# High-order Implicit relaxation schemes for hyperbolic models

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### Outline

Physical and mathematical context

Relaxation methods

Discretization

Numerical results

Conclusion and perspectives





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### Physical and mathematical context



- Fusion DT: At sufficiently high energies, deuterium and tritium can fuse to Helium. Free energy is released. At those energies, the atoms are ionized forming a plasma (which can be controlled by magnetic fields).
- Tokamak: toroidal room where the plasma is confined using powerful magnetic fields.
- The simulation of these instabilities is an important subject for ITER.
- Difficulty: plasma instabilities.
  - Disruptions: Violent instabilities which can critically damage the Tokamak.
  - Edge Localized Modes (ELM): Periodic edge instabilities which can damage the Tokamak.







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# MHD in Tokamak I

#### Simplify Extended MHD

$$\begin{array}{l} & (\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = \boldsymbol{0}, \\ & \rho \partial_t \boldsymbol{u} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla \rho + \nabla \cdot \boldsymbol{\Pi} = \boldsymbol{J} \times \boldsymbol{B}, \\ & \partial_t \rho + \boldsymbol{u} \cdot \nabla \rho + \rho \nabla \cdot \boldsymbol{u} + \nabla \cdot \boldsymbol{q} = \eta \mid \boldsymbol{J} \mid^2 \\ & \partial_t \boldsymbol{B} = -\nabla \times (-\boldsymbol{u} \times \boldsymbol{B} + \eta \boldsymbol{J}), \\ & \nabla \times \boldsymbol{B} = \mu_0 \boldsymbol{J}, \quad \nabla \cdot \boldsymbol{B} = \boldsymbol{0} \end{array}$$

with  $\rho$  the density, *p* the pressure, **u** the velocity, *B* the magnetic field, *J* the current,  $\Pi$  stress tensor and **q** the heat flux.

#### MHD specificities in Tokamak

- Strong anisotropic flows (direction on the magnetic field) ===> complex geometries and aligned meshes (flux surface or magnetic field lines).
- MHD scaling:
  - **B\_{\parallel} direction**: compressible flow and large diffusion.
  - **B**<sub> $\perp$ </sub> direction: quasi incompressible flow and small diffusion.
- □ **MHD Scaling** ===> compressible code with no discontinuities + fast waves.
- Quasi stationary flows + fast waves ===> implicit or semi implicit schemes.



### Hyperbolic systems and implicit schemes

We consider the general problem

 $\partial_t \boldsymbol{U} + \partial_x (\boldsymbol{F}(\boldsymbol{U})) = \nu \partial_x (D(\boldsymbol{U}) \partial_x \boldsymbol{U})$ 

- with  $\boldsymbol{U}: \mathbb{R}^n \longrightarrow \mathbb{R}^n$  (idem for  $\boldsymbol{F}(\boldsymbol{U})$ ) and D a matrix.
- In the following we consider the limit  $\nu << 1$ .

#### Implicit schemes

- **Implicit scheme**: allows to avoid the CFL condition filtering the fast phenomena.
- Problem: Direct solvers are not useful in 3D (too large matrices), we need iterative solvers.
- Conditioning of the implicit matrix: given by the ratio of the maximal and minimal eigenvalues.
- Implicit scheme :

$$\boldsymbol{U} + \Delta t \partial_x (\boldsymbol{F}(\boldsymbol{U})) - \Delta t \nu \partial_x (\boldsymbol{D}(\boldsymbol{U}) \partial_x \boldsymbol{U}) = \boldsymbol{U}^n$$

• At the limit  $\nu \ll 1$  and  $\Delta t \gg 1$  (large time step) we solve  $\partial_x F(U) = 0$ .

#### Issues of implicit schemes

Conclusion: for ν << 1 and Δt >> 1 the condition number of the full system closed to conditioning number of the steady hyperbolic model (the ratio of the speed waves).

