IPP Garching Contributions to the Application and Development of the non-linear MHD code JOREK

Matthias Hölzl
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About JOREK

Overview

- Non-linear MHD code
- Divertor tokamaks including X-point(s)
- Focus on plasma edge simulations
- Originally developed by Guido Huysmans at CEA Cadarache
  
  Huysmans and Czarny [2007]

- Reduced MHD in toroidal geometry (next slide)

- Other models:
  - Two-fluid extensions (M. Becoulet, S. Pamela)
  - Neutrons (C. Reux)
  - Full MHD

- Fortran 90/95

- MPI + OpenMP parallelized
About JOREK

Reduced MHD Equations

\[
\frac{\partial \Psi}{\partial t} = \eta j - R [u, \Psi] - F_0 \frac{\partial u}{\partial \phi}
\]

\[
\frac{\partial \rho}{\partial t} = - \nabla \cdot (\rho v) + \nabla \cdot (D \nabla \rho) + S_{\rho}
\]

\[
\frac{\partial (\rho T)}{\partial t} = - v \cdot \nabla (\rho T) - \gamma \rho T \nabla \cdot v + \nabla \cdot \left( K_\perp \nabla \rho + K_\parallel \nabla || T \right) + S_T
\]

\[
e_{\phi} \cdot \nabla \times \left\{ \rho \frac{\partial v}{\partial t} = -\rho (v \cdot \nabla)v - \nabla p + j \times B + \mu \Delta v \right\}
\]

\[
B \cdot \left\{ \rho \frac{\partial v}{\partial t} = -\rho (v \cdot \nabla)v - \nabla p + j \times B + \mu \Delta v \right\}
\]

\[
j \equiv -j_\phi = \Delta^* \Psi
\]

\[
\omega \equiv -\omega_\phi = \nabla^{2}_{pol} u
\]

Variables: \( \Psi, u, j, \omega, \rho, T, v_\parallel \)

Ideal wall + Bohm boundary conditions

Definitions: \( B = \frac{F_0}{R} e_\phi + \frac{1}{R} \nabla \Psi \times e_\phi \) and \( v = -R \nabla u \times e_\phi + v_\parallel B \)
About JOREK

Typical code run

• Initial grid (Grids shown with reduced resolution)
• Equilibrium data ($F_0$, $\Psi_{bnd}$, profiles for $T$, $\rho$, $FF'$)
• Grad-Shafranov
• Flux aligned grid (may include X-points)
• Radial and poloidal grid meshing
• Grad-Shafranov
• Axisymmetric flows
• Time-integration
• Analysis of restart-files:
  • Poincare plots
  • 2D or 3D VTK files
  • …
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Diagnostics

Monitor a running simulation

- Script plot_live_data.sh using gnuplot
- Allows to plot some data while a simulation is running
- Non-regression testing partly uses this infrastructure [Latu et al. 2012]
- For instance, energy time-traces:

(Hard to continue simulation into non-linear phase)
Diagnostics

Synthetic Magnetics (R. Wenninger)

- Remove ideal-wall boundary conditions from solution in post-processing
- Add effects of AUG conducting structures
- Generate synthetic Mirnov-coil signals
Diagnostics

2D Fourier analysis

- Determine straight field line coordinates
- 2D Fourier analysis in these coordinates
Additional postprocessing

• Run `jorek2_postproc` with simple script or interactively
• For example, density at outboard midplane and flux-surface averaged density:

```plaintext
namelist input1
set linepoints 150
for step 480 to 500 do
  line density psi_n 2.00 0.11 0 2.19 0.11 0 # values along straight line
  average density # flux-surface average
done
```

![Normalized density](image1)

![Normalized density (flux-surface averaged)](image2)
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Edge Localized Mode Simulations

Overview

Simulations performed

- Edge Localized Modes (ELMs) in realistic ASDEX Upgrade geometry
- Focus on early phase until non-linear saturation starts
- Comparably high number of toroidal modes
  - Periodicity 1: $n = 0, 1, 2, \ldots 16$
  - Periodicity 2: $n = 0, 2, 4, \ldots 16$
  - ...

