Numerical issues for nonlinear MHD Jorek code

Emmanuel Franck
Max Planck Institute For Plasma Physics (Munich)
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Physical context and models
**Fusion DT**: Reaction between Deuterium and tritium which product Helium and energy. The deuterium and tritium form a plasma (ionized gas).
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**Magnetic confinement:** The plasma obtained by the reaction is confined in the center of the reactor (tokamak) using a powerful magnetic field.

**Tokamak:** Toroidal room used for the plasma confinement.
The dynamic of the plasmas in Iter is a very difficult multiscale problem.

**Figure:** Spatial and time scales
The dynamic of the plasmas in Iter is a very difficult multiscale problem.

We have different models for the different time and space scales:

- **Kinetic Vlasov-Maxwell equation** not used in practice (CPU cost very important).
- **Gyrokinetic approximation** of the Vlasov-Maxwell equation used for the turbulence in the core Tokamak.
- **MagnetoHydrodynamics fluids models** (resistive MHD, two fluids MHD) used to simulate the edge instabilities.

Figure: Spatial and time scales
ELMs and instabilities

- An edge-localized mode ("ELM’s") is a disruptive instability occurring in the edge region of a tokamak plasma.
- The development of edge-localized modes poses an important challenge in magnetic fusion research with tokamaks. Instabilities can damage wall components due to their extremely high energy transfer rate.
- **Aim**: simulate the ELM’s to estimate the amplitude of these instabilities and understand how control these.

**References**

- Reduced magnetohydrodynamic simulation of toroidally and poloidally localized edge localized modes, M. Hölzl and co-workers, Phys. of Plasmas, 2012.
MHD model

The full - resistive MHD model is given by

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= \nabla \cdot (D_{||} \nabla_{||} \rho + D_{\perp} \nabla_{\perp} \rho) + S_p \\
\rho \partial_t \mathbf{v} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla (\rho T) &= \mathbf{J} \times \mathbf{B} + \nu \nabla \mathbf{v} \\
\rho \partial_t T + \rho \mathbf{v} \cdot \nabla T + (\gamma - 1) \rho T \nabla \mathbf{v} &= \nabla \cdot (K_{||} \nabla_{||} T + K_{\perp} \nabla_{\perp} T) + S_h \\
\partial_t \mathbf{B} &= \nabla \times (\mathbf{v} \times \mathbf{B}) - \nabla \times \eta \mathbf{J} + S_c \\
\nabla \cdot \mathbf{B} &= 0
\end{align*}
\]

with \( \rho \) the density, \( \mathbf{v} \) the velocity, \( T \) the temperature, \( \mathbf{B} \) the magnetic field and \( \mathbf{J} = \nabla \times \mathbf{B} \) the current.

- The terms \( D_{||}, D_{\perp}, K_{||}, K_{\perp} \) are anisotropic diffusion tensors.
- We add source terms. \( S_c \) correspond to the current source, \( S_h \) correspond to the heat source, \( S_p \) correspond to the particle source.
Reduced MHD: assumption and derivation

- We consider the cylindric coordinate \((R, Z, \phi) \in \Omega \times [0, 2\pi]\).
- \((R, Z)\) correspond to the poloidal plan and \(\phi\) the toroidal direction.

**Reduced MHD: assumptions**

\[
\mathbf{B} = \frac{F_0}{R} \mathbf{e}_\phi + \frac{1}{R} \nabla \Psi \times \mathbf{e}_\phi \quad \mathbf{v} = -R \nabla u \times \mathbf{e}_\phi + v_\parallel \mathbf{B}
\]

with \(u\) the electrical potential and \(\psi\) the poloidal magnetic flux.

