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Variational-FEEC discretization for the ideal MHD

EAGSTIM Workshop Pisa

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Outline

Ideal Magneto-Hydrodydamics and variational formulation

- Ideal MHD
- The de Rham complex
- Invariants of the system

Discretization

- Discretes forms and vector fields
- Discrete Lagrangian

Numerical experiments

Outline

Ideal MHD

Compressible Euler + Maxwell + Ideal Conductor + Massless electrons + Electric quasi-equilibrium =

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \,, \tag{1a}$$

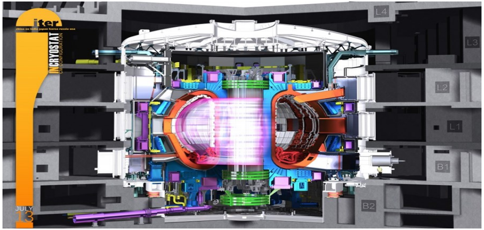
$$\rho \partial_t \mathbf{u} + \rho(\mathbf{u} \cdot \nabla \mathbf{u}) + \nabla p + \mathbf{B} \times \operatorname{curl} \mathbf{B} = 0 \,, \tag{1b}$$

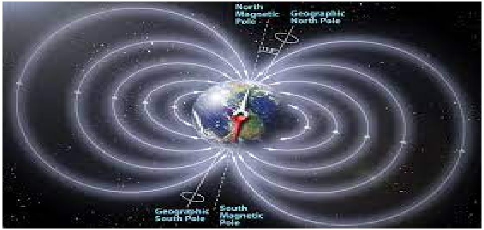
$$\partial_t s + \operatorname{div}(s \mathbf{u}) = 0 \,, \tag{1c}$$

$$\partial_t \mathbf{B} + \operatorname{curl}(\mathbf{B} \times \mathbf{u}) = 0 \,. \tag{1d}$$

Have an equivalent hyperbolic form (usually used for discretizations), using variable $\mathbf{m}$ and E.
Only valid in smooth regime (conservation instead of dissipation of entropy).
No dimensionality (removed all physical constant).
We will not consider boundary conditions here.

A few applications of MDH





Least action principle

Consider the following Lagrangian and action[1,2]

$$l(\mathbf{u}, \rho, s, \mathbf{B}) = \int_\Omega \frac{1}{2}\rho|u|^2 - \rho e(\rho, s) - \frac{1}{2}|\mathbf{B}|^2 dV \ , \tag{2a}$$

$$\Sigma(\mathbf{u}, \rho, s, \mathbf{B}) = \int_0^T l(\mathbf{u}, \rho, s, \mathbf{B}) dt \tag{2b}$$

solution of ideal MHD $\iff$ $\delta\Sigma = 0$ under variation $\delta\mathbf{u} = \partial_t \mathbf{v} + [\mathbf{u}, \mathbf{v}]$, $\delta\rho = -\operatorname{div}(\rho\mathbf{v})$, $\delta s = -\operatorname{div}(s\mathbf{v})$ and $\delta\mathbf{B} = \operatorname{curl}(\mathbf{B} \times \mathbf{v})$ with a curve in $X(\Omega)$ null at both end-points and advection equations :
$\partial_t \rho + \operatorname{div}(\rho\mathbf{u}) = 0 \ , \partial_t s + \operatorname{div}(s\mathbf{u}) = 0 \ , \partial_t \mathbf{B} + \operatorname{curl}(\mathbf{B} \times \mathbf{u}) = 0$.

[1] **Lagrangian and Hamiltonian methods in magnetohydrodynamics**, **William A. Newcomb**, **1961**.
[2] **Topological methods in hydrodynamics**, **Vladimir I. Arnold and Boris A. Khesin**, **2008**.

The de Rham complex

$$H^1 \xrightarrow{\text{grad}} H(curl) \xrightarrow{\text{curl}} H(div) \xrightarrow{\text{div}} L^2 \tag{3}$$

Take smooth subspace and use general notation :

$$V^0 \xrightarrow{d^0} V^1 \xrightarrow{d^1} V^2 \xrightarrow{d^2} V^3 \tag{4}$$

Interior product to go the other way around (for a given vector field **u**)

$$V^0 \xleftarrow{i^1_{\mathbf{u}} = .\cdot\mathbf{u}} V^1 \xleftarrow{i^2_{\mathbf{u}} = .\times\mathbf{u}} V^2 \xleftarrow{i^3_{\mathbf{u}} = .\mathbf{u}} V^3 \tag{5}$$

Mix everything : Lie derivative $\mathcal{L}^i_{\mathbf{u}} = d^{i-1} i^i_{\mathbf{u}} + i^{i+1}_{\mathbf{u}} d^i$

Theorem

$\mathcal{L}_{\mathbf{u}}$ commutes with d

General advection equations :

$$\partial_t \omega^i + \mathcal{L}^i_{\mathbf{u}} \omega^i = 0 \ , \tag{6a}$$

$$\partial_t f + \mathbf{u} \cdot \operatorname{grad} f = 0 \ . \tag{6b}$$

$$\partial_t \mathbf{A} + \operatorname{grad}(\mathbf{A} \cdot \mathbf{u}) + \operatorname{curl}(\mathbf{A}) \times \mathbf{u} \ , \tag{6c}$$

$$\partial_t \mathbf{B} + \operatorname{curl}(\mathbf{B} \times \mathbf{u}) + \operatorname{div}(\mathbf{B})\mathbf{u} = 0 \ . \tag{6d}$$

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \ , \tag{6e}$$

Reformulation of the variational principle

For $\mathbf{u} \in X$, $\rho, s \in V^3$ and $\mathbf{B} \in V^2$,

$$l(\mathbf{u}, \rho, s, \mathbf{B}) = \int_\Omega \frac{1}{2}\rho|u|^2 - \rho e(\rho, s) - \frac{1}{2}|\mathbf{B}|^2 dV \ , \tag{7a}$$

$$\Sigma(\mathbf{u}, \rho, s, \mathbf{B}) = \int_0^T l(\mathbf{u}, \rho, s, \mathbf{B}) dt \ , \tag{7b}$$

$\delta\Sigma = 0$ under variations

$$\delta\mathbf{u} = \partial_t \mathbf{v} + [\mathbf{u}, \mathbf{v}] \ , \tag{8a}$$

$$\delta\rho = -\mathcal{L}_{\mathbf{v}}\rho \ , \tag{8b}$$

$$\delta s = -\mathcal{L}_{\mathbf{v}} s \ , \tag{8c}$$

$$\delta\mathbf{B} = -\mathcal{L}_{\mathbf{v}}\mathbf{B} \ . \tag{8d}$$

Advection equations :

$$\partial_t \rho + \mathcal{L}_{\mathbf{u}}\rho = 0 \ , \tag{9a}$$

$$\partial_t s + \mathcal{L}_{\mathbf{u}} s = 0 \ , \tag{9b}$$

$$\partial_t \mathbf{B} + \mathcal{L}_{\mathbf{u}}\mathbf{B} = 0 \ . \tag{9c}$$

Invariants of the system (1/2)

Total mass and entropy:

$$\partial_t \int_\Omega \rho = 0 \ , \tag{10a}$$

$$\partial_t \int_\Omega s = 0 \ , \tag{10b}$$

comes from $\int_\Omega \mathcal{L}_u \omega^3 = 0$
$\mathbf{B}$ is solenoidal (if $\operatorname{div} \mathbf{B}(t=0) = 0$):

$$\operatorname{div} \mathbf{B} = 0 \ , \tag{11}$$

comes from the commutativity of d and $\mathcal{L}_{\mathbf{u}}$

Invariants of the system (2/2)

Total Energy:

$$\partial_t \int_\Omega \frac{1}{2}\rho|u|^2 + \rho e(\rho, s) + \frac{1}{2}|B|^2 dV = 0 \ , \tag{12}$$

Comes from the duality between the constrained variations and the advection equation for ρ, s and $\mathbf{B}$.
(Write the extrema condition, integrate by part to remove the $\partial_t \mathbf{v}$ and choose $\mathbf{v} = \mathbf{u}$)

Outline

Discretization based on this variational principle

Why ?

