Preconditioning and nonlinear time solvers for the JOREK MHD code

E. Franck, A. Lessig, M. Hölzl, E. Sonnendrücker

Max Planck Institute of Plasma physics, Garching, Germany

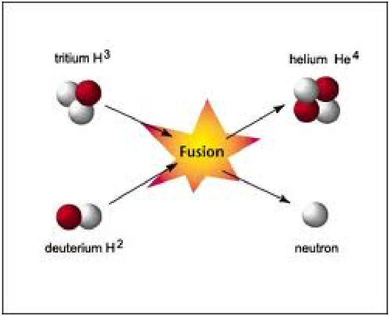
10th AIMS Conference, special session 121, Madrid
10 July 2014

Outline

Physical context and models

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.

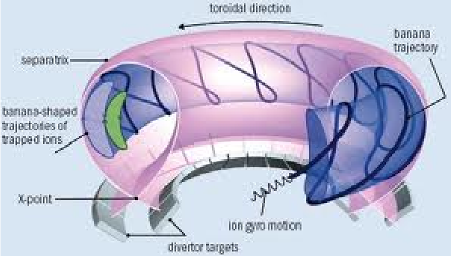
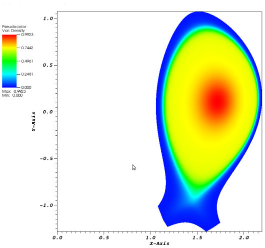


Figure : Tokamak

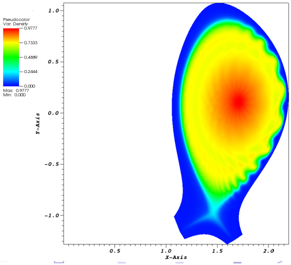
Plasma instabilities

- 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 simuation (MHD models) can help to understand and control ELMs better.

- Initial Density



- Final Density



MHD model

- The full resistive MHD model is given by

$$
\begin{cases}
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = \nabla \cdot (D \nabla \rho) + S_p \\
\rho \partial_t \mathbf{v} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla P = \mathbf{J} \times \mathbf{B} + \nu \triangle \mathbf{v} \\
\partial_t P + \mathbf{v} \cdot \nabla P + \gamma P \nabla \mathbf{v} = \nabla \cdot (K \nabla T) + S_h \\
\partial_t \mathbf{B} = -\nabla \times \mathbf{E} = \nabla \times (\mathbf{v} \times \mathbf{B}) - \eta \nabla \times \mathbf{J} \\
\nabla \cdot \mathbf{B} = \mathbf{0}
\end{cases}
$$

- **Magnetic quantities**: $\mathbf{B}$ the magnetic field, $\mathbf{E}$ the electric field and $\mathbf{J} = \nabla \times \mathbf{B}$ the current.
- **Hydrodynamic quantities**: ρ the density, $\mathbf{v}$ the velocity, T the temperature, and $P = \rho T$ the pressure.
- The terms K and D are anisotropic diffusion tensors.
- Source terms: S_h is a heat source, S_p is a particle source.

Reduced MHD: assumptions and principle of derivation

- **Aim**: Reduce the number of variables and eliminate the fast magnetosonic waves.
- We consider the cylindrical coordinate $(R, Z, \phi) \in \Omega \times [0, 2\pi]$

Reduced MHD: Assumptions

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

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 $\mathbf{v}$ in the equations + some computations. For the equations on u and $v_{||}$ we use the following projections

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

and

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

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

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

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

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

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

Main result: energy estimate

- Correct reduced model : estimation on the energy conservation or dissipation.

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 $\mathbf{v} = -R\nabla u \times \mathbf{e}_\phi + v_{||}\mathbf{B}$.

For the model associated with these fields we obtain

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

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

- The implemented models approximately conserve energy. For exact energy conservation, some neglected cross-terms between poloidal and parallel velocity have to be added which might be important in the non-linear phase.

