Semi-implicit numerical method of arbitrary high order on non-uniform 1D meshes for hyperbolic problems

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Outline

Continuous problem

- Hyperbolic problem
- Relaxation model

Hyperbolic problem

Consider the following 1D hyperbolic system of conservation laws

$$\partial_t \mathbf{u} + \partial_x A(\mathbf{u}) = \mathbf{0} \tag{1}$$

with $\mathbf{u} : \mathbb{R} \times \mathbb{R}_+ \to \mathbb{R}^p$, $p \in \mathbb{N}$ and $A : \mathbb{R}^p \to \mathbb{R}^p$ a Lipschitz continuous flux.

In the context of fluid-structure interactions, the desired properties for the scheme are the following:

- Arbitrarily high order in time and space,
- CFL number larger or equal to unity (unlike fully explicit schemes),
- Computationally explicit scheme (implicit with the same complexity as an explicit one).

Relaxation system

Set the relaxing system

$$\partial_t \mathbf{F} + \partial_x \Lambda \mathbf{F} = \frac{\mathbb{M}(\mathbb{P}\mathbf{F}) - \mathbf{F}}{\varepsilon} \tag{2}$$

with $\mathbf{F} : \mathbb{R} \times \mathbb{R}_+ \to \mathbb{R}^{pk}$, $\mathbb{M} : \mathbb{R}^p \to \mathbb{R}^{pk}$ a Maxwellian function, $\mathbb{P} : \mathbb{R}^{pk} \to \mathbb{R}^p$ a linear operator and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_k) \in \mathcal{M}_{pk,pk}(\mathbb{R})$ a constant matrix.

By construction, the Maxwellian function must satisfy the following properties

- $\mathbb{P}\mathbb{M}(\mathbb{P}\mathbf{F}) = \mathbb{P}\mathbf{F}$,
- $\mathbb{P}\Lambda\mathbb{M}(\mathbb{P}\mathbf{F}) = A(\mathbb{P}\mathbf{F})$,
- Monotone Maxwellian Function:

$$\forall \mathbf{u} \in \mathbb{R}^p,\ \sigma(\mathbb{M}_i'(\mathbf{u})) \subset [0, \infty[, \quad \forall i = 1, \ldots, k.$$

Chapman-Enskog expansion

Consider the relaxation system:

$$\partial_t \mathbf{F} + \partial_x \Lambda \mathbf{F} = \frac{\mathbb{M}(\mathbb{P}\mathbf{F}) - \mathbf{F}}{\varepsilon}. \tag{3}$$

1. Multiplying (3) by $\mathbb{P}$, we obtain

$$\partial_t \mathbb{P}\mathbf{F} + \partial_x \mathbb{P}\Lambda \mathbf{F} = 0.$$

2. Multiply (3) by $\mathbb{P}\Lambda$, then

$$\mathbb{P}\Lambda \mathbf{F} = A(\mathbb{P}\mathbf{F}) + O(\varepsilon).$$

3. It leads to

$$\partial_t \mathbb{P}\mathbf{F} + \partial_x A(\mathbb{P}\mathbf{F}) = O(\varepsilon).$$

Then $\mathbb{P}\mathbf{F} \to \mathbf{u}$ formally when $\varepsilon \to 0$.

For deeper analysis see [Bou99; Nat98].

Maxwellian function

Define the linear operator $\mathbb{P}$ as

$$\mathbb{P}\mathbf{F} := \sum_{i=1}^{k} \mathbf{F}_i.$$

Set $k \geq d + 1$ with d the spacial dimension, and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_k)$ such that $\sum_{i=1}^{k} \lambda_i = 0$. Set $S_\Lambda = \sum_{i=1}^{k} \lambda_i^2$, one can build $\mathbb{M}$ as:

$$\mathbb{M}_i(\mathbb{P}\mathbf{F}) = \frac{1}{k}\mathbb{P}\mathbf{F} + \frac{A(\mathbb{P}\mathbf{F})}{S_\Lambda}\lambda_i, \quad \forall i = 1 \ldots, k.$$

Monotone Maxwellian Function condition

$$\frac{1}{k} + \frac{\lambda_i}{|\Lambda|}\sigma_j \geq 0, \quad \forall i = 1, \ldots, k, \quad \forall j = 1, \ldots, p$$

where σ_j are the eigenvalues of the Jacobian of A.

