

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

Matthias Hölzl

- 1 About JOREK
- 2 Diagnostics
- 3 Edge Localized Mode Simulations
- 4 Resistive Wall Model
- 5 Numerical Aspects (non-expert view)

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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)
  - Neutrals (C. Reux)
  - Full MHD
- Fortran 90/95
- MPI + OpenMP parallelized

## Reduced MHD Equations

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

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) + \nabla \cdot (D_{\perp} \nabla_{\perp} \rho) + S_{\rho}$$

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

$$\mathbf{e}_{\phi} \cdot \nabla \times \left\{ \rho \frac{\partial \mathbf{v}}{\partial t} = -\rho (\mathbf{v} \cdot \nabla) \mathbf{v} - \nabla p + \mathbf{j} \times \mathbf{B} + \mu \Delta \mathbf{v} \right\}$$

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

$$\mathbf{j} \equiv -\mathbf{j}_{\phi} = \Delta^* \Psi$$

$$\boldsymbol{\omega} \equiv -\boldsymbol{\omega}_{\phi} = \nabla_{\text{pol}}^2 \mathbf{u}$$

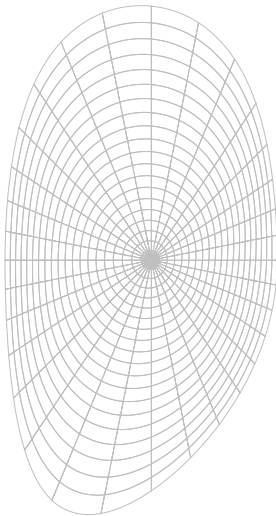
Variables:  $\Psi, \mathbf{u}, j, \boldsymbol{\omega}, \rho, T, v_{\parallel}$

Ideal wall + Bohm boundary conditions

Definitions:  $\mathbf{B} = \frac{F_0}{R} \mathbf{e}_{\phi} + \frac{1}{R} \nabla \Psi \times \mathbf{e}_{\phi}$  and  $\mathbf{v} = -R \nabla \mathbf{u} \times \mathbf{e}_{\phi} + v_{\parallel} \mathbf{B}$

# About JOREK

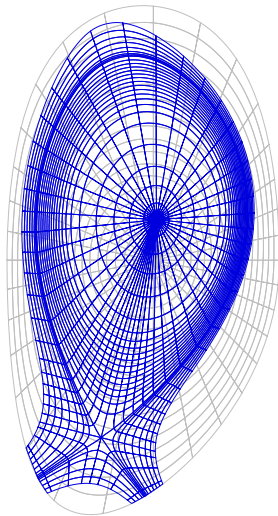
## Typical code run



- Initial grid (Grids shown with reduced resolution)
- Equilibrium data ( $F_0$ ,  $\Psi_{\text{bnd}}$ , 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
  - ...

# About JOEREK

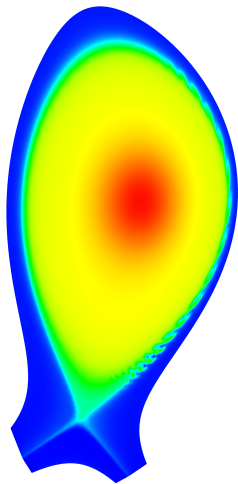
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# About JOEREK

