Hierarchy of fluid models and numerical methods for the JOREK code

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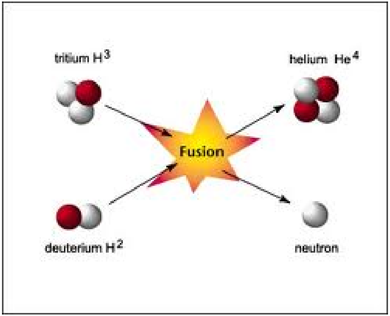
Outline

Physical and mathematical context

Magnetic Confinement Fusion

- **Fusion DT**: At sufficiently high energies, deuterium and tritium can fuse to Helium. A neutron and 17.6 MeV of free energy are released. At those energies, the atoms are ionized forming a plasma.



Magnetic Confinement Fusion

- **Fusion DT**: At sufficiently high energies, deuterium and tritium can fuse to Helium. A neutron and 17.6 MeV of free energy are released. At those energies, the atoms are ionized forming a plasma.
- **Magnetic confinement**: The charged plasma particles can be confined in a toroidal magnetic field configuration, for instance a Tokamak.

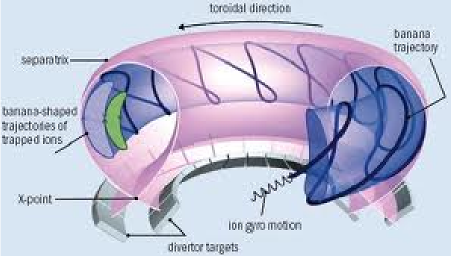
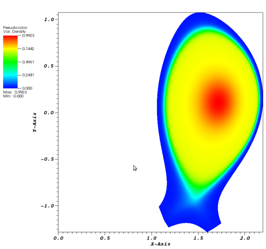


Figure: Tokamak

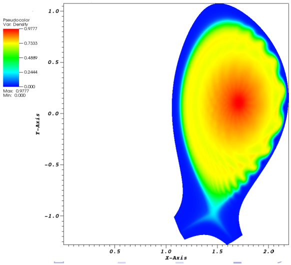
Plasma instabilities

- Edge localized modes (ELMs) are periodic instabilities occurring at the edge of tokamak plasmas.
- They are associated with strong heat and particle losses which could damage wall components in ITER by large heat loads.
- **Aim**: Detailed non-linear modeling and simulation (MHD models) can help to understand and control ELMs better (pellet or massive gas injection).

- Initial Density



- Final Density

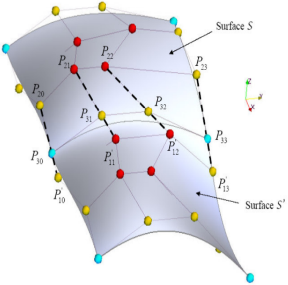


Forewords: JOREK – Overview

- **Closed & open field lines domain**, **X-point geom.**
  - Cubic Finite Elements, flux aligned poloidal grid
  - Isoparametric: elements approaching geometry are used to approach unknowns
  - Fourier series in toroidal direction
  - Non-linear reduced MHD in toroidal geometry

- **Time stepping, solver & parallelism**
  - fully implicit e. g. Crank-Nicholson
  - sparse matrices (PastiX) $\sim 10^7$ degrees of freedom
  - MPI/OpenMP over typically $256 - 1500$ processors

- **ELM simulations consumptions**
  - At **IRFM**, we use 7 Millions CPUH/year
  - Typical simulations: $\sim 20'000 - 200'000$ CPUH
  - A JET simulation ($n_{tor} = 0...10$): $\sim 100'000 - 200'000$ CPUH



Description of the JOREK code I

- Initialization
- Determine the equilibrium
  - Define the boundary of the computational domain.
  - Create a first grid which is used to compute the aligned grid.
  - Compute $\psi(R, Z)$ in the new grid.
- Compute equilibrium.
  - Solve the Grad-Shafranov equation:

$$R\frac{\partial}{\partial R}\left(\frac{1}{R}\frac{\partial \psi}{\partial R}\right)+\frac{\partial^2 \psi}{\partial Z^2}=-R^2\frac{\partial p}{\partial \psi}-F\frac{\partial F}{\partial \psi}$$

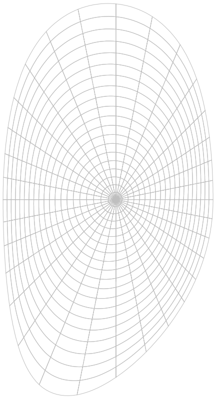


Figure: unaligned grid

Description of the JOREK code II

- Computation of aligned grid
  - Identification of the magnetic flux surfaces.
  - Create the aligned grid (with X-point).
  - Interpolate $\psi(R, Z)$ in the new grid.
- Recompute equilibrium of the new grid.
- **Perturbation of the equilibrium** (small perturbations of non principal harmonics).
- Time-stepping (full implicit):
  - Construction of the matrix and some profiles (diffusion tensors, sources terms).
  - Solve linear system.
  - Update solutions.

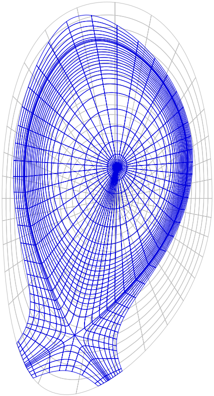


Figure: Aligned grid

Hierarchy of models for plasmas

Vlasov equation

- First model to describe a plasma : **Two species Vlasov-Maxwell** kinetic equation.
- We define $f_s(t, \mathbf{x}, \mathbf{v})$ the distribution function associated with the species s. $\mathbf{x} \in D_{\mathbf{x}}$ and $\mathbf{v} \in \mathbb{R}^3$.

$$\begin{cases} \partial_t f_s + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \dfrac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = C_s = \sum_t C_{st}, \\ \frac{1}{c^2} \partial_t \mathbf{E} - \nabla \times \mathbf{B} = -\mu_0 \mathbf{J}, \\ \partial_t \mathbf{B} = -\nabla \times \mathbf{E}, \\ \nabla \cdot \mathbf{B} = 0, \quad \nabla \cdot \mathbf{E} = \frac{\sigma}{\varepsilon_0}. \end{cases}$$