Semi-implicit numerical scheme

- Time discretization: Deferred Correction method
- Space discretization
  - Finite Difference scheme
  - Finite Volume scheme
  - Equality of FD and FV fluxes

Discretization

Set on the mesh Ω the cells $\mathcal{C}_j$ of centers x_j and vertices $x_{j-\frac{1}{2}}$ and $x_{j+\frac{1}{2}}$ as follows:

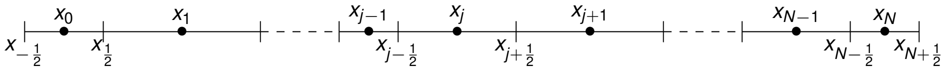


Figure 1: Non uniform mesh example.

Set δ a q-th order spatial derivative operator such that $\Lambda \frac{1}{\Delta x_j} \delta_j \mathbf{F} \approx \Lambda \frac{\partial \mathbf{F}}{\partial x}$. Let us assume that the error is $O(\Delta x^q)$. The relaxation model becomes:

$$\frac{\partial \mathbf{F}_j}{\partial t} + \frac{1}{\Delta x_j} \Lambda \delta_j \mathbf{F} = \frac{\mathbb{M}(\mathbb{P}\mathbf{F}_j) - \mathbf{F}_j}{\varepsilon} + O(\Delta x^q). \quad (4)$$

We will define the operator δ later. Let us focus on the time discretization for now: Deferred Correction [AT22].

Time discretization: Deferred Correction method

Set $q+1$ numbers $0 = c_0 < c_1 < \cdots < c_q = 1$ such that $\mathbf{F}_j^{n,i} \approx \mathbf{F}(x_j, t^n + c_i\Delta t)$ with $\mathbf{F}_j^{n,0} = \mathbf{F}_j^n$ and $\mathbf{F}_j^{n,q} = \mathbf{F}_j^{n+1}$.

Set $\quad \mathcal{F}_j = \begin{pmatrix} \mathbf{F}_j^{n,1} & \dots & \mathbf{F}_j^{n,q} \end{pmatrix}^T \quad$ and $\quad \mathcal{F}_j^{(0)} = \begin{pmatrix} \mathbf{F}_j^{n,0} & \dots & \mathbf{F}_j^{n,0} \end{pmatrix}^T$.

Set $\mathcal{L}^2$ an implicit high order accurate operator, and $\mathcal{L}^1$ an explicit lower order operator. Our objective is to solve $\mathcal{L}^2(\mathcal{F}) = 0$.

Example (Order 2: Crank-Nicolson)

At order 2, set $q = 1$. Then

$$\mathcal{L}^2(\mathbf{F}_j^{n+1}) = \mathbf{F}_j^{n+1} - \mathbf{F}_j^n + \frac{\Delta t}{2\Delta x_j}\left(\delta_j \Lambda \mathbf{F}^n + \delta_j \Lambda \mathbf{F}^{n+1}\right) - \frac{\Delta t}{2\varepsilon} \underbrace{\left((\mathbb{M}(\mathbb{P}\mathbf{F}_j^n) - \mathbf{F}_j^n) + (\mathbb{M}(\mathbb{P}\mathbf{F}_j^{n+1}) - \mathbf{F}_j^{n+1}) \right)}_{\mathcal{S}}.$$

and

$$\mathcal{L}^1(\mathbf{F}_j^{n+1}) = \mathbf{F}_j^{n+1} - \mathbf{F}_j^n + \underbrace{\frac{\Delta t}{\Delta x_j}\delta_j \Lambda \mathbf{F}^n}_{\text{Forward Euler discretization}} - \underbrace{\frac{\Delta t}{2\varepsilon}\mathcal{S}}_{\text{As for } \mathcal{L}^2}.$$

Dec iterations

Deferred Correction method at order $M = q + 1$:

1. set, for any j, $\mathcal{F}_j^{(0)} = \begin{pmatrix} \mathbf{F}_j^n & \dots & \mathbf{F}_j^n \end{pmatrix}^T$;
2. solve, for $p = 0, \dots, M-1$:
$$\mathcal{L}^1(\mathcal{F}_j^{(p+1)}) = \mathcal{L}^1(\mathcal{F}_j^{(p)}) - \mathcal{L}^2(\mathcal{F}_j^{(p)});$$
3. set $\mathcal{F}_j^{n+1} = \mathcal{F}_j^{(M)}$.