## Typical code run



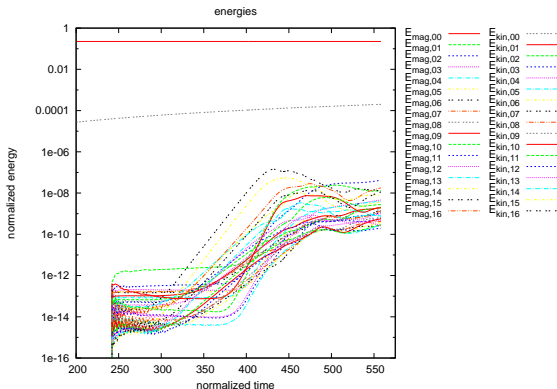
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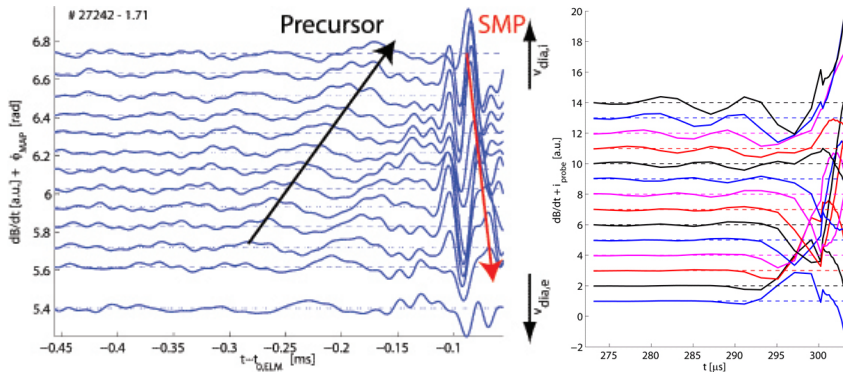
## Monitor a running simulation

- 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)

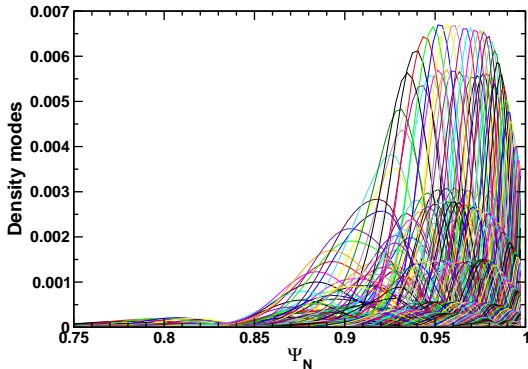
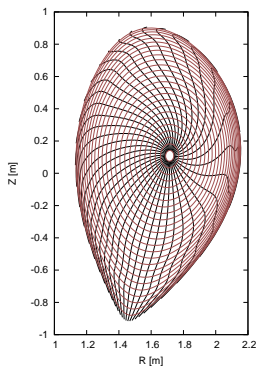
- Remove ideal-wall boundary conditions from solution in post-processing
- Add effects of AUG conducting structures
- Generate synthetic Mirnov-coil signals



# Diagnostics

## 2D Fourier analysis

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



# Diagnostics

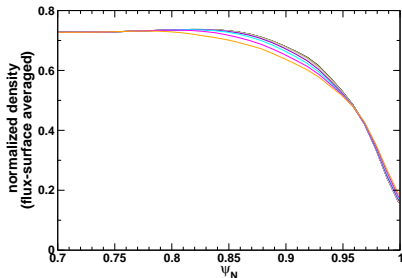
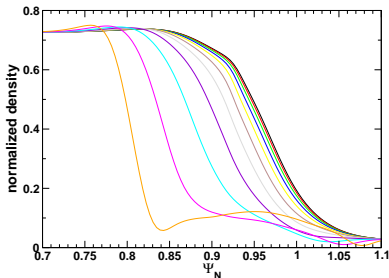
## Additional postprocessing

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

```

namelist input1                                # load input namelist
set linepoints 150                             # set number of points
for step 480 to 500 do                         # loop over time-steps
  line density psi_n 2.00 0.11 0 2.19 0.11 0 # values along straight line
  average density                               # flux-surface average
done

```



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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:  $n = 0, 1, 2, \dots 16$
  - Periodicity 2:  $n = 0, 2, 4, \dots 16$
  - ...

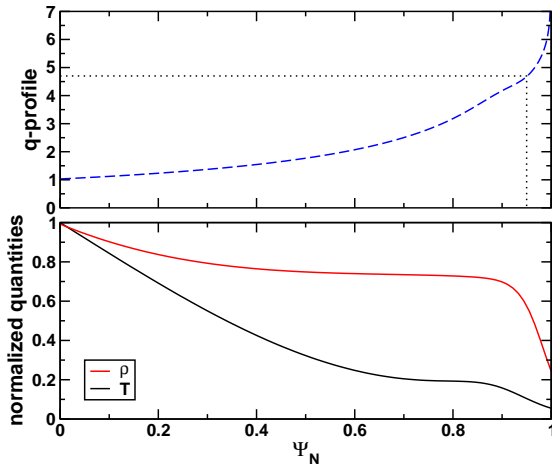
### Questions addressed

- Spatial mode structure?
- Non-linear effects?
- Mode saturation?