- Derivation of two fluid model :
  - We apply this operator $\int_{\mathbb{R}^3} g(\mathbf{v})(\cdot)$ on the equation.
  - $g(\mathbf{v})_s = 1, m_s \mathbf{v}, m_s |\mathbf{v}|^2$.
- Using
  - $\int_{D_{\mathbf{v}}} m_s \mathbf{v} C_{ss} d\mathbf{v} = 0, \quad \int_{D_{\mathbf{v}}} m_s |\mathbf{v}|^2 C_{ss} d\mathbf{v} = 0,$
  - $\int_{D_{\mathbf{v}}} g(\mathbf{v})_s C_{st} d\mathbf{v} + \int_{D_{\mathbf{v}}} g(\mathbf{v})_t C_{ts} d\mathbf{v} = 0.$

Two fluid model

- Computing the moment of the Vlasov equations we obtain the following two fluid model

$$\left\{\begin{array}{l}\partial_t n_s + \nabla\cdot(m_s n_s \mathbf{u}_s) = 0,\\ \partial_t(m_s n_s \mathbf{u}_s) + \nabla_{\mathbf{x}}\cdot(m_s n_s \mathbf{u}_s\otimes\mathbf{u}_s) + \nabla_{\mathbf{x}} p_s + \nabla_{\mathbf{x}}\cdot\Pi_s = \sigma_s\mathbf{E} + \mathbf{J}_s\times\mathbf{B} + \mathbf{R}_s,\\ \partial_t(m_s n_s \epsilon_s) + \nabla_{\mathbf{x}}\cdot(m_s n_s \mathbf{u}_s\epsilon_s + p_s\mathbf{u}_s) + \nabla_{\mathbf{x}}\cdot(\Pi\cdot\mathbf{u}_s + \mathbf{q}_s) = \sigma_s\mathbf{E}\cdot\mathbf{u}_s + Q_{\Delta_s} + \mathbf{R}_s\cdot\mathbf{u}_s,\\ \\ \frac{1}{c^2}\partial_t\mathbf{E} - \nabla\times\mathbf{B} = -\mu_0\mathbf{J},\\ \partial_t\mathbf{B} = -\nabla\times\mathbf{E},\\ \nabla\cdot\mathbf{B} = 0,\quad \nabla\cdot\mathbf{E} = \frac{\sigma}{\varepsilon_0}.\end{array}\right.$$

- $n_s = \int_{D_{\mathbf{v}}} f_s d\mathbf{v}$ the particle number , $m_s n_s \mathbf{u}_s = \int_{D_{\mathbf{v}}} m_s \mathbf{v} f_s d\mathbf{v}$ the momentum, $m_s n_s \epsilon_s = \int_{D_{\mathbf{v}}} m_s |\mathbf{v}|^2 f_s d\mathbf{v}$ the energy.
- The isotropic pressure are p_s, Π_s the stress tensors and $\mathbf{q}_s$ the heat fluxes.
- $\mathbf{R}_s$ and Q_{Δ_s} associated with the collision between two species.
- The current is given by $\mathbf{J} = \sum_s \mathbf{J}_s = \sum_s \sigma_s \mathbf{u}_s$ with $\sigma_s = q_s n_s$.

Extended MHD: assumptions and generalized Ohm law

Extended MHD: assumptions

- **quasi neutrality assumption**: $n_i = n_e$
  - Since $m_e << m_i$ therefore $\rho = m_i n_i + m_e n_e \approx m_i n_i$
  - Since $m_e << m_i$ therefore $\mathbf{u} = \frac{m_i n_i \mathbf{u}_i + m_e n_e \mathbf{u}_e}{\rho} \approx \mathbf{u}_i$
- **Magnetostatic assumption** : $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$

- Taking the electronic density and momentum equations we obtain

$$m_e \left(\partial_t (n_e \mathbf{u}_e) + \nabla \cdot (n_e \mathbf{u}_e \mathbf{u}_e)\right) + \nabla p_e = -e n_e \mathbf{E} + \mathbf{J}_e \times \mathbf{B} - \nabla \cdot \Pi_e + \mathbf{R}_e,$$

- We multiply the previous equation by $-e$ and we define $\mathbf{J}_e = -e n_e \mathbf{u}_e$, we obtain

$$\frac{m_e}{e^2 n_e} \left(\partial_t \mathbf{J}_e + \nabla \cdot (\mathbf{J}_e \mathbf{u}_e)\right) = \mathbf{E} + \mathbf{u}_e \times \mathbf{B} + \frac{1}{e n_e} \nabla p_e + \frac{1}{e n_e} \nabla \cdot \Pi_e - \frac{1}{e n_e} \mathbf{R}_e,$$

- Using the quasi neutrality, $m_e << m_i$ and $\mathbf{R} = -\mathbf{R}_e = -\eta \frac{e}{m_i} \rho \mathbf{J}$, we obtain

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = \eta \mathbf{J} - \frac{m_i}{\rho e} \nabla \cdot \Pi_e + \frac{m_i}{\rho e} \mathbf{J} \times \mathbf{B} - \frac{m_i}{\rho e} \nabla p_e.$$

Extended MHD: model

- Using the generalized Ohm's law and the different assumptions we obtain

Extended MHD

$$
\left\{
\begin{array}{l}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\[2ex]
\rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{J} \times \mathbf{B} - \nabla \cdot \mathbf{\Pi}, \\[2ex]
\frac{1}{\gamma - 1} \partial_t p + \frac{1}{\gamma - 1} \mathbf{u} \cdot \nabla p + \frac{\gamma}{\gamma - 1} p \nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{q} = \frac{1}{\gamma - 1} \frac{m_i}{e\rho} \mathbf{J} \cdot \left(\nabla p_e - \gamma p_e \frac{\nabla \rho}{\rho} \right) \\
- \mathbf{\Pi} : \nabla \mathbf{u} + \mathbf{\Pi}_e : \nabla \left(\frac{m_i}{e\rho} \mathbf{J} \right) + \eta |\mathbf{J}|^2, \\[2ex]
\partial_t \mathbf{B} = -\nabla \times \mathbf{E}, \\[2ex]
\mathbf{E} = \left(-\mathbf{u} \times \mathbf{B} + \eta \mathbf{J} - \frac{m_i}{\rho e} \nabla \cdot \mathbf{\Pi}_e - \frac{m_i}{\rho e} \nabla p_e + \frac{m_i}{\rho e} (\mathbf{J} \times \mathbf{B}) \right), \\[2ex]
\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{B} = \mathbf{J}.
\end{array}
\right.
$$

Extended MHD: energy conservation

- The extended MHD satisfy a total energy conservation law.