Example (Order 2: Crank-Nicolson)

Step 2 of the DeC method gives, for $p \in \{0, 1\}$:

$$\mathbf{F}_j^{n+1,(p+1)} = \left(1 + \frac{\Delta t}{2\varepsilon}\right)^{-1} \left(\frac{\Delta t}{2\varepsilon}\mathbb{M}(\mathbb{P}\mathbf{F}_j^{n+1,(p+1)}) + \mathbf{F}_j^n - \frac{\Delta t}{2\Delta x_j}(\delta_j \Lambda \mathbf{F}^{n+1,(p)} + \delta_j \Lambda \mathbf{F}^n) + \frac{\Delta t}{2\varepsilon}(\mathbb{M}(\mathbb{P}\mathbf{F}_j^n) - \mathbf{F}_j^n)\right),$$

with

$$\mathbb{P}\mathbf{F}_j^{n+1,(p+1)} = \mathbb{P}\mathbf{F}_j^n - \frac{\Delta t}{2\Delta x_j}(\mathbb{P}\delta_j \Lambda \mathbf{F}^{n+1,(p)} + \mathbb{P}\Lambda \delta_j \mathbf{F}^n).$$

This method is:

- computationally explicit;
- L^2 stable on uniform meshes for a CFL condition of a few units;
- compatible with $\varepsilon = 0$.

Space discretization: Finite Differences method

Objective: define δ such that

$$\frac{1}{\Delta x_j}\Lambda\delta_j\mathbf{F} \approx \partial_x\Lambda\mathbf{F}(x_j,t)$$

Set $\mathbf{F}_j \approx \mathbf{F}(x_j)$, and L_j the Lagrange polynomial of degree $q = r + s$ that interpolates $\mathbf{F}$ in $\{\mathbf{F}_{j+i}; i \in S_j\}$, with $|S_j| = q + 1$ such that

$$\lambda L_j(x) = \lambda \sum_{l=-s}^{r} F_{j+l} \prod_{\substack{i=-s\\ i\neq l}}^{r} \frac{x - x_{j+i}}{x_{j+l} - x_{j+i}}, \text{ if } \lambda \geq 0.$$

The spatial derivative operator δ_j is defined as follows: $\frac{1}{\Delta x_j}\lambda\delta_j F = \lambda L_j'(x_j)$.

Properties of the FD scheme

- Arbitrary high order on non-uniform meshes,
- Writes as a difference of fluxes on uniform meshes (conservativity),
- Non conservative on non-uniform meshes,
- Lax-Wendroff theorem under restrictive conditions on the mesh.

Finite Volume scheme

Set $\overline{\mathbf{F}}_j \approx \frac{1}{\Delta x_j} \int_j \mathbf{F}(x)dx$. Consider $\mathbf{P}_j$ a polynomial of degree $q-1$, built such that

$$\frac{1}{\Delta x_j} \int_i \mathbf{P}_j(x)dx = \overline{\mathbf{F}}_i, \quad \forall i \in \mathcal{S}_j,$$

where $\mathcal{S}_j$ is the stencil of the reconstruction ($|\mathcal{S}_j| = q-1$ and if $\lambda \geq 0$, $\mathcal{S}_j = \{j-s+1, \ldots, j+r\}$). Set $\mathbf{F}_{j+\frac{1}{2}} = \mathbf{P}_j(x_{j+\frac{1}{2}})$ the numerical flux. The spatial derivative operator δ_j is given by

$$\frac{1}{\Delta x_j} \Lambda \delta_j \mathbf{F} = \frac{1}{\Delta x_j} \Lambda (\mathbf{F}_{j+\frac{1}{2}} - \mathbf{F}_{j-\frac{1}{2}}).$$

Reconstruction of the flux A: set $\mathcal{P}_j(g_i) \approx A(\mathbf{u}(g_i))$ with g_i the points of Gauss quadrature formula of q-th order in the j-th cell, then

$$\overline{A(\mathbf{u})}_j = \frac{1}{\Delta x_j} \sum_i \omega_i \mathcal{P}_j(g_i).$$

Finite Volume scheme

Properties of the FV scheme

- Arbitrary high order on non-uniform meshes with reconstruction of the flux function $A(\mathbf{u})$,
- Conservative by construction,
- Consistency of the limit scheme ($\varepsilon = 0$) with the initial conservation law (1),
- Consistency of the scheme $\varepsilon \neq 0$ with the relaxing system (3),
- Lax-Wendroff theorem adapted to our problem on non-uniform mesh: $\mathbb{P}\mathbf{F}_h^0 \rightharpoonup \mathbf{u}$ as $h \to 0$.