**Relaxation methods** 







### General principle

We consider the following nonlinear system

$$\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = \nu \partial_x (D(\boldsymbol{U}) \partial_x \boldsymbol{U}) + \boldsymbol{G}(\boldsymbol{U})$$

- with U a vector of N functions.
- Aim: Find a way to approximate this system with a sequence of simple systems.
- Idea: Xin-Jin relaxation method (very popular in the hyperbolic and finite volume community).

$$\begin{cases} \partial_t \boldsymbol{U} + \partial_x \boldsymbol{V} = \boldsymbol{G}(\boldsymbol{U}) \\ \partial_t \boldsymbol{V} + \alpha^2 \partial_x \boldsymbol{U} = \frac{1}{\varepsilon} (\boldsymbol{F}(\boldsymbol{U}) - \boldsymbol{V}) \end{cases}$$

#### Limit of the hyperbolic relaxation scheme

The limit scheme of the relaxation system is

$$\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = \boldsymbol{G}(\boldsymbol{U}) + \epsilon \partial_x ((\alpha^2 - |\boldsymbol{A}(\boldsymbol{U})|^2) \partial_x \boldsymbol{U}) + \epsilon \partial_x \boldsymbol{G}(\boldsymbol{U}) + \boldsymbol{o}(\epsilon^2)$$

 $\square$  with A(U) the Jacobian of F(U).

Conclusion: the relaxation system is an approximation of the hyperbolic original system (error in ε).

Stability: the limit system is dissipative if  $(\alpha^2 - |A(U)|^2) > 0$ .



### General principle II

#### Generalization

The generalized relaxation is given by

$$\begin{cases} \partial_t \boldsymbol{U} + \partial_x \boldsymbol{V} = \boldsymbol{G}(\boldsymbol{U}) \\ \partial_t \boldsymbol{V} + \alpha^2 \partial_x \boldsymbol{U} = \frac{R(\boldsymbol{U})}{\varepsilon} (\boldsymbol{F}(\boldsymbol{U}) - \boldsymbol{V}) + \boldsymbol{H}(\boldsymbol{U}) \end{cases}$$

The limit scheme of the relaxation system is

 $\begin{aligned} \partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) &= \boldsymbol{G}(\boldsymbol{U}) \\ &+ \varepsilon \partial_x (\boldsymbol{R}(\boldsymbol{U})^{-1} (\alpha^2 - |\boldsymbol{A}(\boldsymbol{U})|^2) \partial_x \boldsymbol{U}) + \varepsilon \partial_x (\boldsymbol{A}(\boldsymbol{U}) \boldsymbol{G}(\boldsymbol{U}) - \boldsymbol{H}(\boldsymbol{U})) + \boldsymbol{o}(\varepsilon^2) \end{aligned}$ 

#### Treatment of small diffusion

□ Taking  $R(\boldsymbol{U}) = (\alpha^2 - |A(\boldsymbol{U})|^2)D(\boldsymbol{U})^{-1}$ ,  $\varepsilon = \nu$  and  $H(\boldsymbol{U}) = A(\boldsymbol{U})\boldsymbol{G}(\boldsymbol{U})$ : we obtain the following limit system

 $\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = \boldsymbol{G}(\boldsymbol{U}) + \nu \partial_x (D(\boldsymbol{U}) \partial_x \boldsymbol{U}) + o(\nu^2)$ 

• Limitation of the method: the relaxation model cannot approach PDE with high diffusion.