Questions addressed

- Spatial mode structure?
- Non-linear effects?
- Mode saturation?
Edge Localized Mode Simulations

Input Profiles

- Input profiles taken from typical ASDEX Upgrade discharge:
Edge Localized Mode Simulations
Flux-aligned X-point Grid
Edge Localized Mode Simulations

Ballooning Structure

- Mode-coupling causes localization of ballooning-filaments:

![Normalized density](image)

unperturbed

\( n = 0, 8, 16 \)
Edge Localized Mode Simulations

Ballooning Structure

- Mode-coupling causes localization of ballooning-filaments:

\[
\text{unperturbed} \quad n = 0, 8, 16 \quad n = 0, 1, 2, \ldots, 16
\]
Edge Localized Mode Simulations

Poloidal Flux Perturbation

\[ n = 0, 8, 16 \]

- Red/blue surfaces correspond to 70 percent of maximum/minimum values
Edge Localized Mode Simulations

Poloidal Flux Perturbation

\[ n = 0, 1, 2, 3, 4, \ldots, 16 \]

- Red/blue surfaces correspond to 70 percent of maximum/minimum values
- Perturbation localized due to several strong modes with adjacent \( n \)

≈ Solitary Magnetic Perturbations in ASDEX Upgrade [Wenninger et al. 2012]
• Radial perturbation positions differ between variables
Edge Localized Mode Simulations

Energy Timetraces

- Starting from small random perturbation
- Ballooning-like mode evolves, grows exponentially
- $n = 1$ driven non-linearly to large amplitude
- (Subdominant modes not shown for clarity)
Edge Localized Mode Simulations

Mode Interaction

- Consider a simpler case with $n = 0, 4, 8, 12, 16$
- Can we reproduce and understand this with a simple model?

![Graph showing normalized energy vs. normalized time for different values of n. The graph includes lines for $n=4$, $n=8$, $n=12$, and $n=16$. The x-axis is normalized time ranging from 850 to 1150, and the y-axis is normalized energy ranging from $10^{-22}$ to $10^{-6}$. The distance $d=0.6cm$.](image-url)
Edge Localized Mode Simulations
Mode Interaction (2)

- Non-linear terms lead to mixing of toroidal modes
- Quadratic: \((n_1, n_2) \leftrightarrow n_1 \pm n_2\)
- For instance: \(n = 4\) coupled to \((8, 4), (12, 8), \text{and} (16, 12)\)
Edge Localized Mode Simulations

Mode Interaction (2)

- Non-linear terms lead to mixing of toroidal modes
- Quadratic: \((n_1, n_2) \leftrightarrow n_1 \pm n_2\)
- For instance: \(n = 4\) coupled to \((8, 4), (12, 8),\) and \((16, 12)\)
- Simple model (Mode rigidity, \(n = 0\) fixed):

\[
\dot{A}_4 = \gamma_4 A_4 + \gamma_{8,-4} A_8 A_4 + \gamma_{12,-8} A_{12} A_8 + \gamma_{16,-12} A_{16} A_{12}
\]
Non-linear terms lead to mixing of toroidal modes

Quadratic: \((n_1, n_2) \leftrightarrow n_1 \pm n_2\)

For instance: \(n = 4\) coupled to \((8, 4), (12, 8), \text{and} (16, 12)\)