The total energy for the MHD is given by

$$E = \rho\frac{|\mathbf{u}|^2}{2} + \frac{|\mathbf{B}|^2}{2} + \frac{1}{\gamma-1}p.$$

with $p = \rho T$ and $\gamma = \frac{5}{3}$. The conservation law for the total energy is given by

$$\partial_t E + \nabla\cdot\left[\mathbf{u}\left(\rho\frac{|\mathbf{u}|^2}{2} + \frac{\gamma}{\gamma-1}p\right) - (\mathbf{u}\times\mathbf{B})\times\mathbf{B}\right]$$
$$+\nabla\cdot\left[\frac{m_i}{\rho e}\left((\mathbf{J}\times\mathbf{B})\times\mathbf{B} - \nabla p_e\times\mathbf{B} - \nabla\cdot\Pi_e\times\mathbf{B} - \frac{\gamma}{\gamma-1}p_e\mathbf{J} - \mathbf{J}\cdot\Pi_e\right)\right]$$
$$+\nabla\cdot\mathbf{q} + \nabla\cdot(\Pi\cdot\mathbf{u}) + \eta\nabla\cdot(\mathbf{J}\times\mathbf{B}) = 0.$$

- Neglecting ohmic and viscous heating $-\Pi : \nabla\mathbf{u} + \eta|\mathbf{J}|^2$ we obtain a dissipative estimate energy.

Extended MHD: Diamagnetic MHD I

- In the Extended MHD case, The stress tensor is given by $\Pi = \Pi^v + \Pi^{gv}$.
- The structure of the gyro-viscous tensor Π^{gv} is complicate. To simplify we use **the "gyro-viscous cancellation"** (D.D. Schnack and Al, Physics of Plasmas 2006). For this we use ion velocity:

$$\mathbf{u}_i = -\mathbf{E} + \frac{m_i}{e}(\partial_t \mathbf{u}_i + \mathbf{u}_i \cdot \nabla \mathbf{u}_i) + \frac{1}{n_i e}\nabla p_i + \frac{1}{n_i e}\nabla \cdot \Pi_i - \frac{1}{n_i e}\mathbf{R}_i.$$

- We define the perpendicular ion velocity $\mathbf{u}_{i,\perp} = \frac{\mathbf{B}}{|\mathbf{B}|^2} \times \mathbf{u}_i$. We obtain

$$\mathbf{u}_{i,\perp} = \frac{\mathbf{E}\times\mathbf{B}}{|\mathbf{B}|^2} + \frac{m_i}{e|\mathbf{B}|^2}\mathbf{B} \times (\partial_t \mathbf{u}_i + \mathbf{u}_i \cdot \nabla \mathbf{u}_i) + \frac{\mathbf{B}}{n_i e|\mathbf{B}|^2} \times (\nabla p_i + \nabla \cdot \Pi_i - \mathbf{R}_i).$$

- Now we neglect the term which depend of $\partial_t \mathbf{u}_i + \mathbf{u}_i \cdot \nabla \mathbf{u}_i$, $\nabla \cdot \Pi_i$ and the term which depend of the friction term.
- At the end we obtain the following decomposition of the full velocity

$$\mathbf{u} = \mathbf{u}_E + \mathbf{u}_i^* + \mathbf{u}_{\parallel},$$

with $\mathbf{u}_E = \frac{\mathbf{E}\times\mathbf{B}}{|\mathbf{B}|^2}$, $\mathbf{u}_{\parallel}$ the parallel ion velocity and $\mathbf{u}_i^* = \frac{m_i}{\rho e}\frac{\mathbf{B}\times\nabla p_i}{|\mathbf{B}|^2}$ the diamagnetic ion velocity.

Extended MHD: Diamagnetic MHD II

- Momentum equation

$$\rho\partial_t \mathbf{u} + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{J}\times\mathbf{B} - \nabla\cdot\Pi^v - \nabla\cdot\Pi^{gv}.$$

- Using the decomposition of the velocity we obtain

$$\rho\partial_t(\mathbf{u}_E + \mathbf{u}_{||}) + \rho(\mathbf{u}_E + \mathbf{u}_i^* + \mathbf{u}_{||})\cdot\nabla(\mathbf{u}_E + \mathbf{u}_{||})$$
$$+ \rho\partial_t\mathbf{u}_i^* + \rho(\mathbf{u}_E + \mathbf{u}_i^* + \mathbf{u}_{||})\cdot\nabla\mathbf{u}_i^* = -\nabla p + \mathbf{J}\times\mathbf{B} - \nabla\cdot\Pi^v - \nabla\cdot\Pi^{gv}.$$

- The "Gyro-viscous cancellation" gives

$$\rho\partial_t\mathbf{u}_i^* + \rho(\mathbf{u}_E + \mathbf{u}_i^* + \mathbf{u}_{||})\cdot\nabla\mathbf{u}_i^* + \nabla\cdot\Pi^{gv} \approx \nabla\chi - \rho\mathbf{u}_i^*\cdot\nabla\mathbf{u}_{||}$$

with $\nabla\chi << \nabla p$.