### Kinetic relaxation scheme

We consider the classical Xin-Jin relaxation for a scalar system  $\partial_t u + \partial_x F(u) = 0$ :

$$\begin{cases} \partial_t u + \partial_x v = 0\\ \partial_t v + \alpha^2 \partial_x u = \frac{1}{\varepsilon} (F(u) - v) \end{cases}$$

• We diagonalize the hyperbolic matrix  $\begin{pmatrix} 0 & 1 \\ \alpha^2 & 0 \end{pmatrix}$  and note  $f_+$  and  $f_-$  the new variables. We obtain

$$\begin{cases} \partial_t f_- - \alpha \partial_x f_- = \frac{1}{\varepsilon} (f_{eq}^- - f_-) \\ \partial_t f_+ + \alpha \partial_x f_+ = \frac{1}{\varepsilon} (f_{eq}^+ - f_+) \end{cases}$$

• with 
$$f_{eq}^{\pm} = \frac{u}{2} \pm \frac{F(u)}{2\alpha}$$

#### First Generalization

□ Main property: the transport is diagonal which can easily solved.

#### Remark

□ in the Lattice Boltzmann community the discretization of this model is called D1Q2.



### Generic kinetic relaxation scheme

#### Kinetic relaxation system

Considered model:

$$\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = 0, \qquad \partial_t \eta(\boldsymbol{U}) + \partial_x \zeta(\boldsymbol{U}) \leq 0$$

- Lattice:  $W = \{\lambda_1 ... \lambda_{n_v}\}$  a set of velocities.
- **•** Mapping matrix: P a matrix  $n_c \times n_v$   $(n_c < n_v)$  such that U = Pf, with  $U \in \mathbb{R}^{n_c}$ .
- Kinetic relaxation system:

$$\partial_t \boldsymbol{f} + \Lambda \partial_x \boldsymbol{f} = \frac{R}{\varepsilon} (\boldsymbol{f}^{eq}(\boldsymbol{U}) - \boldsymbol{f})$$

Equilibrium vector operator  $f^{eq}: R^{n_c} \to R^{n_v}$  such that  $Pf^{eq}(U) = U$ .

Consistance with the initial PDE:

$$\mathcal{C} \left\{ \begin{array}{c} P \boldsymbol{f}^{eq}(\boldsymbol{U}) = \boldsymbol{U} \\ P \Lambda \boldsymbol{f}^{eq}(\boldsymbol{U}) = F(\boldsymbol{U}) \end{array} \right.$$

- For source terms and small diffusion terms, it is the same that the first relaxation method.
- In 1D : same property of stability that the classical relaxation method.
- Limit of the system:

$$\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = \varepsilon \partial_x \left( \left( P \Lambda^2 \partial \boldsymbol{f}_{eq} - | \partial \boldsymbol{F}(\boldsymbol{U}) |^2 \right) \partial_x \boldsymbol{U} \right)$$



### Different kinetic models

#### ID models:

□ The  $[D1Q2]^n$  model. Two transport equations (velocities  $\lambda_{\pm}$ ) by physical variable.

□ The  $[D1Q3]^n$  model. Three transport equations (velocities  $\lambda_{\pm}$  and  $\lambda_0$ ) by physical variable. Based on flux-splitting method (Van-Leer etc).

#### Stability:

Kinetic entropy

$$H(\boldsymbol{f}) = \sum_{i=1}^{q} h_i(f_i^1, \dots, f_i^N)$$

is dissipate if

$$\sum_{i=1}^{q} h_i^*(\boldsymbol{\phi}) = \eta^*(\boldsymbol{\phi}), \quad \sum_{i=1}^{q} v_i h_i^*(\boldsymbol{\phi}) = \boldsymbol{\zeta}^*(\boldsymbol{\phi})$$

with  $\eta$  the macroscopic entropy,  $\boldsymbol{\zeta}$  the entropy flux and  $\boldsymbol{\phi} = \eta^{'}(\boldsymbol{U}).$ 

- $\Box$  Entropy stability for the  $[D1Q2]^n$  model.
- Entropy stability for the [D1Q3]<sup>n</sup> model if the flux splitting is entropy). Dissipative stability if not.

#### Models in d-dimension:

- □ The  $[DdQ(2d)]^n$  model. Generalization of  $[D1Q2]^n$  model with the same properties.
- □ The  $[DdQ(2d+1)]^n$  model. Generalization of  $[D1Q3]^n$ . Same properties ?
- □ The  $[DdQ(d^2)]^n$  model. Additional direction to have better accuracy for isotropic problem.