Simple model (Mode rigidity, \(n = 0\) fixed):

\[
\dot{A}_4 = \gamma_{4} A_4 + \gamma_{8,-4} A_8 A_4 + \gamma_{12,-8} A_{12} A_8 + \gamma_{16,-12} A_{16} A_{12}
\]
\[
\dot{A}_8 = \gamma_{8} A_8 + \gamma_{4,4} A_4 A_4 + \gamma_{12,-4} A_{12} A_4 + \gamma_{16,-8} A_{16} A_8
\]
\[
\dot{A}_{12} = \gamma_{12} A_{12} + \gamma_{4,8} A_4 A_8 + \gamma_{16,-4} A_{16} A_4
\]
\[
\dot{A}_{16} = \gamma_{16} A_{16} + \gamma_{8,8} A_8 A_8 + \gamma_{4,12} A_4 A_{12}
\]

Linear growth rates taken from JOREK simulation

Energy conservation \(\Rightarrow\) Six remaining free parameters \(\gamma_{i,j}\)

Determine free parameters numerically by minimizing quadratic difference
• Saturation not covered by the model (of course)
• Same set of interaction-parameters $\gamma_{i,j}$ for both wall-distances
• Non-linear growth of $n = 4$ described well: Interaction of $n = 12$ and $n = 16$
• Same mechanism brings up $n = 1$ in the simulations shown before with poloidally and toroidally localized ELMs!
Edge Localized Mode Simulations

Saturation

Saturation mechanisms:

- Displacement $\xi$ gets significant compared to wall distance
- Modification of background profiles by the instability
ELM simulations for realistic ASDEX Upgrade conditions
Poloidal and toroidal localization of ELM-crash – similar to experiment (requires strong modes with adjacent $n$)
Radial perturbation positions of kinetic and magnetic quantities differ
$n = 1$ grows non-linearly – similar to experiment (requires strong modes with adjacent $n$)
Can be explained by non-linear mode-interaction picture
Saturation mechanisms
Published in Hölz et al. [2012a] and to be published in Krebs et al. [2013]
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Resistive Wall Model

Overview

Physics: Growing or rotating instability

⇒ Time-dependent magnetic perturbation outside the plasma
⇒ Mirror currents in conducting structures
⇒ Changes linear and non-linear behaviour of instability
  • For instance, external kink (∼ μs)
    • With close-fitting ideal wall: Fully stabilized
    • With resistive wall: Becomes a Resistive wall mode (∼ ms)
    • May be stabilized by active feedback-system
  • Aim: Non-linear resistive wall simulations with JOREK

Implementation

• Coupling to STARWALL (described a bit later)
• Showing status of implementation and benchmarking
Resistive Wall Model

Natural boundary condition

- Current definition equation \( j = \Delta^*\Psi \) in weak form (test function \( \nu^* \)):

\[
\int dV \frac{\nu^*}{R^2} j - \int dV \nu^* \nabla \cdot \left( \frac{1}{R^2} \nabla \Psi \right) = 0
\]

- Partial integration:

\[
\int dV \frac{\nu^*}{R^2} j + \int dV \frac{1}{R^2} \nabla \nu^* \cdot \nabla \Psi - \oint dA \frac{\nu^*}{R} \left( \nabla \Psi \cdot \hat{n}/R \right) = 0.
\]

\[\equiv B_{\text{tan}}\]

- Ideal-wall boundary conditions: Boundary integral vanishes in “old” JOREK

- Natural boundary condition: Replace \( B_{\text{tan}} \) by STARWALL response
Resistive Wall Model

STARWALL response

- **STARWALL** Merkel and Sempf [2006]; Strumberger et al. [2011]
  - Solves vacuum field equation outside JOREK domain (Neumann problem)
  - Resistive wall represented by triangles
  - Wall currents described by current potentials $Y_k$ at triangle nodes
  - Response matrices: $\hat{M}^\text{id}$

- Ideal wall (algebraic expression):

\[
B_{\text{tan}} = \sum_i b_i \sum_j \hat{M}_{i,j}^\text{id} \Psi_j
\]

Matthias Hölzl Application and Development of JOREK 4th Summer School on Numerical Modelling for Fusion (10/2012)
Resistive Wall Model

