Hierarchy of fluid models and numerical methods for the JOREK code

E. Franck[1],
A. Lessig [2], M. Hölzl [2], A. Ratnani [2], E. Sonnendrücker [2]

TONUS Day, IRMA, Strasbourg.
4 November 2014

[1]Inria Nancy Grand Est, Tonus team, France.
[2]Max-Planck-Institut für Plasmaphysik, Germany.

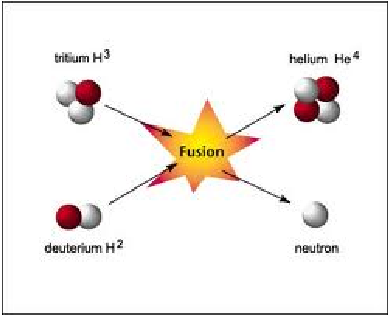
Outline

1. Physical and mathematical context
2. Hierarchy of models for plasmas
3. Nonlinear solvers and preconditioning
4. Future works, perspectives and conclusion

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.

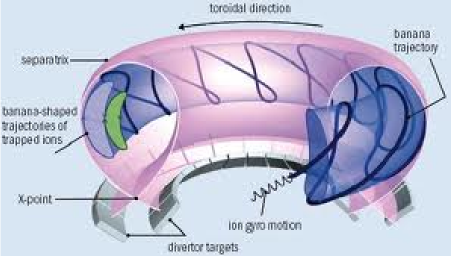
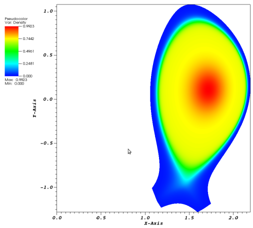


Figure: Tokamak

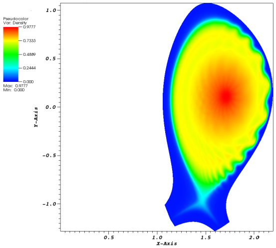
Plasma instabilities

- Edge localized modes (ELMs) are periodic instabilities driven by large pressure gradients and current densities 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 (Pellets injection and Resonant Magnetic Perturbations).

- Initial Density

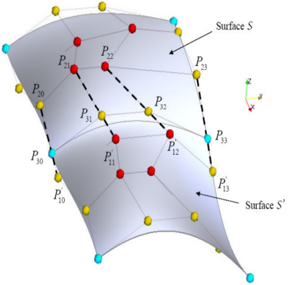


- Final Density



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:

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

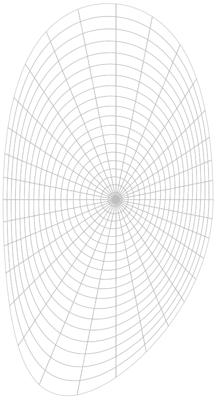


Figure: unaligned grid

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.

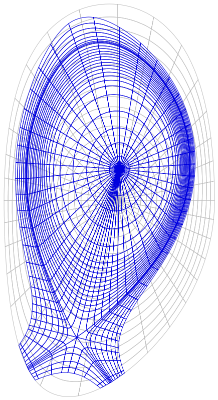


Figure: Aligned grid

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 $\mathbf{v}\in\mathbb{R}^3$.

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

- 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
  - $\int_{D_{\mathbf{v}}} m_s\mathbf{v}C_{ss}d\mathbf{v}=0,\quad \int_{D_{\mathbf{v}}} m_s|\mathbf{v}|^2C_{ss}d\mathbf{v}=0,$
  - $\int_{D_{\mathbf{v}}} g(\mathbf{v})_sC_{st}d\mathbf{v}+\int_{D_{\mathbf{v}}} g(\mathbf{v})_tC_{ts}d\mathbf{v}=0.$

Two fluid model

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

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

- $n_s = \int_{D_{\mathbf{v}}} f_s d\mathbf{v}$ 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, ϵ_s 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_s associated with the collision between two species (force and energy transfer).
- 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

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

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: Stress tensor and closure

- The heat flux is given by

$$\mathbf{q} = -\left[k_{||}\mathbf{b}\times\mathbf{b} + k_{\perp}(I_d - \mathbf{b}\times\mathbf{b})\right]\cdot\nabla T$$

with $\mathbf{b} = \frac{\mathbf{B}}{||\mathbf{B}||}$ and $k_{||} >> k_{\perp}$.