Similarities between FD and FV schemes

Proposition

The FD and FV fluxes are identical on uniform meshes.

Sketch of the proof

- The FD scheme can write as a difference of fluxes on uniform meshes

$$\frac{\lambda}{\Delta x}\delta_j F = \frac{\lambda}{\Delta x}\sum_{l=-s}^{r}\gamma_l F_{j+l} = \frac{\lambda}{\Delta x}(F^D_{j+\frac{1}{2}} - F^D_{j-\frac{1}{2}}),$$

where

$$\begin{aligned} F^D_{j+\frac{1}{2}} &= \sum_{l=-s+1}^{r}(\sum_{i=l}^{r}\gamma_i)F_{j+l}, \\ &= \sum_{\substack{l=-s+1 \\ l\neq 0}}^{r}\left(\sum_{i=l}^{r}\gamma_i\right)\left(F_{j+l}-F_j\right) + \underbrace{\sum_{l=-s+1}^{r}(\sum_{i=l}^{r}\gamma_i)}_{=1} F_j, \\ &= \boldsymbol{\beta}\cdot B_j + F_j. \end{aligned}$$

with for all $l \in \{-s+1,\dots,r\},\ l\neq 0,\ (B_j)_l = F_{j+l}-F_j$ and $\boldsymbol{\beta}_l = \sum_{i=l}^{r}\gamma_i$.

Similarities between FD and FV schemes

- On the other hand, the FV fluxes write

$$F^{v}_{j+\frac{1}{2}} = P_j(x_{j+\frac{1}{2}}) = \sum_{l=0}^{r+s-1} \alpha_j^l e_j^l(x_{j+\frac{1}{2}}) + F_j,$$

where e_j^l is the l-th element of the polynomial basis of degree at most q, and α_j^l are obtained when solving $Q^{-1}B_j$ with for all $i \in \{-s+1, \ldots, r\}$, $i \neq 0$ and $l \in \{1, \ldots, r+s-1\}$

$$Q_{il} = \frac{\Delta x^l}{l+1}\Big(\big(i+\frac{1}{2}\big)^{l+1} - \big(i-\frac{1}{2}\big)^{l+1} - \big(\frac{1}{2}\big)^{l+1} + \big(-\frac{1}{2}\big)^{l+1}\Big).$$

Then

$$\begin{aligned} F^{v}_{j+\frac{1}{2}} &= \sum_{l=0}^{r+s-1} (Q^{-1}B_j)_l e_j^l(x_{j+\frac{1}{2}}) + F_j, \\ &= (Q^{-1}B_j) \cdot E_j(x_{j+\frac{1}{2}}) + F_j, \\ &= B_j \cdot (Q^{-T} E_j(x_{j+\frac{1}{2}})) + F_j. \end{aligned}$$

where $E_j(\cdot) = (e_j^1(\cdot), \ldots, e_j^{r+s-1}(\cdot))^T$.

Similarities between FD and FV schemes

Finally, proving that the FD and FV fluxes are identical on a uniform mesh is equivalent to showing that

$$
\begin{aligned}
& F^D_{j+\frac{1}{2}} = F^V_{j+\frac{1}{2}} \\
\Longleftrightarrow\ & \beta \cdot B_j + F_j = B_j \cdot (Q^{-T} E_j(x_{j+\frac{1}{2}})) + F_j \\
\Longleftrightarrow\ & \beta = Q^{-T} E_j(x_{j+\frac{1}{2}}).
\end{aligned}
$$

Using some properties of the coefficients γ_l of the FD scheme and Bernoulli polynomials, the equality is verified.

$\Rightarrow$ Paper in preparation with the details of the proof.