Giro-viscous cancellation:

- $\rho\partial_t(\mathbf{u}_E + \mathbf{u}_{||}) + \rho(\mathbf{u}_E + \mathbf{u}_{||})\cdot\nabla(\mathbf{u}_E + \mathbf{u}_{||}) + \rho\mathbf{u}_i^*\cdot\nabla\mathbf{u}_E = -\nabla p + \mathbf{J}\times\mathbf{B} - \nabla\cdot\Pi^v$
- Neglect the viscous heating linked to the gyro-viscous tensor in the pressure equation.

Reduced MHD: assumptions and principle of derivation

- **Aim**: Reduce the number of variables and eliminate the fast waves in the resistive MHD model (the two fluid effects, the viscous and resistive heating are neglected).
- We consider the cylindrical coordinate $(R, Z, \phi) \in \Omega \times [0, 2\pi]$

Reduced MHD: Assumptions

$$\mathbf{B} = \frac{F_0}{R}\mathbf{e}_\phi + \frac{1}{R}\nabla\psi \times \mathbf{e}_\phi \quad \mathbf{u} = -R\nabla u \times \mathbf{e}_\phi + v_{||}\mathbf{B}$$

with u the electrical potential, ψ the magnetic poloidal flux, $v_{||}$ the parallel velocity. F_0 is constant.

- To avoid high order operators we introduce the vorticity $w = \triangle_{pol} u$ and the toroidal current $j = \triangle^* \psi = R^2 \nabla \cdot (\frac{1}{R^2}\nabla_{pol}\psi)$.
- Derivation: we plug $\mathbf{B}$ and $\mathbf{u}$ in the equations + some computations. For the equations on u and $v_{||}$ we use the following projections

$$\mathbf{e}_\phi \cdot \nabla \times R^2 \left(\rho\partial_t \mathbf{u} + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{J}\times\mathbf{B} + \nu\triangle\mathbf{u}\right)$$

and

$$\mathbf{B}\cdot \left(\rho\partial_t \mathbf{u} + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{J}\times\mathbf{B} + \nu\triangle\mathbf{u}\right).$$

Reduced MHD without $v_{||}$: simple model

- Example of model: case where $v_{||} = 0$.

$$
\begin{cases}
\partial_t \psi = R[\psi, u] - F_0 \partial_\phi u + \eta(T)\left(j + \frac{1}{R^2} \partial_{\phi\phi} \psi\right) \\
R\nabla \cdot (\hat{\rho} \nabla_{pol}(\partial_t u)) = \frac{1}{2}[R^2 ||\nabla_{pol} u||^2, \hat{\rho}] + [R^2 \hat{\rho} w, u] + [\psi, j] - \frac{F_0}{R} \partial_\phi j - [R^2, p] \\
+\nu R \nabla \cdot (\nabla_{pol} w) \\
\frac{1}{R^2} j - \nabla \cdot \left(\frac{1}{R^2} \nabla_{pol} \psi\right) = 0 \\
w - \nabla \cdot (\nabla_{pol} u) = 0 \\
\partial_t \rho = R[\rho, u] + 2\rho \partial_Z u + \nabla \cdot (D \nabla \rho) \\
\partial_t T = R[T, u] + 2(\gamma - 1) T \partial_Z u + \nabla \cdot (K \nabla T)
\end{cases}
$$

with $\hat{\rho} = R^2 \rho$.

- D and K are anisotropic diffusion tensors (in the direction parallel to **B**).
- $\eta(T)$ is the physical resistivity. ν is the viscosity.

Main result: energy estimate

Model with parallel velocity:

We assume that the boundary conditions are correctly chosen. The fields are defined by $\mathbf{B} = \frac{F_0}{R}\mathbf{e}_\phi + \frac{1}{R}\nabla\psi \times \mathbf{e}_\phi$ and $\mathbf{u} = -R\nabla u \times \mathbf{e}_\phi + v_{||}\mathbf{B}$. We have

$$\frac{d}{dt}\int_\Omega E(t) = -\int_\Omega \eta \frac{|\triangle^*\psi|^2}{R^2} - \int_\Omega \eta |\nabla_{pol}(\frac{\partial_\phi \psi}{R^2})|^2 - \int_\Omega \nu |\triangle_{pol} u|^2$$

with $E(t) = \frac{|\mathbf{B}|^2}{2} + \rho\frac{|\mathbf{u}|^2}{2} + \frac{1}{\gamma-1}P$ the total energy.

- The implemented models conserve approximately the energy. For exact energy conservation, some neglected terms must to be added.
- **Future work** : Derivation and energy estimate for the Reduced Extended MHD

- *Theoretical and numerical stability for the reduced MHD models in JOREK code*, E. Franck, M. Hölzl, A. Lessig, E. Sonnendrücker, submit.

Nonlinear solvers and preconditioning

Time scheme in JOREK code

- The model is $\partial_t A(\mathbf{U}) = B(\mathbf{U}, t)$
- For time stepping we use a Crank Nicholson or Gear scheme :

$$(1+\zeta)A(\mathbf{U}^{n+1}) - \zeta A(\mathbf{U}^{n}) + \zeta A(\mathbf{U}^{n-1}) = \theta \Delta t B(\mathbf{U}^{n+1}) + (1-\theta)\Delta t B(\mathbf{U}^{n}).$$

- Defining $G(\mathbf{U}) = (1+\zeta)A(\mathbf{U}) - \theta \Delta t B(\mathbf{U})$ and

$$b(\mathbf{U}^{n}, \mathbf{U}^{n-1}) = (1+2\zeta)A(\mathbf{U}^{n}) - \zeta A(\mathbf{U}^{n-1}) + (1-\theta)\Delta t B(\mathbf{U}^{n})$$

we obtain the nonlinear problem

$$G(\mathbf{U}^{n+1}) = b(\mathbf{U}^{n}, \mathbf{U}^{n-1}).$$

- First order linearization

$$\left(\frac{\partial G(\mathbf{U}^{n})}{\partial \mathbf{U}^{n}}\right) \delta \mathbf{U}^{n} = -G(\mathbf{U}^{n}) + b(\mathbf{U}^{n}, \mathbf{U}^{n-1}) = R(\mathbf{U}^{n}),$$

with $\delta \mathbf{U}^{n} = \mathbf{U}^{n+1} - \mathbf{U}^{n}$, and $J_n = \frac{\partial G(\mathbf{U}^{n})}{\partial \mathbf{U}^{n}}$ the Jacobian matrix of $G(\mathbf{U}^{n})$.