# Edge Localized Mode Simulations

## Input Profiles

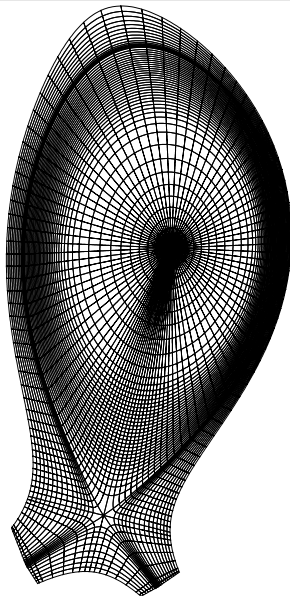
- Input profiles taken from typical ASDEX Upgrade discharge:





# Edge Localized Mode Simulations

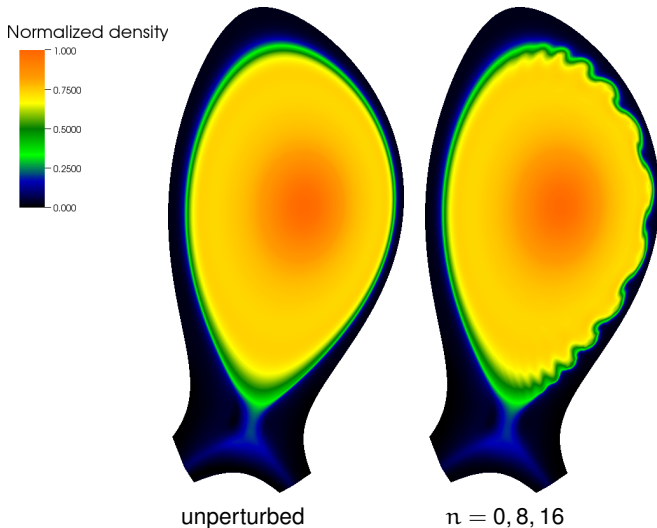
## Flux-aligned X-point Grid



# Edge Localized Mode Simulations

## Ballooning Structure

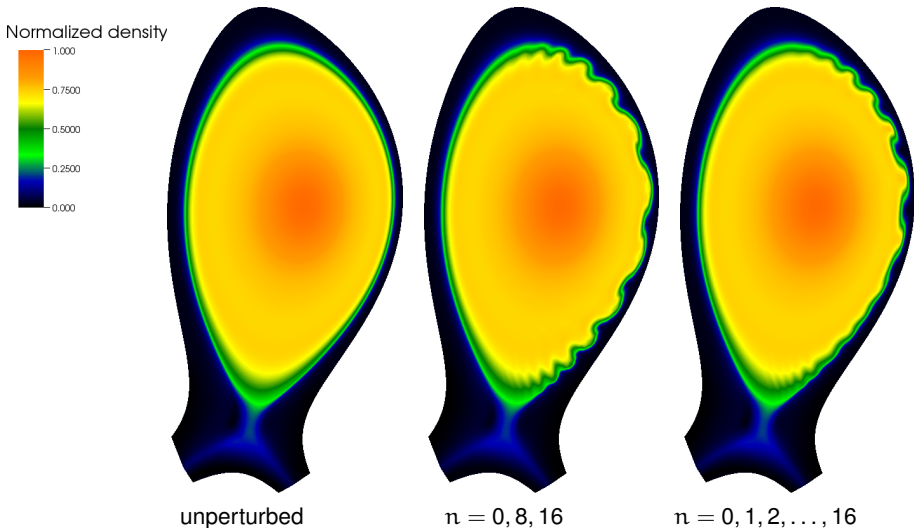
- Mode-coupling causes localization of ballooning-filaments:



