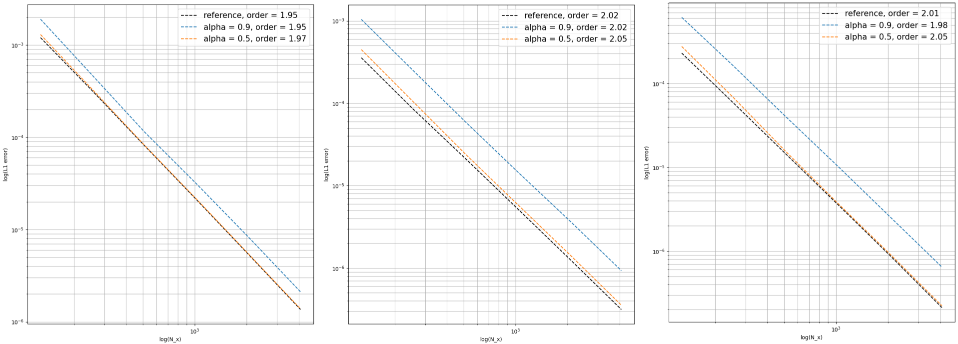

Figure: Test 2, L^1-errors. PP-IMEX method, $CFL_{ac} = 1.9$, $CFL_{mat} = 3.9\alpha$. ρ (left), e (centre), p (centre).

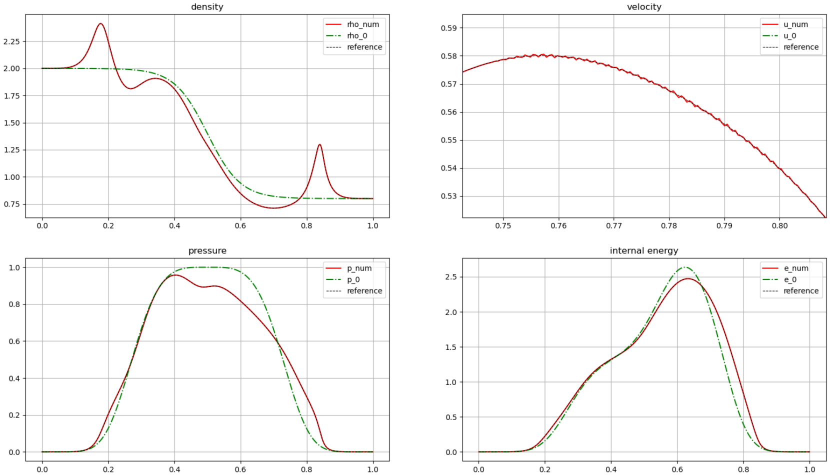

Figure: Test 3: $\lambda_e = 10^{-4}$, $\lambda_{\boldsymbol{u}} = 1/8 \times 10^{-5}$. PP-IMEX method. $\alpha = 0.9$, $CFL_{ac} = 1.9$, $CFL_{mat} = 3.5$, $N_x = 256$.

Numerical results VI

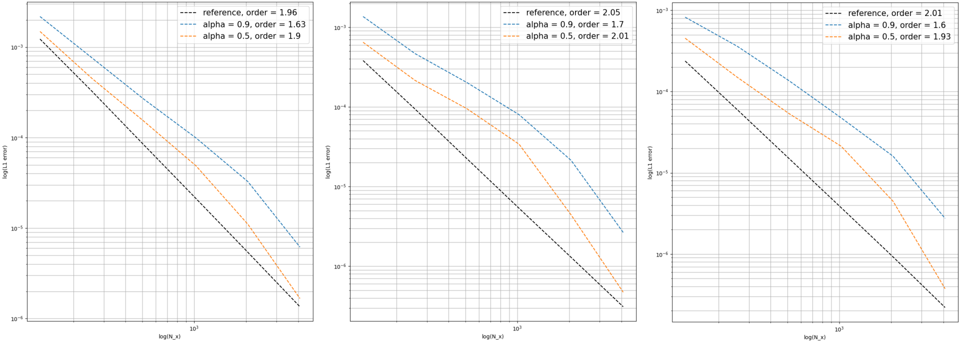

Figure: Test 3, L^1-errors. PP-IMEX method, $CFL_{ac} = 1.9$, $CFL_{mat} = 3.9\alpha$. ρ (left), e (centre), p (centre).

PP-IMEX method:

- numerical scheme for Viscous Euler equations
- second-order accurate when enough diffusion
- efficient: same number of implicit diffusion steps as a implicit/explicit Euler scheme, the inviscid part of the equations is computed fully explicitely.

Issue: when diffusion is too small, oscillations appear because:

- the scheme degenerates to a “bad” solver for Euler equations,
- or the diffusion introduces small oscillations because no parabolic CFL is enforced (the scheme remains stable because the RK method is A-stable).

Merci de votre attention !