Numerical results

- Smooth isentropic test case
- Sod shock tube

Euler equations

Consider the 1D system of conservation laws (1), setting

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} \text{ and } A(\mathbf{u}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(\rho E + p) \end{pmatrix},$$

with the following equation of state for an ideal gas

$$p = (\gamma - 1)\rho\varepsilon \text{ where } \varepsilon = E - \frac{u^2}{2}.$$

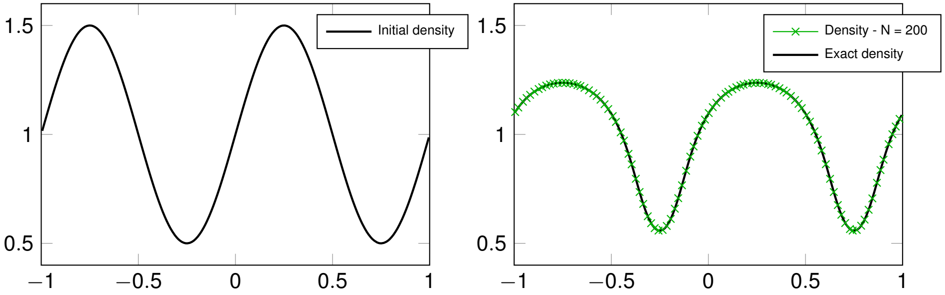
Consider the 2 waves scheme with MMF condition

$$\lambda \geq |u| + c.$$

Smooth isentropic test case

Set the initial condition

$$\begin{cases} \rho_0(x) = 1 + 0.5\sin(2\pi x), \\ u_0(x) = 0, \\ p_0(x) = \rho^\gamma(x, 0) \\ \gamma = 3. \end{cases}$$



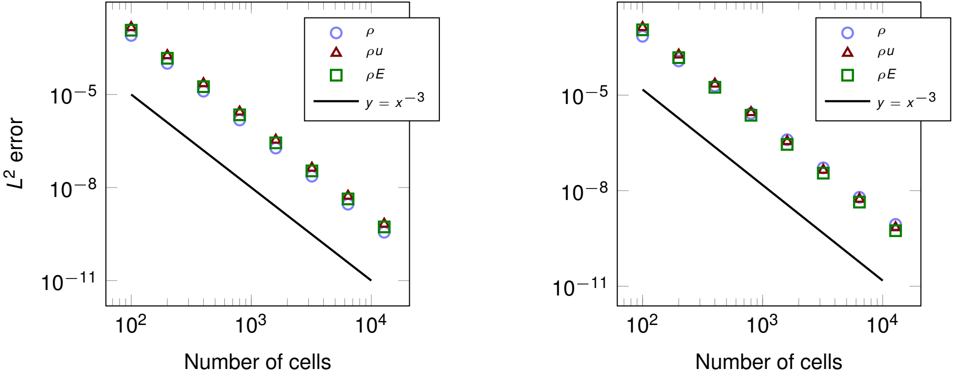
(a) Initial state

(b) Final time T = 0.08

Figure 2: Density of the smooth isentropic test case, 2-waves model, FV scheme, 3rd order, non-uniform mesh.

Smooth isentropic test case

Set the CFL number to 1: $\Delta t = \frac{\Delta x_{\min}}{\lambda}$. Non-uniform mesh: $\frac{\Delta x_{\max}}{\Delta x_{\min}} = 11.35$.



(a) Finite Difference scheme

(b) Finite Volume scheme

Figure 3: L^2-error of the 2 waves FD and FV schemes on non-uniform mesh for the smooth test case at time $T = 0.08$.

Sod test case

Set the initial condition

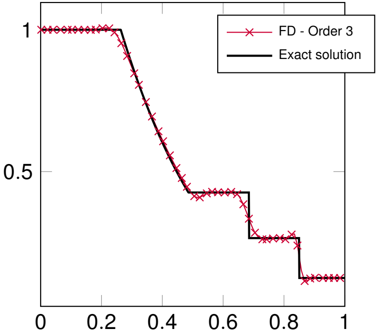
$$\begin{cases} \rho_0(x) = \mathbb{1}_{x<0.5} + 0.125 \times \mathbb{1}_{x\geq 0.5}, \\ u_0(x) = 0, \\ p_0(x) = \mathbb{1}_{x<0.5} + 0.1 \times \mathbb{1}_{x\geq 0.5}. \end{cases}$$

Set $\gamma = 1.4$.

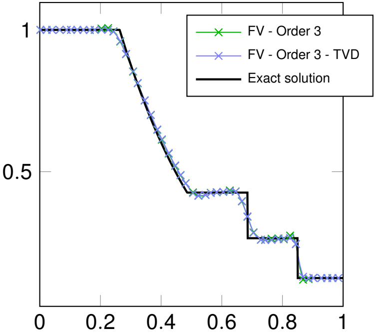
Sod test case

Set the final time $T = 0.2$, $N = 100$ points and the CFL number to 1: $\Delta t = \dfrac{\Delta x_{\min}}{\lambda}$.