STARWALL response

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  - Solves vacuum field equation outside JOREK domain (Neumann problem)
  - Resistive wall represented by triangles
  - Wall currents described by current potentials $Y_k$ at triangle nodes
  - Response matrices: $\hat{M}_{id}$, $\hat{M}_{ee}$, $\hat{M}_{ey}$, $\hat{M}_{ye}$, $\hat{M}_{yy}$

- Ideal wall (algebraic expression):
  \[ B_{\text{tan}} = \sum_i b_i \left( \sum_j \hat{M}_{i,j}^{id} \Psi_j \right) \]

- Resistive wall:
  \[ B_{\text{tan}} = \sum_i b_i \left( \sum_j \hat{M}_{i,j}^{ee} \Psi_j + \sum_k \hat{M}_{i,k}^{ey} Y_k \right) \]
  \[ \dot{Y}_k = -\frac{\eta_w}{d_w} \hat{M}_{k,k}^{yy} Y_k - \sum_j \hat{M}_{k,j}^{ye} \dot{\Psi}_j \]
Resistive Wall Model

Time Discretization

- Discretize wall-current evolution consistent with other JOREK equations where \( Y_{k}^{n+1} = Y_{k}^{n} + \delta Y_{k}^{n} \):

\[
(1 + \xi) \left[ \delta Y_{k}^{n} + \sum_{j} \hat{M}_{k,j}^{ye} \delta \Psi_{j}^{n} \right] + \Delta t \theta \frac{n_{w}}{d_{w}} \hat{M}_{k,k}^{yy} \delta Y_{k}^{n} \\
= -\Delta t \frac{n_{w}}{d_{w}} \hat{M}_{k,k}^{yy} Y_{k}^{n} + \xi \left[ \delta Y_{k}^{n-1} + \sum_{j} \hat{M}_{k,j}^{ye} \delta \Psi_{j}^{n-1} \right]
\]

- Solve for \( \delta Y_{k}^{n} \) and insert into \( B_{\text{tan}} \) at time-step \( n + 1 \):

\[
B_{\text{tan}}^{n+1} = \sum_{i} b_{i} \left[ \sum_{j} \hat{M}_{i,j}^{ee} \cdot (\Psi_{j}^{n} + \delta \Psi_{j}^{n}) + \sum_{k} \hat{M}_{i,k}^{ey} \cdot (Y_{k}^{n} + \delta Y_{k}^{n}) \right]
\]

- Plug result into boundary integral \( \oint dA \left\{ \frac{j^{*}}{R} (\nabla \Psi \cdot \hat{n}/R) \right\} \equiv B_{\text{tan}} \)
Resistive Wall Model

Get this correct in Bezier formulation...

\[
\sum_{i} \int \frac{dV}{R^2} \left( j_{i}^* \delta j^n + \nabla j_{i}^* \cdot \nabla \delta \Psi^n \right) - \sum_{i} \oint dA \frac{j_{i}^*}{R} \sum b_i \sum \hat{E}_{i,j} \delta \Psi^n_j
\]

\[
= - \sum_{i} \int \frac{dV}{R^2} \left( j_{i}^* j^n + \nabla j_{i}^* \cdot \nabla \Psi^n \right)
\]

\[
+ \sum_{i} \oint dA \frac{j_{i}^*}{R} \sum b_i \left[ \sum_{k} \left( \hat{F}_{i,k} \gamma^n_k + \hat{G}_{i,k} \delta \gamma^{n-1}_k \right) + \sum_{j} \left( \hat{H}_{i,j} \psi^n_j + \hat{j}_{i,j} \delta \psi^{n-1}_j \right) \right]
\]

and

\[
\gamma^{n+1}_k = \gamma^n_k + \sum_{j} \hat{A}_{k,j} \delta \Psi^n_j + \hat{B}_{k,k} \gamma^n_k + \hat{C}_{k,k} \delta \gamma^{n-1}_k + \sum_{j} \hat{D}_{k,j} \delta \psi^{n-1}_j
\]