- Invariant/Structure preservation,[3][4]
- Long time stability,
- Easily adaptable to other models,
- No dissipation at all.[5]

How ?

- Discrete de Rham sequence,
- Discrete interior product,
- Discrete Lagrangian and variational principle.

[3] **A variational finite element discretization of compressible flow**, **Evan S. Gawlik and Francois Gay-Balmaz**, **2021**.

[4] **Structure-preserving discretization of incompressible fluids**, **Dmitry Pavlov et Al**, **2011**.

[5] **JOREK3D : An extension of the JOREK nonlinear MHD code to stellarators**, **Nikita Nikulsin et Al**, **2022**.

Discrete De Rham sequence and vector fields

Forms : discrete De Rham sequence (FEEC![6])

$$\begin{array}{ccccccc} V^0 & \xrightarrow{\text{grad}} & V^1 & \xrightarrow{\text{curl}} & V^2 & \xrightarrow{\text{div}} & V^3 \\ \Pi_0 \downarrow & & \Pi_1 \downarrow & & \Pi_2 \downarrow & & \Pi_3 \downarrow \\ V_h^0 & \xrightarrow[\text{grad}]{} & V_h^1 & \xrightarrow[\text{curl}]{} & V_h^2 & \xrightarrow[\text{div}]{} & V_h^3 \end{array} \tag{14}$$

Consider X_h a discrete space of Vector field and $\mathbf{u}_h \in X_h$.
Discrete interior product : $i^i_{h,\mathbf{u}_h}\omega^i = \Pi_i(i^i_{\mathbf{u}_h}\omega^i)$.
Discrete Lie derivative $\mathcal{L}^i_{h,\mathbf{u}_h} = d^{i-1} i^i_{h,\mathbf{u}_h} + i^{i+1}_{\mathbf{u}_h} d^i$.
Discrete Lie derivative also commutes with exterior derivative.

[6] **Finite element exterior calculus**, **Douglas N. Arnold**, **2018**.

Discrete Lagrangian

For $\mathbf{u}_h \in X_h$, $\rho_h, s_h \in V_h^3$ and $\mathbf{B}_h \in V_h^2$,

$$l_h(\mathbf{u}_h, \rho_h, s_h, \mathbf{B}_h) = \int_\Omega \frac{1}{2}\rho_h|\mathbf{u}_h|^2 - \rho_h e(\rho_h, s_h) - \frac{1}{2}|\mathbf{B}_h|^2 dV \ , \tag{15a}$$

$$\Sigma_h(\mathbf{u}_h, \rho_h, s_h, \mathbf{B}_h) = \int_0^T l_h(\mathbf{u}_h, \rho_h, s_h, \mathbf{B}_h) dt \ , \tag{15b}$$

$\delta\Sigma_h = 0$ under variations

$$\delta \mathbf{u}_h = \partial_t \mathbf{v}_h + \widehat{[\mathbf{u}_h, \mathbf{v}_h]} \ , \tag{16a}$$

$$\delta \rho_h = -\mathcal{L}_{\mathbf{v}_h}\rho_h \ , \tag{16b}$$

$$\delta s_h = -\mathcal{L}_{\mathbf{v}_h} s_h \ , \tag{16c}$$

$$\delta \mathbf{B}_h = -\mathcal{L}_{\mathbf{v}_h}\mathbf{B}_h \ . \tag{16d}$$

for $\mathbf{v}_h \in X_h$.

Advection equations :

$$\partial_t \rho_h + \mathcal{L}_{\mathbf{u}_h}\rho_h = 0 \ , \tag{17a}$$

$$\partial_t s_h + \mathcal{L}_{\mathbf{u}_h} s_h = 0 \ , \tag{17b}$$

$$\partial_t \mathbf{B}_h + \mathcal{L}_{\mathbf{u}_h}\mathbf{B}_h = 0 \ . \tag{17c}$$

FEM equations

The semi-discrete scheme reads : find $\mathbf{u}_h \in X_h$, $\rho_h, s_h \in V_h^n$ and $\mathbf{B}_h \in V_h^{n-1}$ such that

$$\begin{aligned} &\int_\Omega \partial_t(\rho_h \mathbf{u}_h) \cdot \mathbf{v}_h - (\rho_h \mathbf{u}_h) \cdot (\widehat{\mathbf{v} \cdot \text{grad}\, u_i - \mathbf{u}} \cdot \text{grad}\, v_i) \\ &+ \Big(\frac{1}{2}|\mathbf{u}_h|^2 - e(\rho_h, s_h) - \rho_h \partial_{\rho_h} e(\rho_h, s_h)\Big) \,\text{div}\, \Pi^2(\rho_h \mathbf{v}_h) \\ &- \rho_h \partial_{s_h} e(\rho_h, s_h) \,\text{div}\, \Pi^2(s_h \mathbf{v}_h) - \mathbf{B}_h \cdot \text{curl}\, \Pi^1(\mathbf{B}_h \times \mathbf{v}_h) = 0 \ \forall \mathbf{v}_h \in X_h \ . \end{aligned} \tag{18}$$

With the following advection equations :

$$\begin{aligned} \partial_t \rho_h + \text{div}\, \Pi^2(\rho_h \mathbf{u}_h) &= 0 \ , \\ \partial_t s_h + \text{div}\, \Pi^2(s_h \mathbf{u}_h) &= 0 \ , \\ \partial_t \mathbf{B}_h + \text{curl}\, \Pi^1(\mathbf{B}_h \times \mathbf{u}_h) &= 0 \ . \end{aligned} \tag{19}$$

Preservation at the semi-discrete level of all the previously mentioned invariants.