**Discretization methods** 







### Time discretization

#### Main property

- Relaxation system: "the nonlinearity is local and the non locality is linear".
- Main idea: splitting scheme between transport and the relaxation.
- Key point: the macroscopic variables are conserved during the relaxation step. Therefore f<sup>eq</sup>(U) explicit.

#### First order scheme

We define the two operators for each step :

$$T_{\Delta t} = I_d + \Delta t \Lambda \partial_x I_d$$

$$R_{\Delta t} = I_d - \Delta t \frac{\Delta t}{\varepsilon} (f^{eq}(U) - I_d)$$

- Asymptotic limit: Chapman-Enskog expansion.
- **Final scheme**:  $T_{\Delta t} \circ R_{\Delta t}$  is consistent with

$$\partial_{t}\boldsymbol{U} + \partial_{x}\boldsymbol{F}(\boldsymbol{U}) = \frac{\Delta t}{2}\partial_{x}(\boldsymbol{P}\Lambda^{2}\partial_{x}\boldsymbol{f}) + \left(\frac{\Delta t}{2} + \varepsilon\right)\partial_{x}\left(\left(\boldsymbol{P}\Lambda^{2}\partial_{\boldsymbol{U}}\boldsymbol{f}^{eq} - \boldsymbol{A}(\boldsymbol{U})^{2}\right)\partial_{x}\boldsymbol{U}\right) \\ + O(\varepsilon\Delta t + \Delta t^{2} + \varepsilon^{2})$$



### High-Order time schemes

#### Second-order scheme

- □ Scheme for transport step  $T(\Delta t)$ : Crank Nicolson or exact time scheme.
- □ Scheme for relaxation step  $R(\Delta t)$ : Crank Nicolson.
- Classical full second order scheme:

$$\Psi(\Delta t) = T\left(\frac{\Delta t}{2}\right) \circ R(\Delta t) \circ T\left(\frac{\Delta t}{2}\right).$$

AP full second order scheme:

$$\Psi_{ap}(\Delta t) = T\left(\frac{\Delta t}{4}\right) \circ R\left(\frac{\Delta t}{2}\right) \circ T\left(\frac{\Delta t}{2}\right) \circ R\left(\frac{\Delta t}{2}\right) \circ T\left(\frac{\Delta t}{4}\right).$$

 $\ \ \square \ \ \Psi \ \ \text{and} \ \ \Psi_{ap}(0) = \textit{I}_d.$ 

#### High order scheme

Using composition method

$$M_{\rho}(\Delta t) = \Psi_{a\rho}(\gamma_{1}\Delta t) \circ \Psi_{a\rho}(\gamma_{2}\Delta t) \dots \circ \Psi_{a\rho}(\gamma_{s}\Delta t)$$

- □ with  $\gamma_i \in [-1, 1]$ , we obtain a *p*-order schemes.
- Susuki scheme : s = 5, p = 4. Kahan-Li scheme: s = 9, p = 6.



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### Space discretization - transport scheme

### Whishlist

- Complex geometry, curved meshes (if possible),
- Flexibility, hp refinement,
- CFL-free,
- Matrix-free.

### Candidates for transport discretization

- Implicit FV-DG schemes,
- Semi-Lagrangian schemes,
- Stochastic schemes (Glimm or particle methods).

#### Choice on Cartesian meshes: SL-scheme.

- Choice on Complex geometry: Implicit DG schemes.
  - Implicit Cranck-Nicholson scheme
  - Block -Triangular matrix (Upwind scheme) solved avoiding storage of the matrix.





### Parallel transport solver

### Complex algorithm

- Velocities: the transport equations are independent. Possible parallelism.
- Transport step: partial parallelism given the implicit upwind scheme.
- Two parallelism: complex to manage.