Non-uniform mesh: $\dfrac{\Delta x_{\max}}{\Delta x_{\min}} = 11.35$.



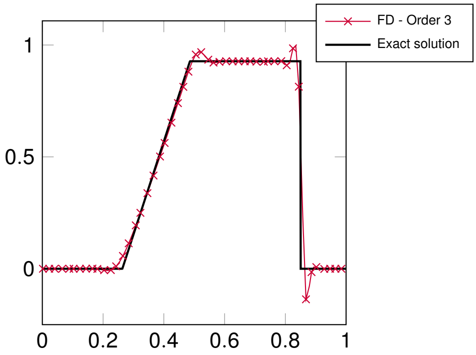
(a) Finite Difference scheme



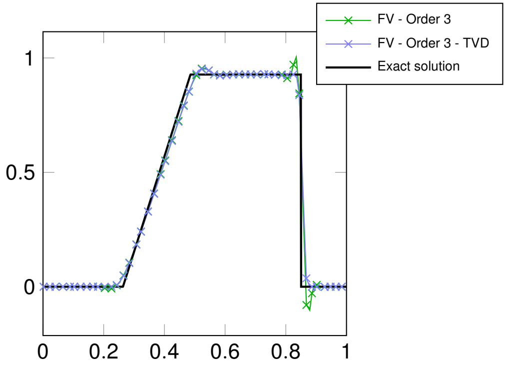
(b) Finite Volume scheme

Figure 4: Density, Sod shock tube with 2-waves model, FD and FV scheme of third order with and without TVD flux limitation on non-uniform mesh. Solution displayed with $N = 100$ cells.

Sod test case



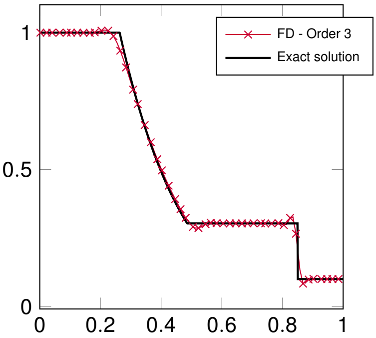
(a) Finite Difference scheme



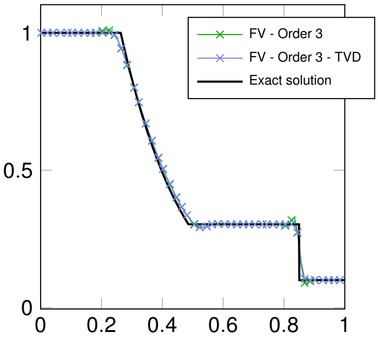
(b) Finite Volume scheme

Figure 5: Velocity, Sod shock tube with 2-waves model, FD and FV scheme of third order with and without TVD flux limitation on non-uniform mesh. Solution displayed with $N = 100$ cells.

Sod test case



(a) Finite Difference scheme



(b) Finite Volume scheme

Figure 6: Pressure, Sod shock tube with 2-waves model, FD and FV scheme of third order with and without TVD flux limitation on non-uniform mesh. Solution displayed with $N = 100$ cells.

Conclusion and perspectives

Conclusion

- Two computationally explicit schemes of arbitrary high order on **non-uniform** meshes that share the same fluxes on uniform meshes.
- Finite Differences scheme:
  - good results despite non-conservativity,
  - Lax-Wendroff theorem under restrictive conditions.
- Finite Volume scheme:
  - consistency of the limit scheme ($\varepsilon = 0$) with the initial conservation law (1),
  - consistency of the scheme $\varepsilon \neq 0$ with the relaxing system (3),
  - Lax-Wendroff theorem on non-uniform mesh.
- k-waves scheme implemented at order up to 3 in time and space for scalar (transport, Burgers) and vector (waves equation, Euler) problems.

Perspectives

- Lagrangian scheme: 1st results at order 1,
- Hyperelasticity model, fluid-structure coupling,
- 2D, unstructured meshes.

Thank you for your attention

[AT22] Rémi Abgrall and Davide Torlo. "Some preliminary results on a high order asymptotic preserving computationally explicit kinetic scheme". In: *Communications in Mathematical Sciences* 20.2 (2022), pp. 297–326. DOI: 10.4310/cms.2022.v20.n2.a1.

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