# Edge Localized Mode Simulations

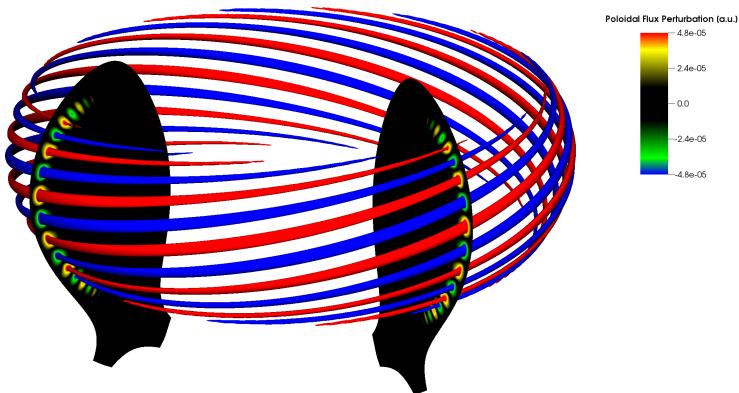
## Ballooning Structure

- Mode-coupling causes localization of ballooning-filaments:



# Edge Localized Mode Simulations

## Poloidal Flux Perturbation

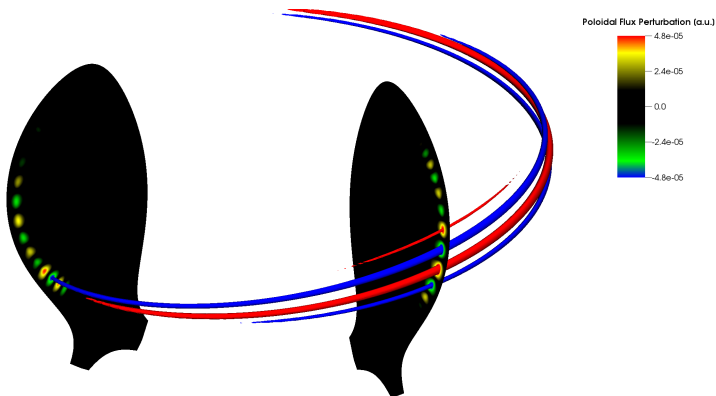


$$n = 0, 8, 16$$

- Red/blue surfaces correspond to 70 percent of maximum/minimum values

# Edge Localized Mode Simulations

## Poloidal Flux Perturbation



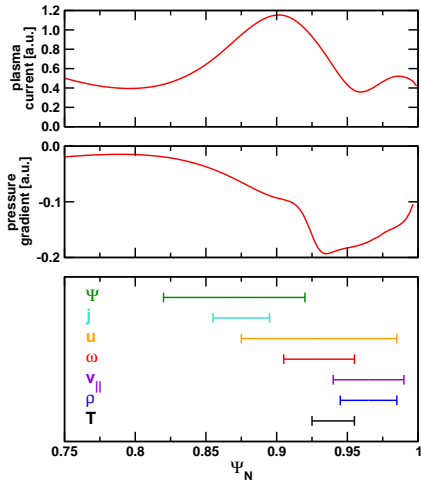
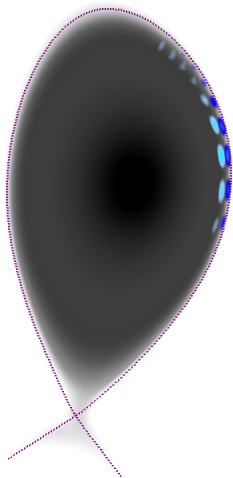
$$n = 0, 1, 2, 3, 4, \dots, 16$$

- 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. \[2012\]](#)

# Edge Localized Mode Simulations

## Position of Perturbations

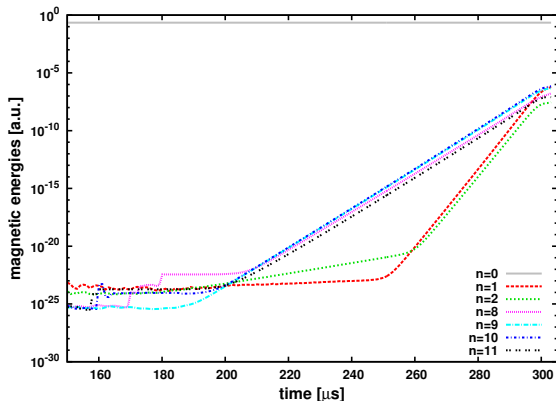
- Radial perturbation positions differ between variables