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

Jorek code and time solvers

Description of the JOREK code I

- JOREK: Fortran 90 code, parallel (MPI+OpenMP) + algebraic libraries (Pastix, MUMPS ...)
- 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

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

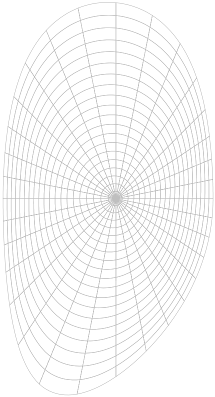


Figure : unaligned grid

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)
  - **Poloidal discretization**: 2D Cubic Bezier finite elements.
  - **Toroidal discretization**: Fourier expansion.
  - Construction of the matrix and some profiles (diffusion tensors, sources terms).
  - Solve linear system.
  - Update solutions.

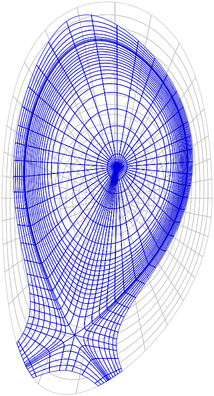


Figure : Aligned grid

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.

JOREK code: convergence issues

Problem :

- For some test cases the linear solver does not converge in the nonlinear phase even for small time steps.

- **Why** ?
  - Because some violent numerical instabilities appear in the nonlinear phase and generate ill-conditioned matrices.

- **Critical time for simulation**: the beginning of nonlinear phase. It is necessary to capture correctly the stabilization of ∇P and $\mathbf{J}$.
- **Aim**: minimize the numerical error and numerical spurious behaviours at this time to avoid critical numerical instabilities and non convergence issues.

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

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

  - 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.

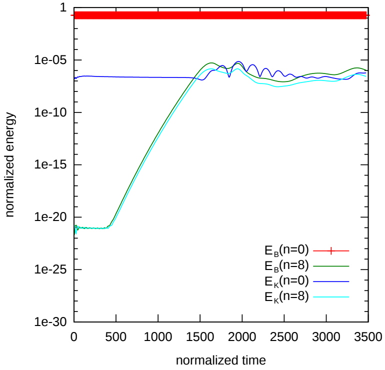


Figure : Reference solution: kinetic and magnetic energies for $\Delta t = 5$ gives by the Newton method.

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.

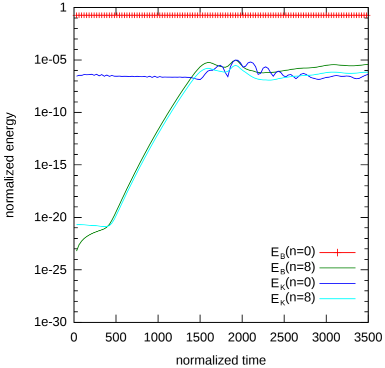


Figure : Kinetic and magnetic energies for Linearization method for $\Delta t = 30$.

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.

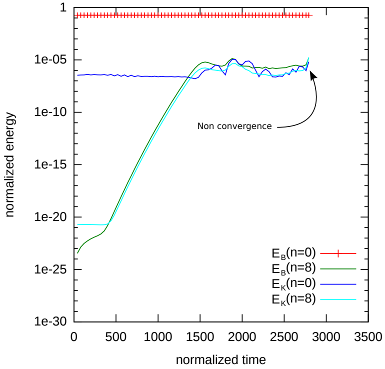


Figure : Kinetic and magnetic energies for Linearization method for $\Delta t = 40$.

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.

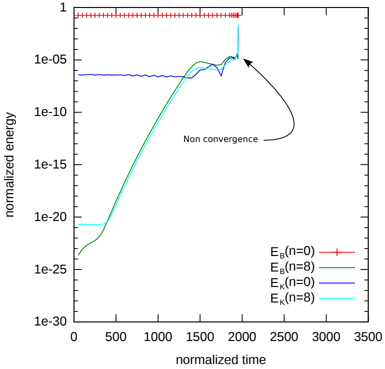


Figure : Kinetic and magnetic energies for Linearization method for $\Delta t = 50$.

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.

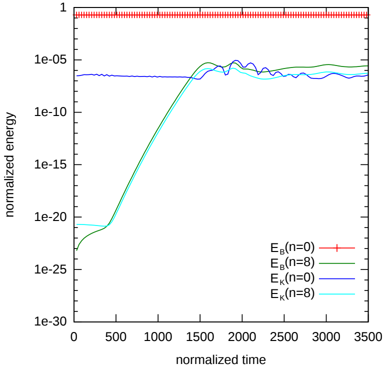


Figure : Kinetic and magnetic energies for Newton method for $\Delta t = 30$.