- For the reduced MHD the quantities are \(\rho, T, \Psi, u, v_\parallel\) the parallel velocity, \(w\) the vorticity and \(z_j\) the toroidal current.
- Derivation: Plug \(\mathbf{B}\) and \(\mathbf{v}\) in the density, magnetic and energy equations. For the equations on \(u\) and \(v_\parallel\) we use

\[
\mathbf{e}_\phi \cdot \nabla \times (\rho \partial_t \mathbf{v} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla (\rho T) = \mathbf{J} \times \mathbf{B} + \nu \Delta \mathbf{v})
\]

and

\[
\mathbf{B} \cdot (\rho \partial_t \mathbf{v} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla (\rho T) = \mathbf{J} \times \mathbf{B} + \nu \Delta \mathbf{v}).
\]
With $\nu_\parallel = 0$ we obtain the model 199 considered in this talk.

We solve $\partial_t A(U) = B(U, t)$ with

$$B(U) = \begin{pmatrix}
[\Psi, u] - \frac{\epsilon F_0}{R} \partial_{\phi} u + \frac{\eta(T)}{R} (z_j - S_c(\Psi)) - \eta_n \nabla . (\nabla z_j) \\
\frac{1}{2} [R^2 \| \nabla u \|^2, \hat{\rho}] + [R^2 \hat{\rho} w, u] + [\Psi, z_j] - \frac{\epsilon F_0}{R} \partial_{\phi} z_j - [R^2, p] \\
+ \nabla . (R \nu(T) \nabla w) - \nu_n \nabla . (\nabla w) \\
\frac{1}{R^2} z_j - \nabla . \left( \frac{1}{R^2} \nabla \Phi \right) \\
w - \nabla . (\nabla u) \\
R^2 [\rho, u] + 2 R \rho \partial_Z u + \nabla . (D_\parallel \nabla \parallel \rho + D_\perp \nabla \perp \rho) + S_p(\Psi) \\
R^2 [T, u] + 2(\gamma - 1) R T \partial_Z u + \nabla . (K_\parallel \nabla \parallel T + K_\perp \nabla \perp T) + S_h(\Psi)
\end{pmatrix}$$

with $\hat{\rho} = R^2 \rho$ and $\partial_t A(U) = (\frac{1}{R} \partial_t \Psi, R \nabla . (\hat{\rho} \nabla (\partial_t u)), 0, 0, R \partial_t \rho, R \partial_t T))$.

Physical and numerical resistivity: $\eta$ and $\eta_n$, viscosity coefficients: $\nu$ and $\nu_n$. 
Jorek Code: description
**Description of the jorek code I**

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

- **Initialization**

- **Determinate 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

\[
R \frac{\partial}{\partial R} \left( \frac{1}{R} \frac{\partial \Psi}{\partial R} \right) + \frac{\partial^2 \Psi}{\partial Z^2} = -R^2 \frac{\partial p}{\partial \Psi} - F \frac{\partial F}{\partial \Psi}
\]
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.

- Time-stepping (restart)
  - Construction of the matrix and some profiles (diffusion tensors, sources terms)
  - Solve linear system
  - Update solutions
  - Plot kinetic magnetic energies and restart files.

Figure: Aligned grid
The equation in the **poloidal plane** are discretized using finite element method. For the **toroidal direction**: Fourier expansion.

**Basis functions**: Cubic Bezier elements

- Generalization of cubic Hermite elements.
- The generalization allows the local refinement of each element essential for adaptive mesh refinement.
- 4 degrees of freedom by node to describe a function (9 for Lagrange cubic finite element).
- With the isoparametric formulation (discretization of \((R, Z)\) using the Bezier elements) the finite elements can be accurately aligned with the equilibrium flux surfaces.
- The Cubic Bezier elements assure a \(C^1\) polynomial reconstruction.