where

\[
\hat{S}_{k,k} = 1 + \xi + \Delta t \theta \frac{\partial w}{\partial t} \hat{M}^{yy}_{k,k}
\]

\[
\hat{A}_{k,j} = - \left( 1 + \xi \right) \frac{\hat{M}^{ye}_{k,j}}{\hat{S}_{k,k}}
\]

\[
\hat{B}_{k,k} = - \Delta t \frac{\partial w}{\partial t} \hat{M}^{yy}_{k,k} / \hat{S}_{k,k}
\]

\[
\hat{C}_{k,k} = \xi / \hat{S}_{k,k}
\]

\[
\hat{D}_{k,j} = \xi \hat{M}^{ye}_{k,j} / \hat{S}_{k,k}
\]

\[
\hat{E}_{i,k} = \hat{M}^{ee}_{i,k} + \sum \hat{M}^{ey}_{i,k} \hat{A}_{k,j}
\]

\[
\hat{F}_{i,k} = \hat{M}^{ey}_{i,k} (1 + \hat{B}_{k,k})
\]

\[
\hat{G}_{i,k} = \hat{M}^{ey}_{i,k} \hat{C}_{k,k}
\]

\[
\hat{H}_{i,j} = \hat{M}^{ee}_{i,j}
\]

\[
\hat{j}_{i,j} = \sum \hat{M}^{ey}_{i,k} \hat{D}_{k,j}
\]

and

\[
\int dV = \sum_{i} \int ds \int dt \int d\phi J_2 R
\]

\[
\oint dA = \sum_{i} \int dt \int d\phi R \sqrt{\left( \frac{\partial R}{\partial t} \right)^2 + \left( \frac{\partial Z}{\partial t} \right)^2}
\]
Resistive Wall Model

Freeboundary Equilibrium

- Same boundary-integral in Grad-Shafranov equation
- Allows to test parts (no time-evolution, no wall-currents)
- ITER-like limiter case as first test

- Flux-surfaces and q-profile agree very well with CEDRES++
Resistive Wall Model

Tearing Mode

- 2/1 tearing mode in a circular plasma \((R = 10, \alpha = 1)\)
- Concentric ideally conducting wall
- Linear growth rates:

![Graph showing linear growth rates for CASTOR, CASTOR + STARWALL_C, and JOREK + STARWALL_J.]

- Excellent agreement with linear CASTOR code for a variety of plasma resistivities and wall distances
- Resistive wall with zero resistivity is consistent
Resistive Wall Model

Resistive Wall Mode

- 2/1 resistive wall mode in circular plasma \((R = 10, \alpha = 1)\)
- Concentric resistive wall
- To be compared to analytical theory and linear simulations…

Linear growth rates for different wall radii and wall resistivities
2/1 resistive wall mode in circular plasma ($R = 10$, $a = 1$)

Concentric resistive wall

To be compared to analytical theory and linear simulations...

Linear growth rates for different wall radii and wall resistivities

Example for non-linear saturation (stable, small time-steps required)
Resistive Wall Model

Summary for this Part

- Plasma instabilities induce mirror currents in conducting structures
- These act back onto the instabilities affecting linear and non-linear behaviour
- Aim: Non-linear investigations
- Coupling JOREK and STARWALL via natural boundary condition
- Full-implicitness of JOREK time-integration is kept
- First tests:
  - Free-boundary equilibrium
  - Tearing mode with ideal wall
  - Resistive wall mode
- Described in Höflzl et al. [2012b]
About JOREK

Diagnostics

Edge Localized Mode Simulations

Resistive Wall Model

Numerical Aspects (non-expert view)
Numerical Aspects (non-expert view)

Spatial Discretization

- Toroidal Fourier-decomposition
- 2D Bezier finite elements [Czarny and Huysmans [2008]]
  - Bicubic Bezier surfaces: 3rd order Bernstein polynomials
  - \( C^0 \) and \( C^1 \) continuity reduces degrees of freedom per node
  - Isoparametric formulation \( \rightarrow \) alignment to flux-surfaces
  - Allows for local refinement