Energy preserving time discretization

$$\int_\Omega \frac{\rho_h^{n+1}\mathbf{u}_h^{n+1} - \rho_h^n \mathbf{u}_h^n}{\Delta t} \cdot \mathbf{v}_h - \sum_{i=1}^{n} \rho_h^{n+\frac{1}{2}} \mathbf{u}_h^{n+\frac{1}{2},i} \cdot (\mathbf{u}_h^{n+\frac{1}{2}} \cdot \nabla \mathbf{v}_h^i - \mathbf{v}_h \cdot \nabla \mathbf{u}_h^{n+\frac{1}{2},i}))$$
$$+ (\frac{\mathbf{u}_h^n \cdot \mathbf{u}_h^{n+1}}{2} - \frac{1}{2}(\frac{\rho_h^{n+1} e(\rho_h^{n+1}, s_h^{n+1}) - \rho_h^n e(\rho_h^n, s_h^{n+1})}{\rho_h^{n+1} - \rho_h^n} + \frac{\rho_h^{n+1} e(\rho_h^{n+1}, s_h^n) - \rho_h^n e(\rho_h^n, s_h^n)}{\rho_h^{n+1} - \rho_h^n})) \operatorname{div} \Pi(\rho_h^{n+\frac{1}{2}} \mathbf{v}_h)$$
$$- \frac{1}{2}(\frac{\rho_h^{n+1} e(\rho_h^{n+1}, s_h^{n+1}) - \rho_h^{n+1} e(\rho_h^{n+1}, s_h^n)}{s_h^{n+1} - s_h^n} + \frac{\rho_h^n e(\rho_h^n, s_h^{n+1}) - \rho_h^n e(\rho_h^n, s_h^n)}{s_h^{n+1} - s_h^n}) \operatorname{div} \Pi(s_h^{n+\frac{1}{2}} \mathbf{v}_h)$$
$$- B_h^{n+\frac{1}{2}} \cdot \operatorname{curl} \Pi(B_h^{n+\frac{1}{2}} \times \mathbf{v}_h) \ \forall \mathbf{v}_h \in (V_h^0)^m \ , \qquad (20)$$

$$\frac{\rho_h^{n+1} - \rho_h^n}{\Delta t} + \operatorname{div} \Pi(\rho_h^{n+\frac{1}{2}} \mathbf{u}_h^{n+\frac{1}{2}}) = 0 \ , \qquad (21)$$

$$\frac{s_h^{n+1} - s_h^n}{\Delta t} + \operatorname{div} \Pi(s_h^{n+\frac{1}{2}} \mathbf{u}_h^{n+\frac{1}{2}}) = 0 \ , \qquad (22)$$

$$\frac{B_h^{n+1} - B_h^n}{\Delta t} + \operatorname{curl} \Pi(B_h^{n+\frac{1}{2}} \times \mathbf{u}_h^{n+\frac{1}{2}}) = 0 \ , \qquad (23)$$

Outline

Implementation details

Tensor product splines spaces.

$$S_{p+1} \bigotimes S_{p+1} \bigotimes S_{p+1} \xrightarrow{\text{grad}} \begin{pmatrix} S_p \bigotimes S_{p+1} \bigotimes S_{p+1} \\ S_{p+1} \bigotimes S_p \bigotimes S_{p+1} \\ S_{p+1} \bigotimes S_{p+1} \bigotimes S_p \end{pmatrix} \xrightarrow{\text{curl}} \begin{pmatrix} S_{p+1} \bigotimes S_p \bigotimes S_p \\ S_p \bigotimes S_{p+1} \bigotimes S_p \\ S_p \bigotimes S_p \bigotimes S_{p+1} \end{pmatrix} \xrightarrow{\text{div}} S_p \bigotimes S_p \bigotimes S_p$$

$X_h = (V_h^0)^3$
Projectors are interpolation/histopolation projections.
Implemented using the psydac library[7]

[7] **PSYDAC: a high-performance IGA library in Python**, **Yaman Guclu et Al**, **2022**.

Taylor-Green Vortex

Barotropic Euler, $e(\rho) = \frac{1}{2}\rho$.
$\Omega = [0, \Pi]^2$ periodic boundary conditions.

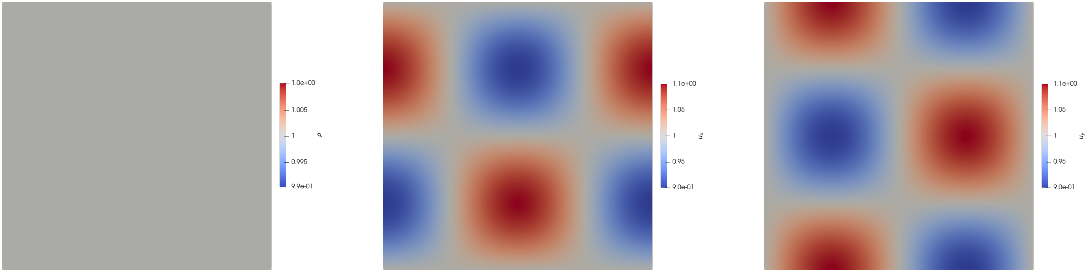


Figure: $p = 3,\ n_c = 128$

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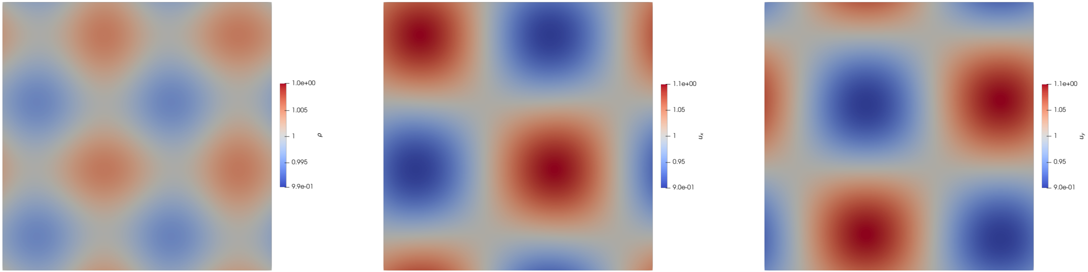

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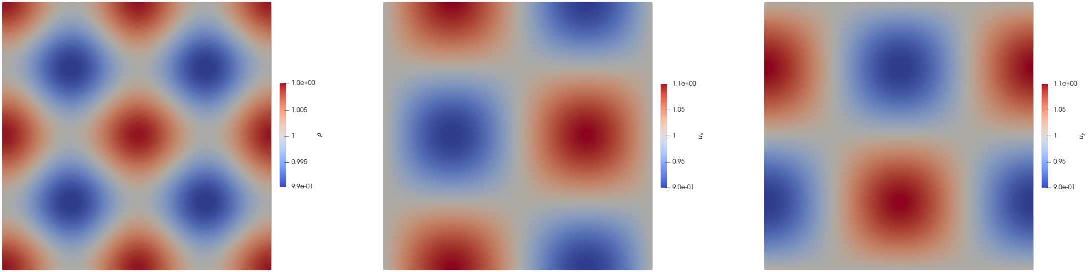

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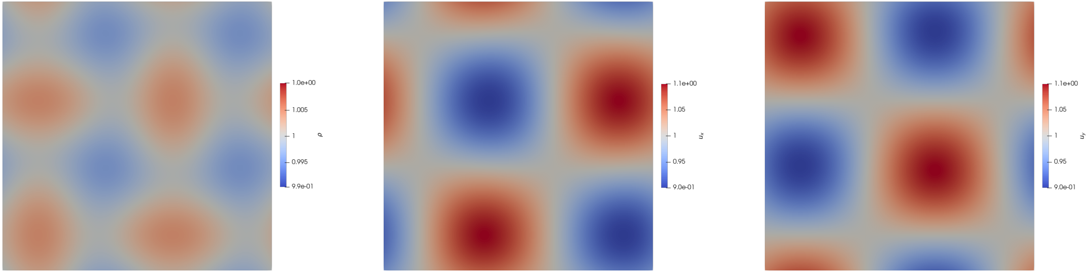