Linear Solvers

- Linear solver in JOREK: Left Preconditioning + GMRES iterative solver.
- Principle of the preconditioning step:
  - Replace the problem $J_k\delta\mathbf{U}_k = R(\mathbf{U}^n)$ by $P_k(P_k^{-1}J_k)\delta\mathbf{U}_k = R(\mathbf{U}^n)$.
  - Solve the new system with two steps $P_k\delta\mathbf{U}_k^* = R(\mathbf{U}^n)$ and $(P_k^{-1}J_k)\delta\mathbf{U}_k = \delta\mathbf{U}_k^*$
- If P_k is easier to invert than J_k and $P_k \approx J_k$ the linear solving step is more robust and efficient.
- Construction and inversion of P_k
  - P_k: diagonal block matrix where the sub-matrices are associated with each toroidal harmonic.
  - Inversion of P_k: We use a LU factorization and invert exactly each subsystem.
- This preconditioning is based on the assumption that the coupling between the toroidal harmonics is weak.
- In practice for some test cases this coupling is strong in the nonlinear phase.

Inexact Newton scheme

- For nonlinear problem is not necessary to solve each linear system with high accuracy.
- **Inexact Newton method**: The convergence criterion for linear solver depends of the nonlinear convergence. Minimization of the number of GMRES iteration for each linear step.
- We choose $\mathbf{U}_0 = \mathbf{U}^n$ and ε_0.
- Step k of the Newton procedure
  - We solve the linear system with GMRES

$$\left(\frac{\partial G(\mathbf{U}_k)}{\partial \mathbf{U}_k}\right)\delta\mathbf{U}_k = R(\mathbf{U}_k) = b(\mathbf{U}^n, \mathbf{U}^{n-1}) - G(\mathbf{U}_k)$$

  and the following convergence criterion

$$||\left(\frac{\partial G}{\partial \mathbf{U}_k}\right)\delta\mathbf{U}_k + R(\mathbf{U}_k)|| \leq \varepsilon_k ||R(\mathbf{U}_k)||, \quad \varepsilon_k = \gamma\left(\frac{||R(\mathbf{U}_k)||}{||R(\mathbf{U}_{k-1})||}\right)^{\alpha}$$

  - We iterate with $\mathbf{U}_{k+1} = \mathbf{U}_k + \delta\mathbf{U}_k$.
  - We apply the convergence test (for example $||R(\mathbf{U}_k)|| < \varepsilon_a + \varepsilon_r ||R(\mathbf{U}^n)||$)
- If the Newton procedure stop we define $\mathbf{U}^{n+1} = \mathbf{U}_{k+1}$.

First test case: model without parallel velocity

- First test case: simplified equilibrium configuration for the reactor JET.
- Additional cost with Inexact Newton procedure (in comparison to linearization) : between 1.5 and 2.

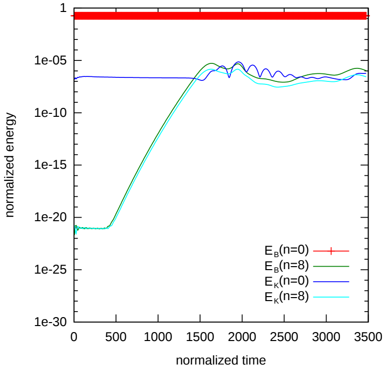


Figure: Reference solution: kinetic and magnetic energies for $\Delta t = 5$ gives by the Newton method.

First test case: model without parallel velocity

- First test case: simplified equilibrium configuration for the reactor JET.
- Additional cost with Inexact Newton procedure (in comparison to linearization) : between 1.5 and 2.

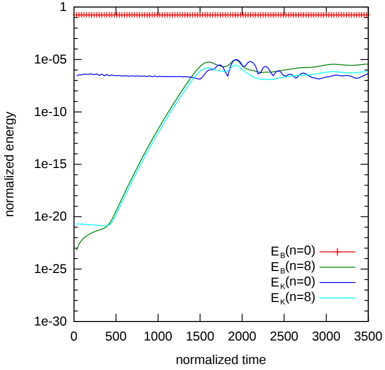


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 30$.

First test case: model without parallel velocity

- First test case: simplified equilibrium configuration for the reactor JET.
- Additional cost with Inexact Newton procedure (in comparison to linearization) : between 1.5 and 2.

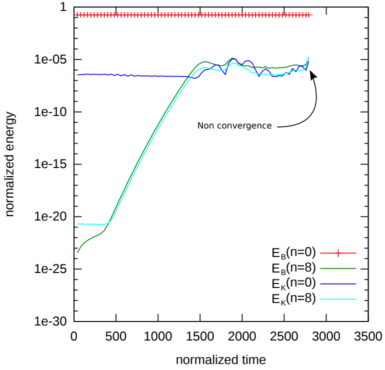


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 40$.

First test case: model without parallel velocity

- First test case: simplified equilibrium configuration for the reactor JET.
- Additional cost with Inexact Newton procedure (in comparison to linearization) : between 1.5 and 2.

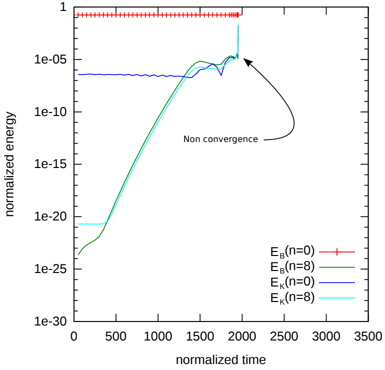


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 50$.

First test case: model without parallel velocity

- First test case: simplified equilibrium configuration for the reactor JET.
- Additional cost with Inexact Newton procedure (in comparison to linearization) : between 1.5 and 2.