- For the Extended MHD, the stress tensor (viscosity) is given by $\Pi = \Pi_{||} + \Pi_c + \Pi_{\perp}$ with :
  - $\Pi_{||}$ the parallel part $(\mathbf{b}\times\mathbf{b})$,
  - Π_c the cross part $(\mathbf{b}\times I_d)$,
  - $\Pi_{\perp}$ the perpendicular part $(I_d - \mathbf{b}\times\mathbf{b})$.

- The perpendicular viscosity is smaller than the parallel one. We replace the perpendicular viscosity by isotropic viscosity $\Pi^v = -\nu(\nabla\mathbf{u} + \nabla\mathbf{u}^t)$.

- The parallel part is approximate by the neoclassical theory Π^{nc}. This tensor is not to complicate to write.

- The structure of the gyro-viscous tensor (cross tensor) Π^{gv} is more complicate.

Extended MHD: Diamagnetic MHD I

- 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

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

with $\mathbf{u}_E = \frac{\mathbf{E}\times\mathbf{B}}{|\mathbf{B}|^2}$, $\mathbf{u}_{||}$ 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

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

- Using the decomposition of the velocity we obtain

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

- 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:

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

- 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 $v_{||} = 0$.

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

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.

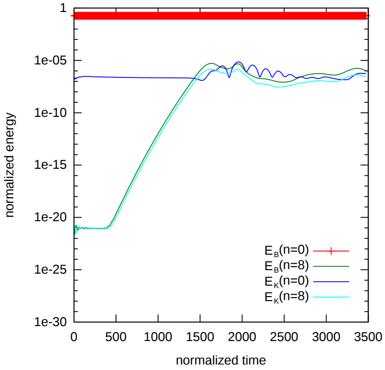


Figure: Reference solution: kinetic and magnetic energies for $\Delta t = 5$ gives by the Newton method.

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.

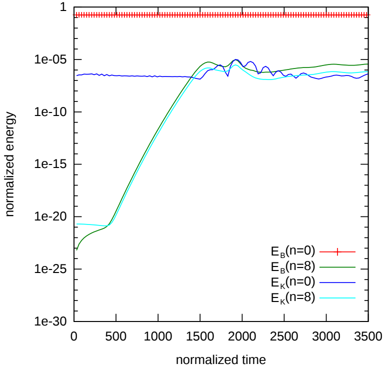


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 30$.

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.

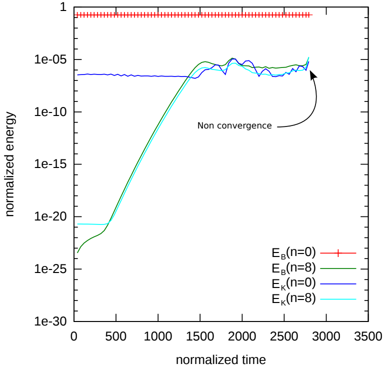


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 40$.

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.

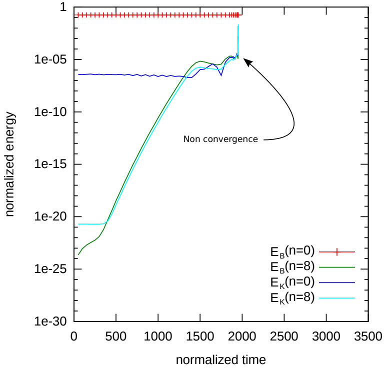


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 50$.

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.

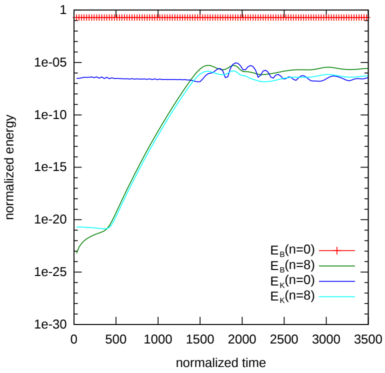


Figure: Kinetic and magnetic energies for Newton method for $\Delta t = 30$.

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.

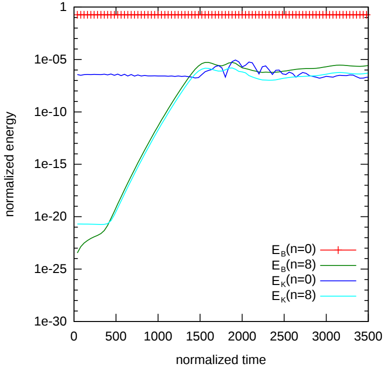


Figure: Kinetic and magnetic energies for Newton method for $\Delta t = 40$.