# Edge Localized Mode Simulations

## Energy Timetraces

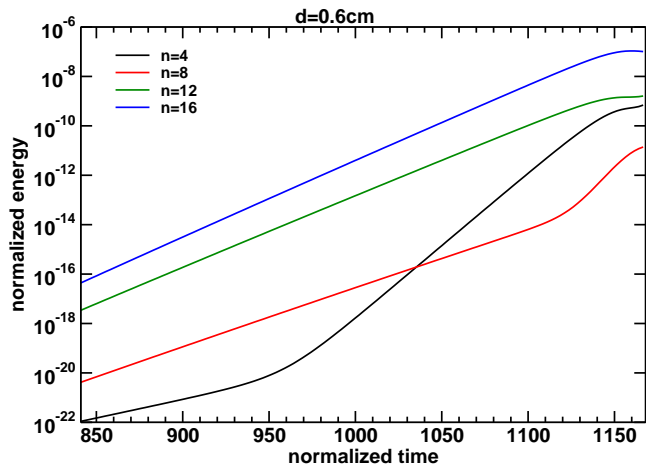
- Starting from small random perturbation
- Ballooning-like mode evolves, grows exponentially
- $n = 1$  driven non-linearly to large amplitude
- (Subdominant modes not shown for clarity)



# 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?





# 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  $(16, 12)$

# Edge Localized Mode Simulations

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- For instance:  $n = 4$  coupled to  $(8, 4)$ ,  $(12, 8)$ , and  $(16, 12)$
- Simple model (Mode rigidity,  $n = 0$  fixed):

$$\dot{A}_4 = \underbrace{\gamma_4 A_4}_{\text{linear}} + \underbrace{\gamma_{8,-4} A_8 A_4 + \gamma_{12,-8} A_{12} A_8 + \gamma_{16,-12} A_{16} A_{12}}_{\text{non-linear interaction}}$$

# Edge Localized Mode Simulations

## Mode Interaction (2)

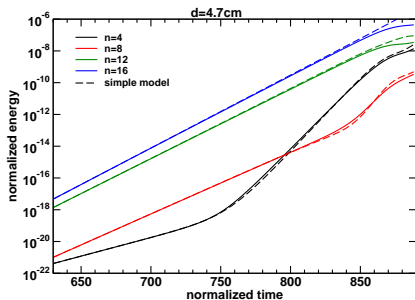
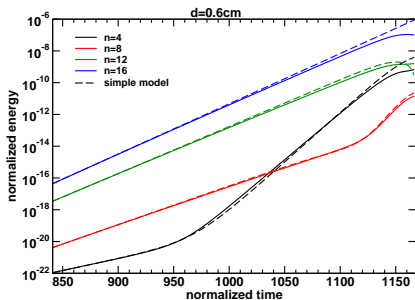
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- Simple model (Mode rigidity,  $n = 0$  fixed):

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 \dot{A}_4 &= \underbrace{\gamma_4 A_4}_{\text{linear}} + \underbrace{\gamma_{8,-4} A_8 A_4 + \gamma_{12,-8} A_{12} A_8 + \gamma_{16,-12} A_{16} A_{12}}_{\text{non-linear interaction}} \\
 \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}
 \end{aligned}$$

- 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

# Edge Localized Mode Simulations

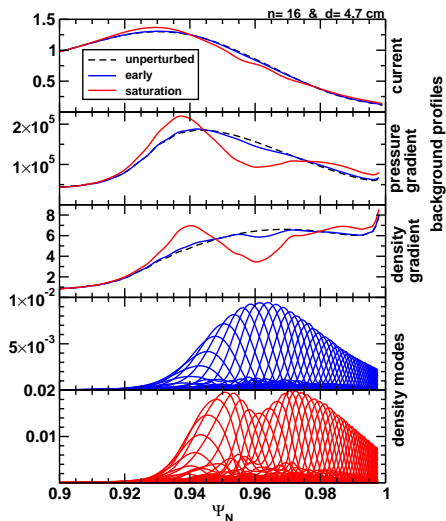
## Mode Interaction (3)