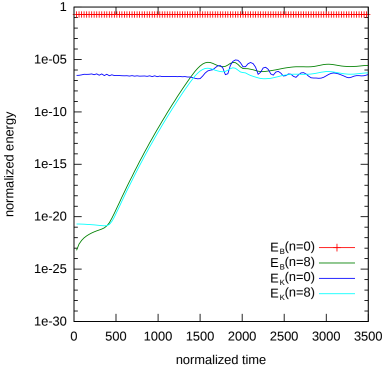


Figure: Kinetic and magnetic energies for Newton method for $\Delta t = 30$.

First test case: model without parallel velocity

- First test case: simplified equilibrium configuration for the reactor JET.
- Additional cost with Inexact Newton procedure (in comparison to linearization) : between 1.5 and 2.

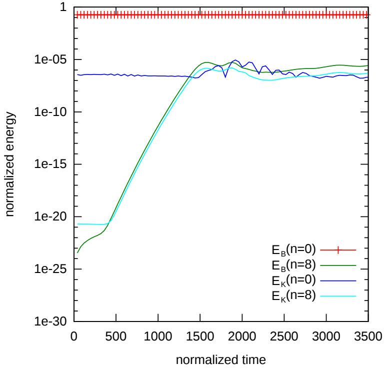


Figure: Kinetic and magnetic energies for Newton method for $\Delta t = 40$.

First test case: model without parallel velocity

- First test case: simplified equilibrium configuration for the reactor JET.
- Additional cost with Inexact Newton procedure (in comparison to linearization) : between 1.5 and 2.

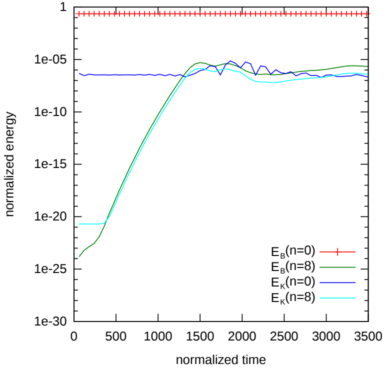


Figure: Kinetic and magnetic energies for Newton method for $\Delta t = 60$.

Second test case

- Second test case: realistic equilibrium configuration for ASDEX Upgrade with large resistivity which generate strong instabilities.
- Reduction of the cost with Inexact Newton procedure (in comparison to linearization): around 1.5.

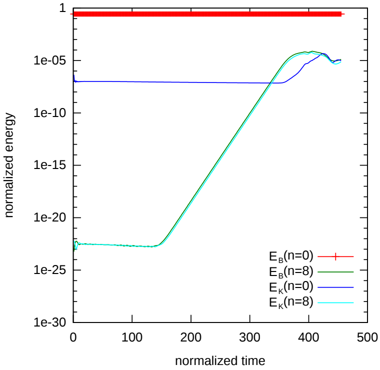


Figure: Reference solution: kinetic and magnetic energies for $\Delta t = 1$ gives by the Linearization method

Second test case

- Second test case: realistic equilibrium configuration for ASDEX Upgrade with large resistivity which generate strong instabilities.
- Reduction of the cost with Inexact Newton procedure (in comparison to linearization): around 1.5.

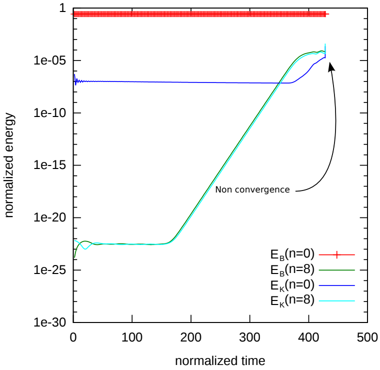


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 2$.

Second test case

- Second test case: realistic equilibrium configuration for ASDEX Upgrade with large resistivity which generate strong instabilities.
- Reduction of the cost with Inexact Newton procedure (in comparison to linearization): around 1.5.

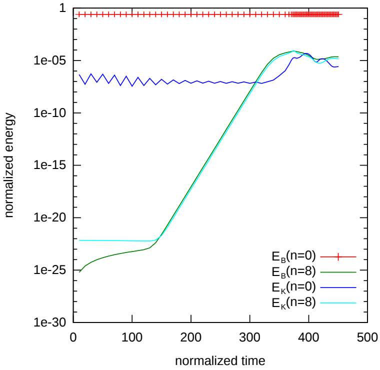


Figure: Kinetic and magnetic energies for Newton method for initial $\Delta t = 10$. Final time step around 2.

Preconditioning: Principle

- *An optimal, parallel fully implicit Newton-Krylov solver for 3D viscoresistive Magnetohydrodynamics*, L. Chacon, Phys. of plasma, 2008.

- **Right preconditioning**: We solve $J_k P_k^{-1} P_k = R(\mathbf{U}_k)$.
- **Aim**: Find P_k easy to invert with $P_k \approx P_k^{-1}$ and more efficient in the nonlinear phase as the preconditioning used.

- **Idea**: Operator splitting + parabolic formulation of the MHD + multigrid methods.
- Example

$$\left\{ \begin{array}{l} \partial_t u = \partial_x v \\ \partial_t v = \partial_x u \end{array} \right. \longrightarrow \left\{ \begin{array}{l} u^{n+1} = u^n + \Delta t \partial_x v^{n+1} \\ v^{n+1} = v^n + \Delta t \partial_x u^{n+1} \end{array} \right.$$

- We obtain $(1 - \Delta t^2 \partial_{xx}) u^{n+1} = u^n + \Delta t \partial_x v^n$.
- The matrix associated to $(1 - \Delta t^2 \partial_{xx})$ is a diagonally dominant matrix and well conditioned.
- This type of operator is easy to invert with algebraic preconditioning as multigrid methods.