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.

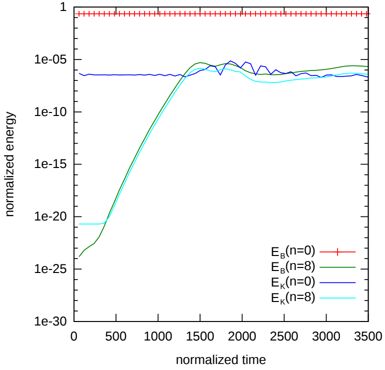


Figure: Kinetic and magnetic energies for Newton method for $\Delta t = 60$.

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.

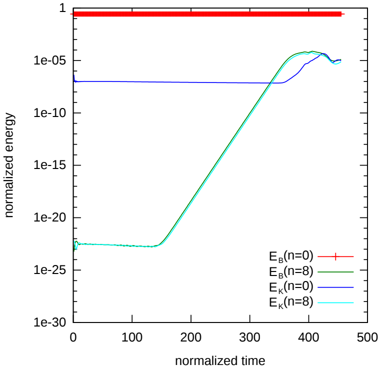


Figure: Reference solution: kinetic and magnetic energies for $\Delta t = 1$ gives by the Linearization method

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.

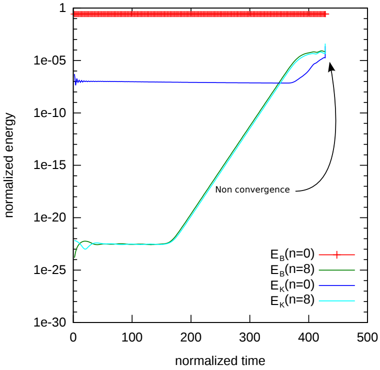


Figure: Kinetic and magnetic energies for Linearization method for $\Delta t = 2$.

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.

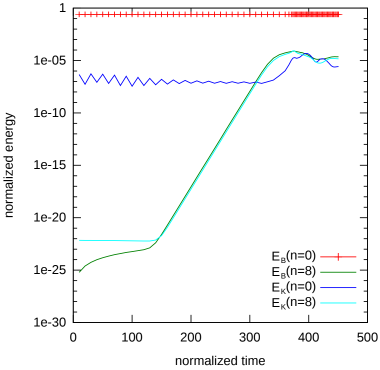


Figure: Kinetic and magnetic energies for Newton method for initial $\Delta t = 10$. Final time step around 2.

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

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

  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

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

  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:

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

- 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 $M^{-1} \approx \Delta t$

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

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

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

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**: $M^{-1} \approx \Delta t$.

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

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

Future works, perspectives 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)

Perspectives on models

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.
  - More realistic stress tensors and viscosity for the reduced MHD models
  - Design of time schemes which preserve the energy estimates (for example the Cranck Nicholson scheme does not preserve energy for the reduced model with parallel velocity).

Perspectives on time scheme and preconditioning

Time scheme and preconditioning

- **Results Time 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.
- **Future works**:
  - Compare the new preconditioning with the old one for the Current Hole.
  - Write the preconditioning for the single and bi-fluid models (reduced and full MHD).
  - Couple the preconditioning with the Jacobian-free method useful to reduce the memory consumption (main problem) and increase scalability.
  - Use semi-implicit schemes to simplify the Jacobian, reduce the CPU time and have better conditioned matrices.
  - Design of adapted time method for extended MHD to treat the singularity close the vacuum.

Perspectives on spatial discretization

Spatial discretization

- **Default of FE and Spectral methods** :
  - These methods are not adapted to conserve the different quantity and to preserve the positivity of the variables (Gibbs phenomenon).
- **First possibility: modification of the FE and spectral methods**
  - Some technic like filtering allows to reduced the Gibbs phenomenon (ref: *The Gibbs Phenomenon in Fourier Analysis, Splines and Wavelet Approximations*)
- **Second possibility: DG methods**
  - **Advantages** : methods efficient to treat the hyperbolic (ideal or extended MHD) systems, preserve the positivity and the conservation laws.
  - **Possible future works**: design DG methods for high order operators (anisotropic diffusion, resistivity terms and stress tensors). Actually they are few results on these problems.

Thanks

Thanks for your attention