*Bezier surfaces and finite elements for MHD simulations*, O. Czarny, G. Huysmans, JCP 2088.
Time scheme in Jorek code

- We recall the model $\partial_t A(U) = B(U, t)$
- For time stepping we use a Crank Nicholson or BDF2 scheme:

$$
(1 + \zeta)A(U^{n+1}) - \zeta A(U^n) + \zeta A(U^{n-1}) = \theta \Delta tB(U^{n+1}) + (1 - \theta)\Delta tB(U^n)
$$

- Defining $G(U) = (1 + \zeta)A(U) - \theta \Delta tB(U)$ and

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

we obtain the non linear problem

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

- First order linearization

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

with $\delta U^n = U^{n+1} - U^n$ and $\frac{\partial G(U^n)}{\partial U^n}$ the Jacobian of $G(U^n)$. 
Time scheme in Jorek code

- **Linear solver in Jorek:**
  - Case 1: Direct solver using Pastix (using when $n_{tor} = 1$)
  - Case 2: Iterative solver

- **Iterative Solver step 1: Preconditioning**
  - Extraction of submatrices associated to each toroidal harmonics.
  - Factorization of each submatrix
  - We solve exactly (with Pastix) each subsystems.
  - We construct the initial vector of GMRES using the solutions of these systems.

- **Iterative solver step 2: GMRES solver for the global matrix.**
  - The matrix product vector is preconditioned with the solutions of each subsystems.

- **Principle:** Construction of initial GMRES data + right preconditioning with an approximation of the Jacobian where the coupling between the Fourier modes are neglected.

- In practice for some test cases this coupling is strongly nonlinear.
Problem:

- For some test cases the GMRES method does not converge in the nonlinear phase for large time step.

Why?

- The preconditioning is not adapted to obtain a robust GMRES method?
- The spatial poloidal and toroidal discretizations is not adapted?
- The mesh is not adapted?
- The models are not stables?
Numerical example

- Evolution of energy in time

![Graph showing energy evolution over time](image)

- Density

![Density distribution](image)
Numerical example

- Density

- Evolution of energy in time

![Graph showing the evolution of energy in time and a density map.](image-url)
Numerical example

- Density

- Evolution of energy in time
Current works on the time discretization
Inexact Newton scheme

- At the time step $n$, we compute $b(U^n, U^{n-1})$, $G(U^n)$
- We choose $U_0 = U^n$ and $\varepsilon_0$.
- Step $k$ of the Newton procedure
  - We compute $G(U_k)$ and $\left( \frac{\partial G}{\partial U_k} \right)$
  - We solve the linear system with GMRES
    \[
    \left( \frac{\partial G(U_k)}{\partial U_k} \right) \delta U_k = \tilde{G}(U_k) = b(U^n, U^{n-1}) - G(U_k)
    \]
    and the following convergence criterion
    \[
    \frac{\left\| \left( \frac{\partial G}{\partial U_k} \right) \delta U_k + \tilde{G}(U_k) \right\|}{\left\| \tilde{G}(U_k) \right\|} \leq \varepsilon_k, \quad \varepsilon_k = \gamma \left( \frac{\left\| \tilde{G}(U_k) \right\|}{\left\| \tilde{G}(U_{k-1}) \right\|} \right) \alpha
    \]
  - We iterate with $U_{k+1} = U_k + \delta U_k$.
  - We apply the convergence test (for example $\left\| \tilde{G}(U_k) \right\| < \varepsilon_a + \varepsilon_r \left\| \tilde{G}(U^n) \right\|$)
  - If the newton procedure stop we define $U^{n+1} = U_{k+1}$.
Preconditioning idea I


**Aim:** Construct an algorithm which give a good prediction of the solution and which is easy to solve.
- The algorithm must give a solution of $A\delta U^n = -G(U^n) + b(U^n, U^{n-1})$
  with $A \approx \frac{\partial G(U^n)}{\partial U^n}$.
- $A$ must be well-conditioned. **Idea:** parabolization of the coupled hyperbolic equations.

**Example**

\[
\begin{align*}
\partial_t u &= \partial_x v \\
\partial_t v &= \partial_x u
\end{align*}
\]

\[
\begin{align*}
u^{n+1} &= u^n + \Delta t \partial_x v^{n+1} \\
v^{n+1} &= v^n + \Delta t \partial_x u^{n+1}
\end{align*}
\]

- 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 diagonal dominant matrix.
Preconditioning idea II

To apply easily this method for more complicated equations, we propose a other interpretation.