Simple example: Low β model

- We assume that the profile of ρ is given, the pressure is small, and the fields are $\mathbf{B} = \frac{F_0}{R} e_\phi + \frac{1}{R}\nabla\psi \times e_\phi$, $\rho\mathbf{u} = -\frac{1}{R}\nabla u \times e_\phi$ and $\rho = \frac{1}{R^2}$.
- The model is

$$\left\{ \begin{array}{l} \partial_t\psi = R[\psi, u] + \eta\triangle^*\psi - F_0\partial_\phi u \\ \\ \partial_t\triangle_{pol} u = \frac{1}{R}[R^2\triangle_{pol} u, u] + \frac{1}{R}[\psi, \triangle^*\psi] - \frac{F_0}{R^2}\triangle^*\partial_\phi\psi + \nu\triangle^2_{pol} u \end{array} \right.$$

  with $w = \triangle_{pol} u$ and $j = \triangle^*\psi$.
- In this formulation we separate the evolution and elliptic equations.
- **Time scheme**: Cranck-Nicholson scheme.
- The Jacobian associated with the evolution equations is

$$\frac{\partial G(\mathbf{U}^n)}{\partial \mathbf{U}^n}\delta\mathbf{U}^n = J_n\delta\mathbf{U}^n = \left(\begin{array}{cc} M & U \\ L & D \end{array} \right) \delta\mathbf{U}^n$$

  with $\delta\mathbf{U}^n = (\delta\psi^n, \delta u^n)$
- M and D the matrices of the diffusion and advection operators for ψ et $\triangle_{pol} u$.
- L and U the matrices of the coupling operators between ψ and u.

Preconditioning : Algorithm

- The final system with Schur decomposition is given by

$$\delta \mathbf{U}^n = J_k^{-1} R(\mathbf{U}^n) = \begin{pmatrix} M & U \\ L & D \end{pmatrix}^{-1} R(\mathbf{U}^n)$$

$$= \begin{pmatrix} I & M^{-1}U \\ 0 & I \end{pmatrix} \begin{pmatrix} M^{-1} & 0 \\ 0 & P_{schur}^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -LM^{-1} & I \end{pmatrix} R(\mathbf{U}^n)$$

  with $P_{schur} = D - LM^{-1}U$.
- We obtain the following algorithm which solve $J_k \delta \mathbf{U}_k = R(\mathbf{U}^n)$ + elliptic equations:

$$\begin{cases} \text{Predictor : } & M\delta\psi_p^n = R_\psi \\ \text{potential update : } & P_{schur}\delta u^n = (-L\delta\psi_p^n + R_u)) \\ \text{Corrector : } & M\delta\psi^n = M\delta\psi_p^n - U\delta u^n \\ \text{Current update : } & \delta z_j^n = D^*\delta\psi^n \\ \text{Vorticity update : } & \delta w^n = D_{pol}\delta u^n \end{cases}$$

- with R_ψ and R_u are the right hand side associated with the equations on ψ and u. D^* and D_{pol} the elliptic operators.

An example of Schur complement approximation

- To compute $P_{schur} = D - LM^{-1}U$ we must compute M^{-1}.
- Solving the previous algorithm with an approximation of the Schur complement gives the preconditioning P_n.

- **"Small flow" approximation**
  - In P_{schur} we assume that $M^{-1} \approx \Delta t$

$$P_{schur} = \frac{\triangle_{pol}\delta u}{\Delta t} + \rho \mathbf{u}^n \cdot \nabla(\frac{1}{\rho}\triangle_{pol}\delta u) + \rho\delta\mathbf{u}\cdot\nabla(\frac{1}{\rho}\triangle_{pol}u^n) - \theta\nu\triangle^2_{pol}\delta u - \theta^2\Delta t LU$$

- Operator $LU = \mathbf{B}^n \cdot \nabla(\triangle^*(\frac{1}{\rho}\mathbf{B}^n \cdot \nabla\delta u)) + \frac{\partial j^n}{\partial\psi^n}\mathbf{B}^n_{\perp} \cdot \nabla(\frac{1}{\rho}\mathbf{B}^n \cdot \nabla\delta u)$ with $\rho = \frac{1}{R^2}$

$\mathbf{B}^n \cdot \nabla\delta u = -\frac{1}{R}[\psi^n, \delta u] + \frac{F_0}{R}\partial_\phi \delta u,$

$\mathbf{u}^n \cdot \nabla\delta u = -R[\delta u, u^n]$ et $\delta\mathbf{u} \cdot \nabla u^n = -R[u^n, \delta u]$.

- **Remark**: the LU operator is the parabolization of coupling hyperbolic terms.

LU operator: properties

- The reduced model contains only the Alfvén waves (rigorous proof missing).
- Idem for the LU operator introduced previously.

Properties of LU operator

- We consider the L^2 space. The operator LU is not positive for all δu

$$< LU\delta u, \delta u >_{L^2} = \int \rho |\nabla(\frac{1}{\rho}\mathbf{B}^n.\nabla\delta u)|^2 - \int \frac{1}{\rho}\frac{\partial j^n}{\partial \psi^n}(\mathbf{B}^n_{\perp}.\nabla\delta u)(\mathbf{B}^n\ .\nabla\delta u)$$

- The LU operator is not self-adjoint : $< LU\delta u, \delta v >_{L^2} \neq < \delta u, LU\delta v >_{L^2}$

LU approximation

- We propose the following approximation $LU^{approx} = \mathbf{B}^n \cdot \nabla(\triangle^*(\frac{1}{\rho}\mathbf{B}^n \cdot \nabla\delta u))$
- The operator LU^{approx} is positive an self-adjoint.

- Remark in physical books and papers: the spectrums of LU^{approx} and LU are essentially close (not rigorous proof).