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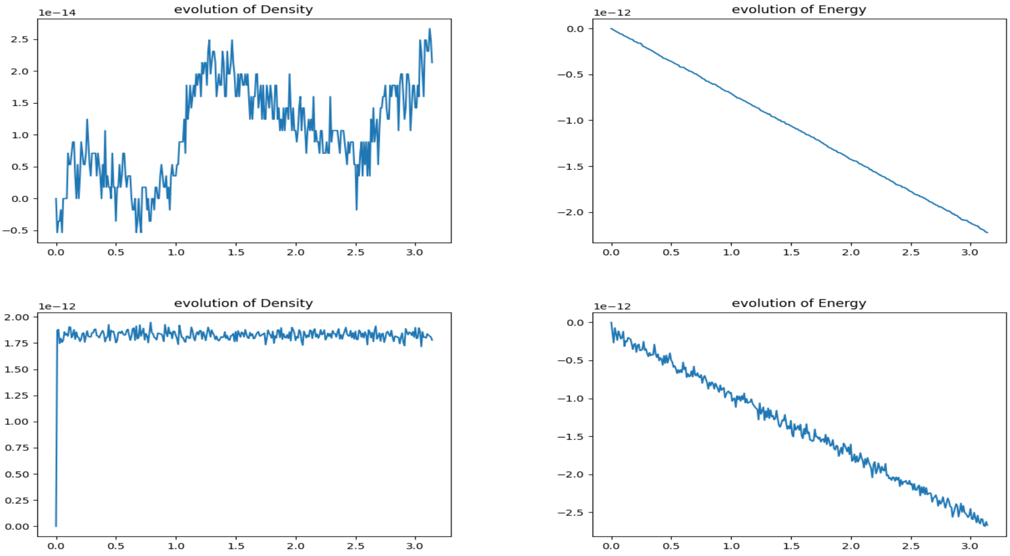
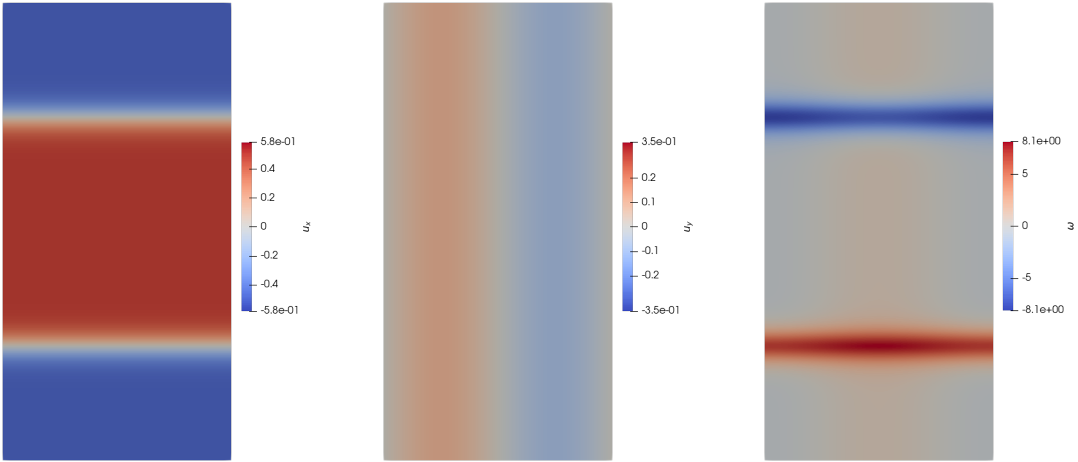


Figure: Numerical evolution of the claimed invariant for a coarse and a finer discretization

Barotropic Kelvin-Helmholtz instability



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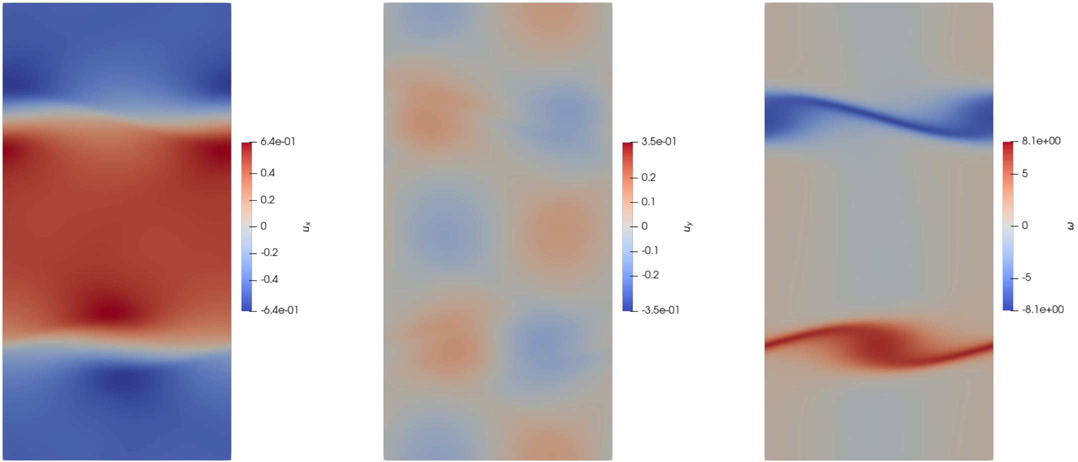

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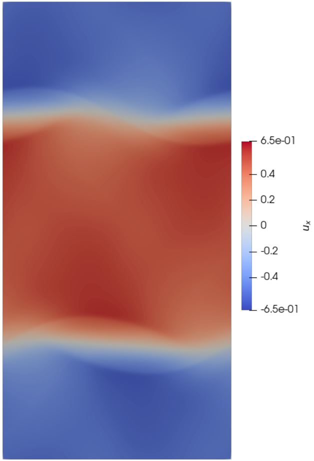

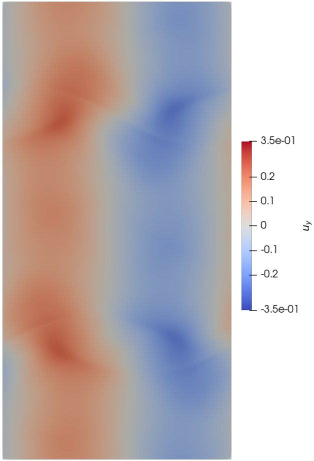

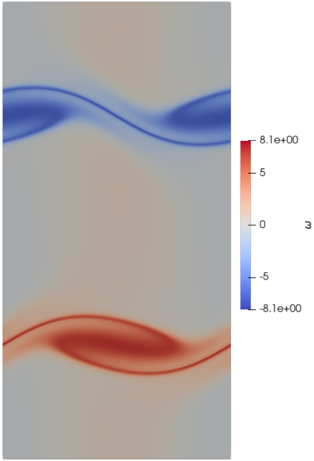

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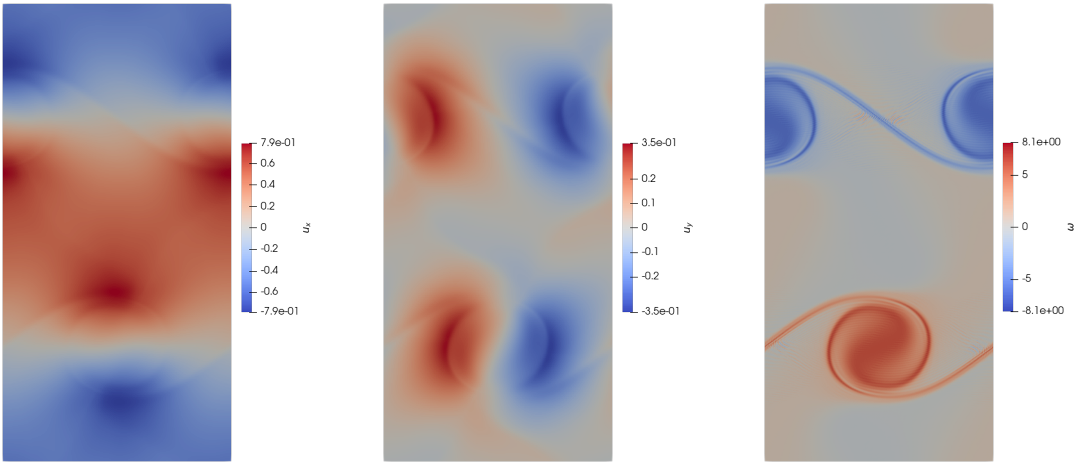