- Remaining problems:
  - Fourier basis-functions non-local
  - Problems at axis and X-point (not \( C^1 \))
  - Positivity not guaranteed
Numerical Aspects (non-expert view)

Time evolution: Fully implicit

- Set of equations for variables $u$:
  \[
  \dot{A}(u(t)) = B(u(t))
  \]
- Time-Discretization ($u^{n+1} = u^n + \delta u^n$):
  \[
  \left[ (1 + \xi) \left( \frac{\partial A}{\partial u} \right)^n - \Delta t \theta \left( \frac{\partial B}{\partial u} \right)^n \right] \delta u^n = \Delta t B^n + \xi \left( \frac{\partial A}{\partial u} \right)^{n-1} \delta u^{n-1}
  \]
  - Already involves a linearization (can be understood as a Newton iteration stopped after one step)
  - Crank-Nicholson: $\theta = 0.5$, $\xi = 0$ or Gears: $\theta = 1$, $\xi = 0.5$

$\Rightarrow$ Large sparse system of equations $\hat{M} \ x = b$
Generalized Minimum Residual Method (GMRES)

- \( \hat{M} \cdot x = b \) solved iteratively with GMRES
- Implementation by CERFACS (France) used which requests the following operations via reverse communication (“black box”):
  - Matrix-vector product \( \rightarrow \) BLAS with OpenMP parallelization
  - Dot-product between two vectors \( \rightarrow \) BLAS
  - Calculation of \( f = \hat{P}^{-1}g \) for some vector \( g \), where \( \hat{P} \) is the left preconditioning matrix
Numerical Aspects (non-expert view)

Time evolution: GMRES and preconditioning

Generalized Minimum Residual Method (GMRES)

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Left Preconditioning

- Need to solve $\hat{P} \mathbf{f} = \mathbf{g}$
- $\hat{P}$: Matrix $\hat{M}$ without coupling terms between toroidal modes
  $\Rightarrow$ Block-diagonal matrix with few large sparse blocks
- Solve decoupled block-systems with direct solver PaStiX
Numerical Aspects (non-expert view)

Time evolution: Pros and Cons

Pro Implicitness
- Time step not restricted by CFL condition
  → Large time steps possible

Con Convergence
- Preconditioning based on linearization
  → Inefficient at strong non-linearities

Con Efficiency
- Direct solver in preconditioning
  → Limited scalability and excessive memory consumption

Con Implementation
- Derivatives of physical equations implemented (Jacobian)
- Mixed with spatial and temporal discretization
  → Hard to verify and extend
Numerical Aspects (non-expert view)

Time evolution: What to change?

Four Levels:

- Loop over timesteps
- Linearization → Newton-iterations?
- GMRES → Jacobian-free?
- Preconditioner → Matrix-free method?

Other possibilities

- Optimize GMRES (convergence criterion, restarts)?
- Better preconditioning for strong non-linearity?
- Improve toroidal/poloidal finite elements?
- Split into explicit and implicit parts?
References


see also: www.ipp.mpg.de/~mhoelzl

Contributions from

P. Merkel
I. Krebs
R. Wenninger
G. Huysmans
E. Nardon
S. Günter
K. Lackner
W.-C. Müller
E. Strumberger
\[ \frac{\partial p}{\partial t} = -\mathbf{v} \cdot \nabla p - \gamma p \nabla \cdot \mathbf{v} + \text{Diffusion} + \text{Source} \]

\[ \frac{\partial (\rho T)}{\partial t} = -\mathbf{v} \cdot \nabla (\rho T) - \gamma \rho T \nabla \cdot \mathbf{v} + \nabla \cdot (K_{\perp} \nabla_{\perp} T + K_{\parallel} \nabla_{\parallel} T) + S_T \]