Semi implicit scheme

- We define $f^{n+\frac{1}{2}} = \frac{1}{2}(f^n + f^{n+1})$. The semi-implicit scheme is

$$\begin{cases} \frac{\psi^{n+1}-\psi^n}{\Delta t}\psi = R[\psi^n, u^{n+\frac{1}{2}}] + \eta\triangle^*\psi^{n+\frac{1}{2}} - F_0\partial_\phi u^{n+\frac{1}{2}} \\ \frac{\triangle_{pol}(u^{n+1}-u^n)}{\Delta t} = \frac{1}{R}[R^2 w^n, u^{n+\frac{1}{2}}] + \frac{1}{R}[\psi^n, \triangle^*\psi^{n+\frac{1}{2}}] - \frac{F_0}{R^2}\triangle^*\partial_\phi\psi^{n+\frac{1}{2}} + \nu\triangle^2_{pol}u^{n+\frac{1}{2}} \\ w^{n+1} = \triangle_{pol}u^{n+1}, \quad j^{n+1} = \triangle^*\psi^{n+1} \end{cases}$$

Energy dissipation

We define $E = \int_\Omega \frac{|\nabla_{pol}\psi|^2}{2R^2} + \frac{|\nabla_{pol}u|^2}{2}$. The scheme satisfy $E^{n+1} - E^n \leq 0$

- We can apply the previous preconditioning to the semi-implicit scheme
- **"Small flow" approximation**: $M^{-1} \approx \Delta t$.

$$P_{schur} = \frac{\triangle_{pol}\delta u}{\Delta t} + \rho\delta\mathbf{u}\cdot\nabla(\frac{1}{\rho}\triangle_{pol}u^n) - \theta\nu\triangle^2_{pol}\delta u - \theta^2\Delta t\mathbf{B}^n\cdot\nabla(\triangle^*(\frac{1}{\rho}\mathbf{B}^n\cdot\nabla\delta u))$$

- We obtain direct a positive and symmetric operator LU.
- The Jacobian is more simple and the preconditioning use less approximations.

Remark about radiative transfer

- The preconditioning can be use for radiative problem as P_1 model:

$$\begin{cases} \partial_t u + \frac{1}{\varepsilon}\partial_x v = 0 \\ \partial_t v + \frac{1}{\varepsilon}\partial_x u = -\frac{\sigma}{\varepsilon^2} v \end{cases} \longrightarrow \begin{cases} u^{n+1} = u^n - \frac{\Delta t}{\varepsilon}\partial_x v^{n+1} \\ v^{n+1} = v^n - \frac{\Delta t}{\varepsilon}\partial_x u^{n+1} - \frac{\sigma \Delta t}{\varepsilon^2} v^{n+1} \end{cases}$$

- We obtain the following scheme on the v equation :

$$\left(1 + \frac{\sigma \Delta t}{\varepsilon^2}\right) v^{n+1} = v^n - \frac{\Delta t}{\varepsilon}\partial_x u^{n+1}$$

- Plugging this equation in the equation on u we obtain the preconditioning.

Preconditioning algorithm

$$\begin{cases} u \text{ update:} \quad P u^{n+1} = u^n - \left(\frac{\varepsilon \Delta t}{\varepsilon^2 + \sigma \Delta t}\right) v^n \\ v \text{ update :} \quad v^{n+1} = \left(\frac{\varepsilon^2}{\varepsilon^2 + \sigma \Delta t}\right) v^n - \left(\frac{\varepsilon \Delta t}{\varepsilon^2 + \sigma \Delta t}\right) u^{n+1} \end{cases}$$

with $P = \left(1 - \frac{\Delta t^2}{\varepsilon^2 + \sigma \Delta t}\partial_{xx}\right)$ a well-conditioned operator.

Other numerical studies and conclusion

Current developing: JOREK-Django

JOREK-Django: experimental version of JOREK for numeric research and validation

- Dedidacted for implementing and testing
  - Numerical schemes
  - Spatial discretization
  - Time stepping
- HPC using MPI

Current work on numerical method in Django :

- In the Poloidal plane
  - B splines of any order and regularity (A. Ratnani)
  - Box splines of any order, based on Hexa-meshes (L. S. Mendoza)
  - Spectral Elements (J. Vildes & B. Nkonga)
- In the Toroidal direction
  - Fourier, B-splines (A. Ratnani, E. F.)
- Domain Decomposition (A. Ratnani & B. Nkonga)
- Coupling with Selalib (A. Ratnani & L. S. Mendoza)

Current work on the model in Django

- Poisson equation (A. Ratnani & B. Nkonga)
- Grad-Shafranov equation (using 2 formulations + Picard/Newton)
- Anisotropic Diffusion (A. Ratnani & B. Nkonga)
- Low β reduced MHD like Current Hole (E. F.)
- Reduced resistive and extended MHD (E. F)

Long term projects :

- DeRham complex using B-splines (A. Ratnani)
- Time Domain Maxwell solver
- Fast Solvers based on Kronecker product
- Physic based preconditioners (E. F & A. Ratnani)
- Geometric Multigrid Method (A. Ratnani)
- Full resistive and extended MHD (B. Nkonga)
- Taylor-Galerkin stabilization (B. Nkonga)

internship proposal

internship proposal:

- **Institut** : IPP (Munich)
- **Supervisors** : Eric Sonnendrücker, A. Ratnani
- **Subject** : Study and implementation of $H(curl)$ and $H(div)$ spaces for the Splines in Django JOREK. Application to Maxwell equations

Conclusion and Outlook

Models

- **Results on models**:
  - Formal derivation of hierarchy of fluid models for tokamak with the energy estimates associated.
  - Rigorous derivation of single fluid reduced MHD and energy estimate.
- **Future works**:
  - Rigorous derivation with an energy estimate of diamagnetic (generalized Ohm's law) and two fluid extended reduced MHD.
  - Design of time schemes which preserve the energy estimates.

Nonlinear solvers:

- **Conclusion**: nonlinear inexact Newton solver + adaptive time stepping allows to capture easier the nonlinear phase and avoid some numerical instabilities.
- **Advantages** : larger time step and efficient adaptive time stepping.
- **Possible future works:** Globalization techniques to obtain more robust nonlinear solvers.

Conclusion and Outlook

Preconditioning:

- **Conclusion**: preconditioning based on some approximations to the MHD operators.
- **Question**: new preconditioning more efficient than the old one in the nonlinear phase where the coupling between harmonics is strong ?
- Compatible with Jacobian-free method to reduce memory consumption and increase scalability. This will allow to use higher grid resolutions and more toroidal harmonics.
- **Future works**: validate the algorithm for models without parallel velocity and write the preconditioning for the single and bi-fluid models.

Thanks

Thanks for your attention