We assume that the matrix associated to the previous linear system is

\[
\begin{pmatrix}
D_1 & U \\
L & D_2
\end{pmatrix}
\]

Using a Schur decomposition we obtain

\[
\begin{pmatrix}
D_1 & U \\
L & D_2
\end{pmatrix} = \begin{pmatrix}
I & UD_2^{-1} \\
0 & I
\end{pmatrix} \begin{pmatrix}
P_{schur} & 0 \\
0 & D_2
\end{pmatrix} \begin{pmatrix}
I & 0 \\
D_2^{-1}L & I
\end{pmatrix}
\]

\[
\begin{pmatrix}
I & -\Delta t \partial_x \\
-\Delta t \partial_x & I
\end{pmatrix} = \begin{pmatrix}
I & -\Delta t \partial_x \\
0 & I
\end{pmatrix} \begin{pmatrix}
P_{schur} & 0 \\
0 & I
\end{pmatrix} \begin{pmatrix}
I & 0 \\
-\Delta t \partial_x & I
\end{pmatrix}
\]

The first and third matrices are triangular and easily to invert.

\[P_{schur} = D_1 - UD_2^{-1}L = (1 - \Delta t^2 \partial_{xx})\] is diagonal dominant matrix.
Physical context and models
Jorek Code: description
Current works on the time discretization
Other way for the future
Conclusion

Preconditioning with Schur decomposition for MHD

- We apply the Schur decomposition to the model 199. The system solved is

\[
\frac{\partial G(U^n)}{\partial U^n} \delta U^n = \left( \begin{array}{cccccc}
D_\psi & 0 & D_\psi, T & D_\psi, z_j & 0 & U_{\psi, u} \\
0 & D_\rho & 0 & 0 & 0 & U_{\rho, u} \\
0 & 0 & D_T & 0 & 0 & U_{T, u} \\
D_{z_j, \psi} & 0 & 0 & D_{z_j} & 0 & 0 \\
0 & 0 & 0 & 0 & D_w & D_{w, u} \\
L_{u, \psi} & L_{u, \rho} & L_{u, T} & L_{u, z} & L_{u, w} & D_u \\
\end{array} \right) \delta U^n = \tilde{G}(U^n)
\]

with \( \delta U^n = (\delta \psi, \delta \rho, \delta T, \delta z_j, \delta w, \delta u) \) and \( \tilde{G}(U^n) = -G(U^n) + b(U^n, U^{n-1}) \).

- The terms \( D \) contains advection and diffusion operators.
- The terms \( L \) and \( U \) contains non linear coupling hyperbolic operators.
- We reduce the number on variable using the definition of \( w \) and \( z_j \).

\[
\frac{\partial G(U^n)}{\partial U^n} \delta U^* = \left( \begin{array}{cccc}
D^{*}_\psi & 0 & D^{*}_\psi, T & U_{\psi, u} \\
0 & D_\rho & 0 & U_{\rho, u} \\
0 & 0 & D_T & U_{T, u} \\
L^{*}_{u, \psi} & L^{*}_{u, \rho} & L^{*}_{u, T} & D^{*}_u \\
\end{array} \right) \delta U^*
\]

with \( \delta U = (\delta \psi, \delta \rho, \delta T, \delta u) \)
Preconditioning : Algorithm

The final system with Schur decomposition is given by

$$\delta U^n = \frac{\partial G(U^n)}{\partial U^n}^{-1} \tilde{G}(U^n) = \left( \begin{array}{cc} M & U \\ L & D_u \end{array} \right)^{-1} \tilde{G}(U^n)$$

$$= \left( \begin{array}{cc} I & M^{-1}U \\ 0 & I \end{array} \right) \left( \begin{array}{cc} M^{-1} & 0 \\ 0 & P_{schur}^{-1} \end{array} \right) \left( \begin{array}{cc} I & 0 \\ -LM^{-1} & I \end{array} \right) \tilde{G}(U^n)$$

with $P_{schur} = D_u^* - LM^{-1}U$.