#### Solution: StarPu

- Task-based scheduling library developed at INRIA Bordeaux.
- User submits tasks in a sequential order. StarPU schedules the tasks in parallel if possible.
- Possible MPI extension



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Figure: task graph for a 3D Torus.

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### Parallelism results

- Full D2Q9 scheme on square grids. Constant dof number per macrocell. Number N of macrocells N from 1 to 64 = 8×8.
  - □ for 1 macrocell : saturation at  $n_{core} = n_v$ . This is expected.
  - $\Box$  efficiency grows with N due to topological parallelism.



MPI scaling

□ Toroidal mesh : 720 macroelements × 3335 dof

Nthreads/Nmpi	1	2	3	4
14	6862	2772	1491	1014





### Parallelism results

- D3Q15, D3Q19, D3Q27 models on a cube with 4x4x4 elements and 8000 dof per elements with eager scheduler.
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  - $\Box$  efficiency grows with *N* due to topological parallelism.



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Numerical results





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### Burgers : quantitatives results

Model: Viscous Burgers equations

$$\partial_t \rho + \partial_x \left(\frac{\rho}{2}\right) = 0$$

- Kinetic model: (D1Q2) or D1Q3.
- Spatial discretization: SL-scheme, 5000 cells, order 7 space, order 2 time.
- Test 1:  $\rho(t = 0, x) = sin(2\pi x)$ , viscosity=  $10^{-4}$ .



Figure: Left: comparison between different D1Q2 and D1Q3 for different time step ( second order in time). Left up:  $\Delta t = 0.001$  (CFL 5-10), Right up:  $\Delta t = 0.005$  (CFL 20-50)



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- Test 2: rarefaction wave, no viscosity.



Figure: Left: comparison between different velocity set and time step . Left up:  $\Delta t = 0.001$  (CFL 1-5).  $V = \{-2.1, 2.1\}$  (violet)  $V = \{0.9, 2.1\}$  (green) ,  $V = \{-2.1, 0, 2.1\}$  (yellow) and  $V = \{0.9, 1.5, 2.1\}$  (blue), Right up: same for  $\Delta t = 0.01$  (CFL 10-50).



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- **Remark**: Choice of kinetic model important to minimize time numerical dispersion.
- **Remark:** Time numerical dispersion comes from to second order relaxation scheme  $f^* = 2f^{eq} f^n$ . More the wave structure is close to the original one more  $|f^{eq} f^n|$  is small. Reduce the oscillations around  $f^{eq}$ .



### 1D isothermal Euler : Convergence

Model: isothermal Euler equation

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0\\ \partial_t \rho u + \partial_x (\rho u^2 + c^2 \rho) = 0 \end{cases}$$

- **Lattice**:  $(D1 Q2)^n$  Lattice scheme.
- For the transport (and relaxations step) we use 6-order DG scheme in space.
- **Time step**:  $\Delta t = \beta \frac{\Delta x}{\lambda}$  with  $\lambda$  the lattice velocity.  $\beta = 1$  explicit time step.
- First test: acoustic wave with  $\beta = 50$  and  $T_f = 0.4$ , Second test: smooth contact wave with  $\beta = 100$  and  $T_f = 20$ .



Figure: convergence rates for the first test (left) and for the second test (right).



### 1D Euler equations: quantitatives results

Model: Euler equation

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0 \\ \partial_t \rho u + \partial_x (\rho u^2 + p) = 0 \\ \partial_t \rho E + \partial_x (\rho E u + p u) = 0 \end{cases}$$

- Kinetic model: (D1Q2) or D1Q3.
- For the transport (and relaxations step) we use 11-order SL scheme in space.

$$\begin{aligned} u(t = 0, x) &= -\sqrt{\gamma} \operatorname{sign}(x) M (1.0 - \cos(2\pi x/L)) \\ p(t = 0, x) &= \frac{1}{M^2} (1.0 + M\gamma (1.0 - \cos(2\pi x/L))) \quad M = \frac{1}{11} \end{aligned}$$

**Discretization**: 4000 cells (for a domain L = [-20, 20]) and order 11.



Figure: Density for the different scheme and order 2 time scheme: D1Q2 with  $\lambda = 16$  (violet), D1Q3 with  $\lambda = 26$  (green) and reference (black). Left :  $\Delta t = 0.01$  (CFL 1-5). Right:  $\Delta t = 0.05$  (CFL 5-20).