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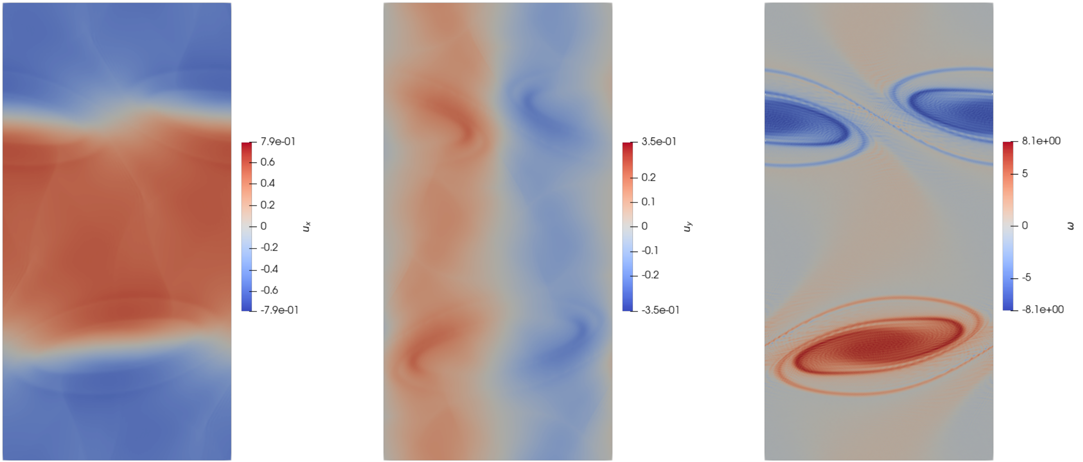
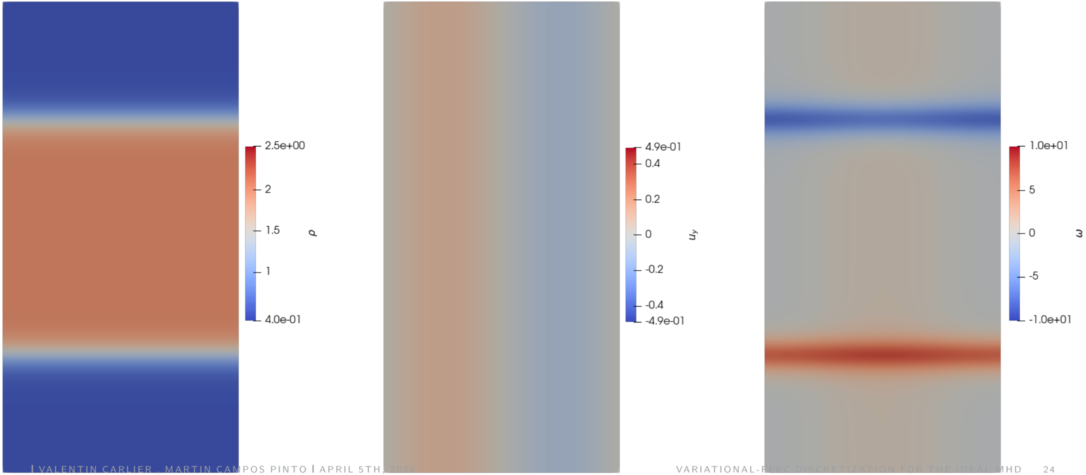


Figure: $p = 3, \; n_c = 256 \times 512$

Fully compressible ($e(\rho, s) = \rho^{\gamma-1} exp(s/\rho)$) Kelvin-Helmholtz instability

Reversibility test



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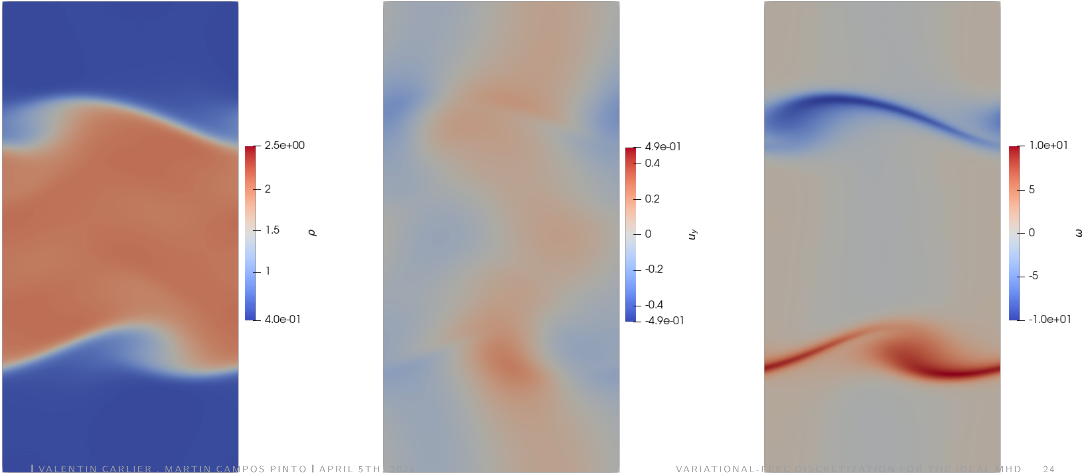

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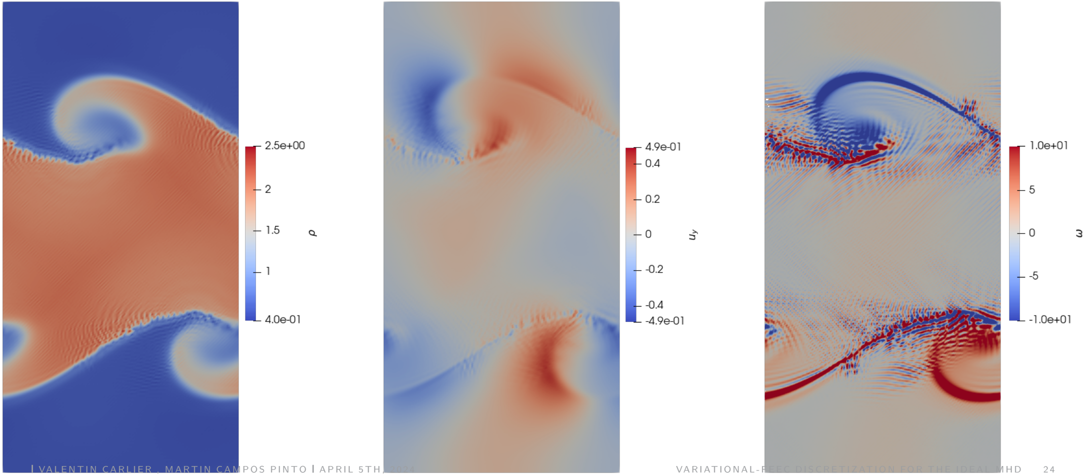