$M$, $D_u^*$ are associated to the advection and diffusion operators. $L$, $U$ are associated to the hyperbolic coupling operators.

Final PC-Algorithm

$$\begin{cases} 
\text{Predictor :} & M \delta v^n_p = (-G^n_v + B^n_v) \\
\text{potential update :} & P_{schur} \delta u^n = (-L \delta v^n_p - G^n_u + B^n_u) \\
\text{Corrector :} & M \delta v^n = M \delta v^n_p - U \delta u^n \\
\text{diffusion, update :} & D_{z_j} \delta z^n_j = D_{z_j} \psi \delta \psi^n \\
& D_w \delta w^n = D_{w,u} \delta u^n
\end{cases}$$

with $\delta v_p = (\delta \Psi, \delta \rho, \delta T)$, $G_v$ and $B_v$ the right hand side associated to the equations on $\Psi$, $\rho$ and $T$. 
Preconditioning: Approximation of the Schur complement

- The Schur complement $P_{\text{schur}} = D_u^* - LM^{-1}U$ necessitates knowing the matrix $M^{-1}$.

- Consequently, we must approximate $P_{\text{schur}}$. Two approximations:

  - Small flow approximation (L. Chacon)
    - In $P_{\text{schur}}$, we assume that $M^{-1} \approx \Delta t$
    - Mathematical problem: estimate the operator $LU$.

  - Arbitrary flow approximation (L. Chacon).
    - We introduce an operator $M_*$ (in $u$-space) with $UM_* \approx MU$.
    - Consequently, $P_{\text{Schur}} = (D_uM_* - LU)M_*^{-1}$ with $LU$ given by the small flow approximation.
    - In this case, the Potential update step is given by

      \[
      \begin{align*}
      \text{potential update I} : \quad & (D_uM_* - LU)\delta u^{*,n} = (-L\delta v^p_n - G^u_n + B^u_n) \\
      \text{potential update II} : \quad & \delta u^n = M_* \delta u^{*,n}
      \end{align*}
      \]

    - Mathematical problem: estimate the operator $M_*$.

- Other choices are possible to approximate the Schur complement.
The PC preconditioning method uses a prediction of the solution based on the approximation of the Schur complement.

It is probable that this prediction of the solution is better than the previous method used in Jorek.

However, it is possible that each step of the PC algorithm admits also a problem of conditioning. But since we have a parabolization of the equations and diagonal dominant matrices, adding algebraic preconditioning as multigrid methods can be performing.

For the step where we solve diffusion and advection operators, the previous preconditioning method can be used.
Other way for the future
After the model 199, it will be important to extend the PC-algorithm for the models with parallel velocity and full MHD.

For the models with parallel velocity the operators $U$ and $P_{Schur}$ are applied on $u$ and $v_{||}$.

For the full-MHD the operators $U$ and $P_{Schur}$ are applied on the complete velocity field.

For the full-MHD we have

\[ \mathbf{v} = R \nabla u \times \mathbf{e}_\phi + R w \mathbf{e}_\phi + \frac{1}{R^2} \nabla_\perp \chi \]

with $u$, $w$, $\chi$ scalar fluxes.

- $u$ is associated mainly with the Alfven wave.
- $w$ is associated mainly with the slow wave.
- $\chi$ is associated mainly with the fast wave.
Extension for others reduced MHD and full MHD

- In the model 199, the choice of the velocity field show the Alfven wave dominate.

- In the reduced MHD with parallel velocity and the full-MHD, the different types of waves are present.

- The ratio between the different waves can be very important. Consequently the conditioning is impacted by the ratio.