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.

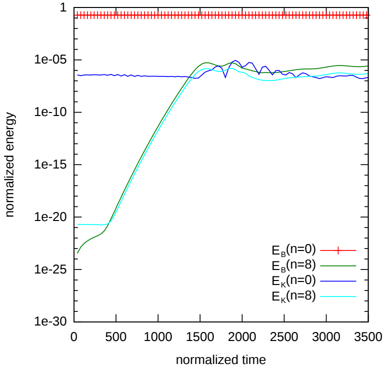


Figure : Kinetic and magnetic energies for Newton method for $\Delta t = 40$.

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.

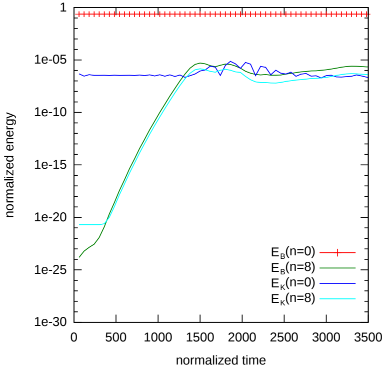


Figure : Kinetic and magnetic energies for Newton method for $\Delta t = 60$.

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.

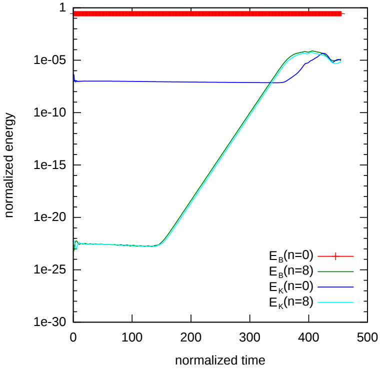


Figure : Reference solution: kinetic and magnetic energies for $\Delta t = 1$ gives by the Linearization method.

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.

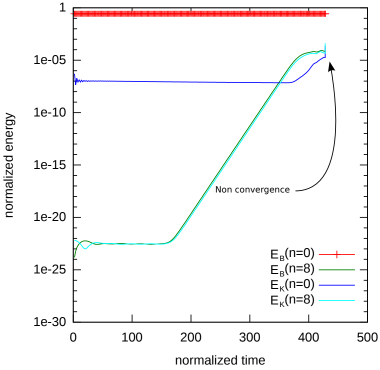


Figure : Kinetic and magnetic energies for Linearization method for $\Delta t = 2$.

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.

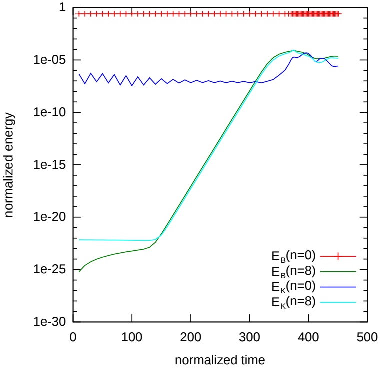


Figure : Kinetic and magnetic energies for Newton method for initial $\Delta t = 10$. Final time step around 2.

Preconditioning

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 $\mathbf{B} = \frac{F_0}{R} e_\phi + \frac{1}{R}\nabla\psi \times e_\phi$ and $\mathbf{v} = -R\nabla u \times e_\phi$.
- The model is

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

  with $w = \triangle_{pol} u$ and $j = \triangle^* \psi$.
- In this formulation we separate the evolution and elliptic equations
- 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}.
- An approximation of the Schur complement gives the preconditioning P_n.
- **"Small flow" approximation**
  - In P_{schur} we assume that $M^{-1} \approx \Delta t$

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

- 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 $\rho = \frac{1}{R^2}$

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

  $\mathbf{v}^n \cdot \nabla \delta u = -R[\delta u, u^n]$ et $\delta \mathbf{v} \cdot \nabla u^n = -R[u^n, \delta u]$.
- **Remark**: the LU operator is the parabolization of coupling hyperbolic terms.

LU operator: properties

- For this reduced model the magnetosonic waves are filtered, it contains only the Aflvén 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).

Conclusion and Outlook

Models :

- **Conclusion**: 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 fluids 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 technics to obtain more robust nonlinear solvers.

Conclusion and Outlook

Preconditioning:

- **Conclusion**: preconditioning based on 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