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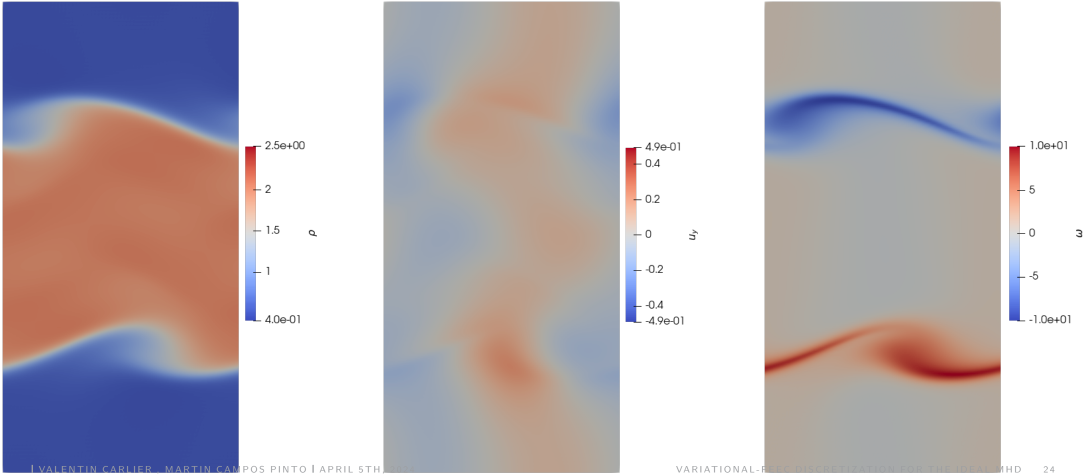

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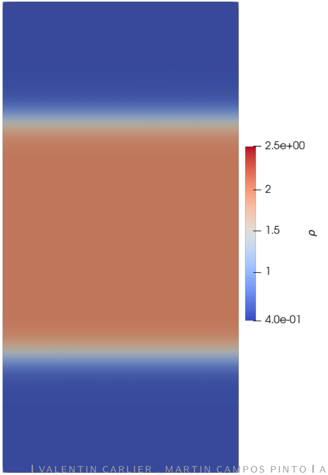
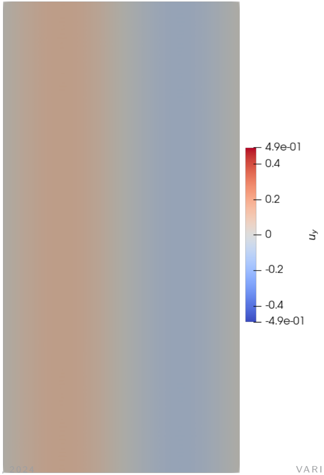
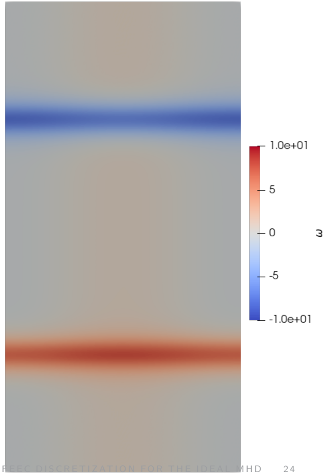
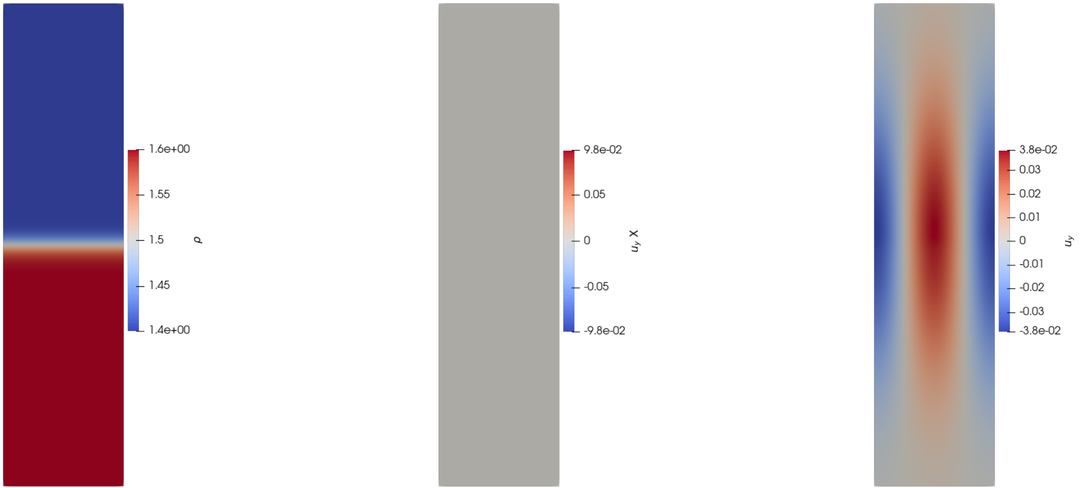






Rayleigh-Taylor Instability



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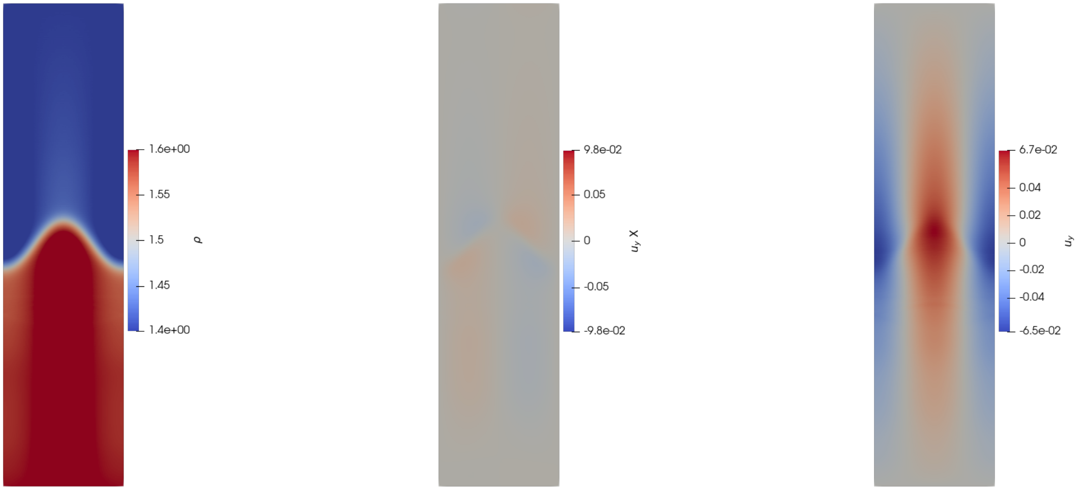

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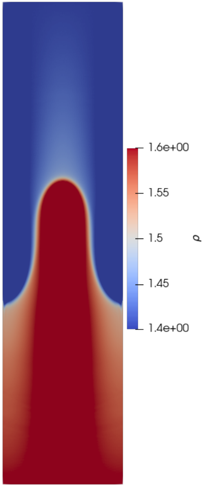