- If this problem impact the efficiency of the PC-algorithm we can use a method proposed by S. Jardin coupled with the previous algorithm.

**Jardin method for Schur matrix**

- This technic use projection operator to isolate the physics associated with the different wave types in different blocks in the matrix weakly coupled.

- Each submatrix are corrected conditioned.
AP schemes for anisotropic diffusion in Jorek

- Anisotropic diffusion

\[ \partial_t \rho - \nabla \cdot (D_\parallel \nabla \parallel \rho + D_\perp \nabla \perp \rho) = 0 \quad \text{with} \quad D_\perp / D_\parallel << 1 \]

- It is known that the anisotropic diffusion operators are *ill-conditioned*.
- For instance the big problem of non convergence come from hyperbolic coupling. But it is possible the anisotropic diffusion can be give problem for some test case.

- In the PC-algorithm the anisotropic diffusion operators are contained in the matrix $M$
- The initial Preconditioning algorithm of Jorek is efficient to treat these terms but the CPU time associated with this algorithm is important.

We propose:
- Determine if the conditioning of $M$ (advection and diffusion terms) is mainly impacted by the anisotropic diffusion.
- **Use AP scheme for these terms** to avoid to use a preconditioning and decrease the CPU time.
Application in the jorek code. Diffusion operator:

\[-\nabla \cdot \left((D_\parallel - D_\perp) \frac{B \otimes B}{||B||^2} \nabla \rho + D_\perp \nabla \rho \right) = 0\]

with for example the constants $D_\parallel = O(1)$, $D_\perp^1 = O(\varepsilon)$, $D_\perp^2 = O(1)$, $D_\perp^3 = O(1)$ and

\[D_\perp = D_\perp^1 (1 - D_\perp^2 + D_\perp^2 (0.5 - 0.5 \tanh(f(\Psi) - D_\perp^3)))\]

We define $\varepsilon = D_\perp^1$, $\nabla_\parallel = \frac{B}{||B||} \cdot (\frac{B}{||B||} \cdot \nabla T)$ to obtain

\[-\nabla \cdot \left(\frac{1}{\varepsilon} A_\parallel \nabla_\parallel \rho + A_\perp \nabla_\perp \rho \right) = 0\]

with $A_\parallel = \varepsilon D_\parallel$ and $A_\perp = D_\perp = O(\varepsilon)$.

In this formulation we can apply the AP scheme.

Recently B. Després and R. Sart have proposed a more rigorous method to
deduce the reduced MHD models (the moment method).
The authors show that to obtain an energy estimate we must had a term on the
poloidal magnetic flux $\psi$ equation.
For the model 199 the equation $\psi$ come from

$$\partial_t \frac{\psi}{R} = [\psi, u] - \epsilon \frac{F_0}{R} \partial_\phi u + \frac{\eta(T)}{R} (z_j - S_c(\psi)) - \eta_n \nabla \cdot (\nabla z_j) + Q$$

with $\triangle Q = 0$.
For the model 199 the stabilization term depends to the boundary conditions.
For the models with parallel velocity the term $Q$ satisfy $\triangle Q = b(F_0, \nu_{||}, \psi)$.
It will be interesting to add this term in jorek and study the stability of time
schemes.

Derivation of hierarchies of reduced MHD models in Tokamak geometry, B.
Després, Rémy Sart, 2013.
Conclusion
Ongoing and future works

- Determine the approximations of $P_{Schur}$
- Finish the code of PC-algorithm for the different approximations of $P_{Schur}$.
- Analyze the conditioning of the matrix $M$.
- If the conditioning is impacted by the anisotropic diffusion operators, try to reduced the computational cost using AP schemes.
- Analyze the conditioning of the matrix $P_{schur}$.
- If this matrix is ill-conditioned, use classical method as ILU method or multigrid method in the "update velocity" step.
- Add the stabilization terms in the reduced MHD models with parallel velocity.
- Adapt the PC-algorithm for the reduced MHD models with parallel velocity.