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Figure: Density for the different scheme and order 4 time scheme: D1Q2 with  $\lambda = 16$  (violet), D1Q3 with  $\lambda = 26$  (green) and reference (black). Left :  $\Delta t = 0.05$  (CFL 5-20). Right:  $\Delta t = 0.1$  (CFL 10-50).



- Model : compressible ideal MHD.
- Kinetic model : (D2 Q4)<sup>n</sup>. Symmetric Lattice.
- Transport scheme : 2 order Implicit DG scheme. 4th order ins space. CFL around 20.
- **Test case** : advection of the vortex (steady state without drift).
- Parameters :  $\rho = 1.0$ ,  $p_0 = 1$ ,  $u_0 = b_0 = 0.5$ ,  $\mathbf{u}_{drift} = [1, 1]^t$ ,  $h(r) = exp[(1 r^2)/2]$





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- Test case : advection of the vortex (steady state without drift).
- Parameters :  $\rho = 1.0$ ,  $p_0 = 1$ ,  $u_0 = b_0 = 0.5$ ,  $\mathbf{u}_{drift} = [1, 1]^t$ ,  $h(r) = exp[(1 r^2)/2]$



Magnetic field



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### Numerical results: 2D-3D fluid models

- Model : liquid-gas Euler model with gravity.
- Kinetic model :  $(D2 Q4)^n$ . Symmetric Lattice.
- **Transport scheme** : 2 order Implicit DG scheme. 3th order in space. CFL around 6.
- **Test case** : Rayleigh-Taylor instability.

2D case in annulus

3D case in cylinder





Figure: Plot of the mass fraction of gas

Figure: Plot of the mass fraction of gas



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2D cut of the 3D case





Figure: Plot of the mass fraction of gas

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**Conclusion and perspectives** 





Inia

### Conclusion

#### Idea

- Aim: solve a strongly coupled nonlinear problem N.
- We construct linear problem with source term  $L_{\varepsilon}$  such that  $|| N L_{\varepsilon} || = O(\nu^2)$ .
- We solve  $L_{\varepsilon}$  with the discretization  $L_{\varepsilon}^{h}$  simple to solve such that  $\|L_{\varepsilon} L_{\varepsilon}^{h}\| = O(h^{\rho})$ .
- We obtain an error homogeneous with  $O(h^p + \varepsilon)$ .

#### Computing

- The linear problem  $L_{\varepsilon}^{h}$  can be split between simple problems.
- Best implicit solver: SL, Glimm scheme or DG for transport (IKR) ?
- Parallelism: additional parallelism with the uncoupled simple models.

#### Advantages/defaults

- Advantages: CFL- free method, High order method, Matrix free method, complex geometry compatible method.
- Defaults: Large diffusion/dispersion at the order one/more. No limiting for discontinuities.



<sup>6</sup>/27

### Perspectives

#### Numerical dispersion in time

- Main problem: for large time step (aim for implicit scheme) high dispersion for fast scales ( acoustic for example).
- Solution:
  - □ Higher order scheme (4th and 6th).
  - □ Construct more efficient kinetic representation (additional zero velocity etc): current work.
  - □ Limiting or entropy dissipation methods for the relaxation step: future work.

#### Equilibrium

- This method not able to preserve steady states.
- Future work: modify the kinetic representation to preserve steady states.

#### Other future works

- Treatment of Complex boundary condition.
- AP method for low-mach regime.
- Convergence in the linear case.