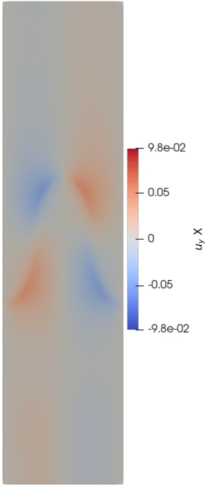

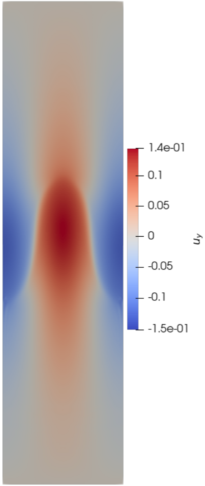

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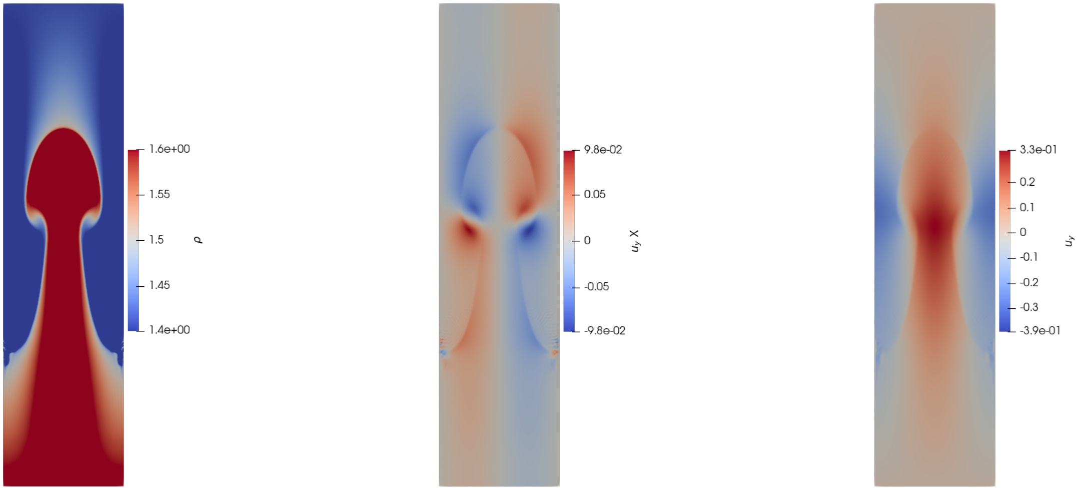

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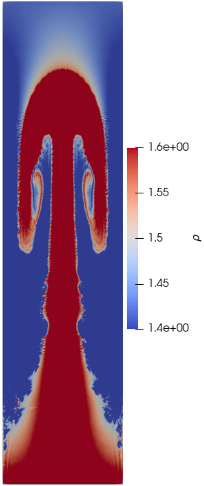
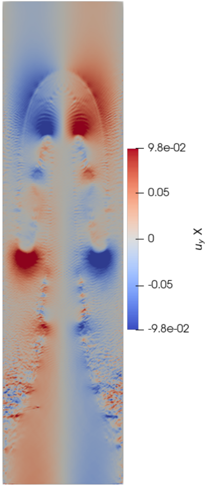
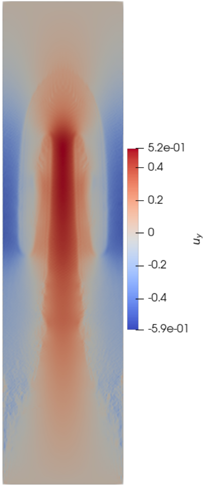






Alven Wave

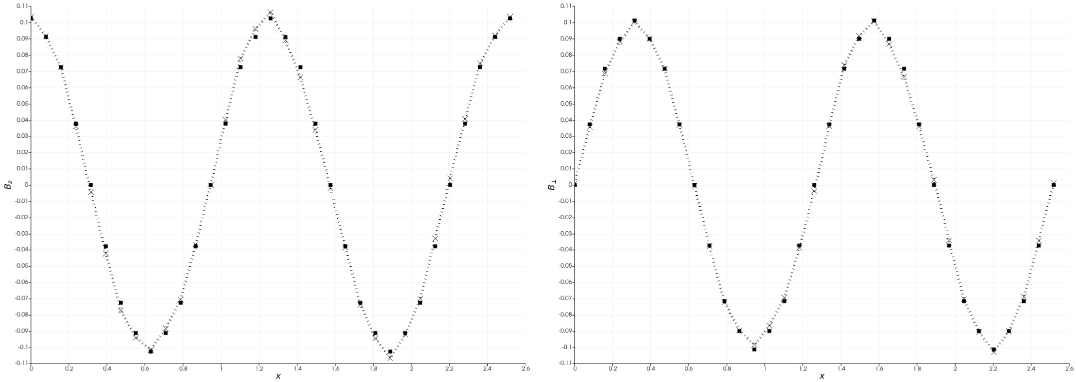
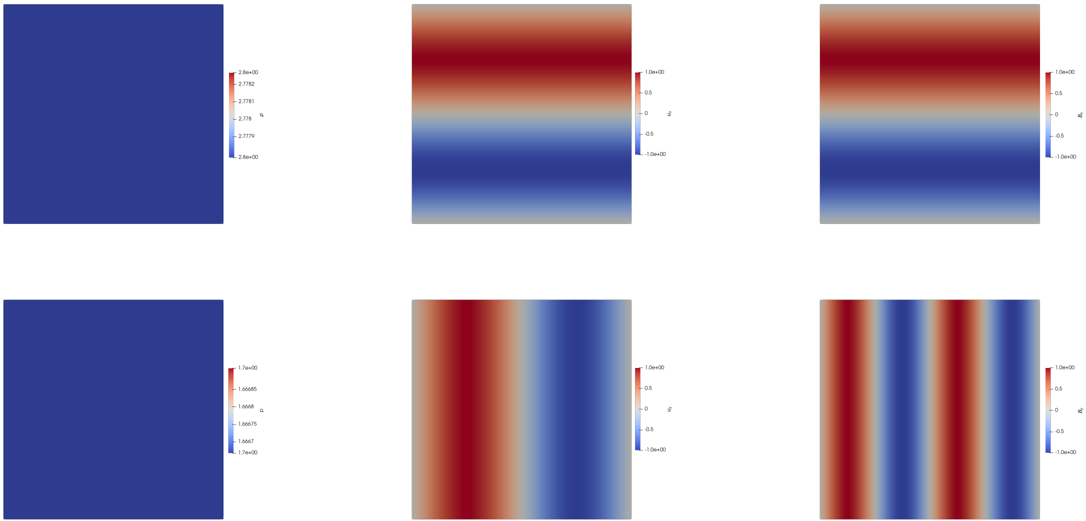
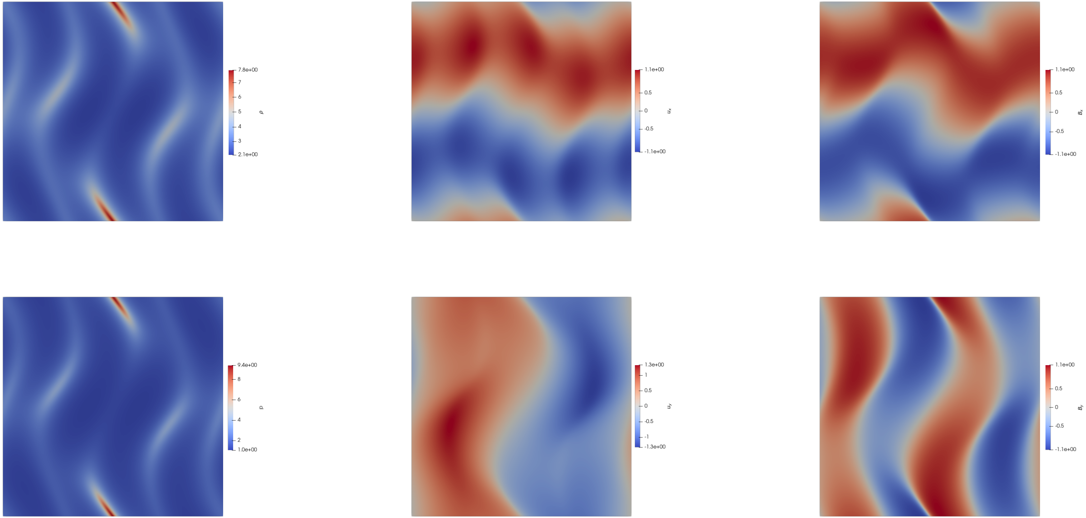


Figure: Plot of B_z and $B_\perp = \cos\alpha B_y - \sin\alpha B_x$ at $t = 75$ (after 75 periods of the wave), cuts at $y = 0$ with a coarse discretization ($N = 16$). The squares are the reference at $t = 0$ and the crosses are the result at $t = 75$

Orszag-Tang Vortex



Orszag-Tang Vortex



Orszag-Tang Vortex

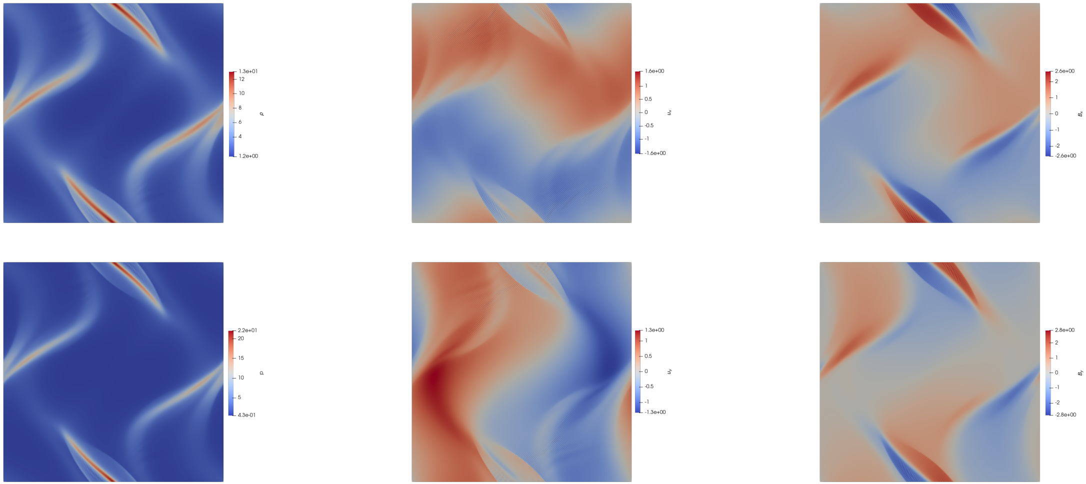


Figure: $p = 3, \; n_c = 256 \times 256$

Conclusion and perspectives

-Alternative method with nice theoretical properties.

-Good results on academic tests cases.

-In implementation in an HPC code (struphy) to test on real physically relevant configuration (Tokamaks/Stelerators).

-To be coupled with kinetic solver for more physics.

-Small dissipation to be added because real life is not ideal.

-arXiv:2402.02905

Supplementary slides

Lagrangian POV for MHD

$\Omega \subset \mathbf{R}^n$, $D(\Omega)$: set of diffeomorphisms (smooth bijection) of Ω,
$X(\Omega)$: set of vector fields of Ω.
Evolution of a plasma in Ω : curve (ϕ_t) in $D(\Omega)$

- $\phi_t(x)$: position at time t of the fluid particle that was located at x at $t = 0$.
- $\partial_t \phi_t(x)$: velocity at time t of the particle that was in x at $t = 0$.
- Classic (eulerian) velocity field $\mathbf{u}(x, t) = (\partial_t \phi_t) \circ \phi_t^{-1}$.

The other fields are then transported (not as functions but as differential forms) :
$\rho(t, \phi_t(x)) = \rho(0, x)/det(D\phi_t(x))$
$s(t, \phi_t(x)) = s(0, x)/det(D\phi_t(x))$
$\mathbf{B}(t, \phi_t(x)) = D\phi_t(x)\mathbf{B}(0, x)/det(D\phi_t(x))$

Variational formulation in Lagragian POV

Consider the following functional (Lagrangian) on $D(\Omega)$, for a given $\rho_0, s_0, \mathbf{B}_0$

$$L(\phi, \partial_t \phi) = \int_\Omega \frac{1}{2}\rho_0 |\partial_t \phi|^2 - \rho_0 e\left(\frac{\rho_0}{det(D\phi_t(x))}, \frac{s_0}{det(D\phi_t(x))}\right) - \frac{1}{2det(D\phi_t(x))}|D_\phi \mathbf{B}_0|^2 dV \ . \tag{24}$$

And its corresponding action :

$$S(\phi, \partial_t \phi) = \int_0^T L(\phi(t), \partial_t \phi(t)) dt \tag{25}$$

Theorem

Solution to the ideal MHD equations correspond to extremizers of S.

Lagrangian reduction

Change of variable :
$\mathbf{u} = (\partial_t \phi_t) \circ \phi_t^{-1}$,
$\rho = (\rho_0 / det(D\phi_t)) \circ \phi_t^{-1}$,
$s = (s_0 / det(D\phi_t)) \circ \phi_t^{-1}$,
$\mathbf{B} = (D\phi_t \mathbf{B}_0 / det(D\phi_t)) \circ \phi_t^{-1}$

$$l(\mathbf{u}, \rho, s, \mathbf{B}) = \int_\Omega \frac{1}{2}\rho|u|^2 - \rho e(\rho, s) - \frac{1}{2}|\mathbf{B}|^2 dV \ , \tag{26a}$$

$$\Sigma(\mathbf{u}, \rho, s, \mathbf{B}) = \int_0^T l(\mathbf{u}, \rho, s, \mathbf{B}) dt \tag{26b}$$

$\delta S = 0$ under free variation of $\phi \iff \delta\Sigma = 0$ under variation $\delta\mathbf{u} = \partial_t \mathbf{v} + [\mathbf{u}, \mathbf{v}]$, $\delta\rho = -\operatorname{div}(\rho\mathbf{v})$, $\delta s = -\operatorname{div}(s\mathbf{v})$ and $\delta\mathbf{B} = \operatorname{curl}(\mathbf{B} \times \mathbf{v})$ with $\mathbf{v} = \delta\phi \circ \phi^{-1}$, curve in $X(\Omega)$ null at both end-points. We also recover the advection equations :
$\partial_t \rho + \operatorname{div}(\rho\mathbf{u}) = 0 \ , \partial_t s + \operatorname{div}(s\mathbf{u}) = 0 \ , \partial_t \mathbf{B} + \operatorname{curl}(\mathbf{B} \times \mathbf{u}) = 0$.

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