- 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

# Edge Localized Mode Simulations

## Summary for this Part

- 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 [Hözl et al. \[2012a\]](#) and to be published in [Krebs et al. \[2013\]](#)

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## 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 ( $\sim \mu\text{s}$ )
    - With close-fitting ideal wall: Fully stabilized
    - With resistive wall: Becomes a Resistive wall mode ( $\sim \text{ms}$ )
    - May be stabilized by active feedback-system
  - Aim: Non-linear resistive wall simulations with JOEREK

## 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  $v^*$ ):

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

- Partial integration:

$$\int dV \frac{v^*}{R^2} j + \int dV \frac{1}{R^2} \nabla v^* \cdot \nabla \Psi - \oint dA \frac{v^*}{R} \underbrace{(\nabla \Psi \cdot \hat{\mathbf{n}}/R)}_{\equiv B_{\text{tan}}} = 0.$$

- Ideal-wall boundary conditions: Boundary integral vanishes in “old” JOEKEK
- 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 JOEKE 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):

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

# 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:  $\hat{M}^{id}$ ,  $\hat{M}^{ee}$ ,  $\hat{M}^{ey}$ ,  $\hat{M}^{ye}$ ,  $\hat{M}^{yy}$
- Ideal wall (algebraic expression):

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

- 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 JOEREK equations where  $Y_k^{n+1} = Y_k^n + \delta Y_k^n$ :

$$\begin{aligned}
 & (1 + \xi) \left[ \delta Y_k^n + \sum_j \hat{M}_{k,j}^{ye} \delta \Psi_j^n \right] + \Delta t \theta \frac{\eta_w}{d_w} \hat{M}_{k,k}^{yy} \delta Y_k^n \\
 & = - \Delta t \frac{\eta_w}{d_w} \hat{M}_{k,k}^{yy} Y_k^n + \xi \left[ \delta Y_k^{n-1} + \sum_j \hat{M}_{k,j}^{ye} \delta \Psi_j^{n-1} \right]
 \end{aligned}$$

- 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  $\oint dA \frac{j_1^*}{R} \underbrace{(\nabla \Psi \cdot \hat{\mathbf{n}}/R)}_{\equiv B_{\text{tan}}}$

## Resistive Wall Model

## Get this correct in Bezier formulation...

$$\begin{aligned}
& \sum_{i_{\text{elem}}} \int \frac{dV}{R^2} (j_i^* \delta j^n + \nabla j_i^* \cdot \nabla \delta \Psi^n) - \sum_{i_{\text{bnd}}} \oint dA \frac{j_i^*}{R} \sum_i b_i \sum_j \hat{E}_{i,j} \delta \Psi_j^n \\
&= - \sum_{i_{\text{elem}}} \int \frac{dV}{R^2} (j_i^* j^n + \nabla j_i^* \cdot \nabla \Psi^n) \\
&+ \sum_{i_{\text{bnd}}} \oint dA \frac{j_i^*}{R} \sum_i b_i \left[ \sum_k (\hat{F}_{i,k} Y_k^n + \hat{G}_{i,k} \delta Y_k^{n-1}) + \sum_j (\hat{H}_{i,j} \Psi_j^n + \hat{J}_{i,j} \delta \Psi_j^{n-1}) \right]
\end{aligned}$$

and

$$Y_k^{n+1} = Y_k^n + \sum_j \hat{A}_{k,j} \delta \Psi_j^n + \hat{B}_{k,k} Y_k^n + \hat{C}_{k,k} \delta Y_k^{n-1} + \sum_j \hat{D}_{k,j} \delta \Psi_j^{n-1}$$

where

$$\begin{aligned}
\hat{S}_{k,k} &= 1 + \xi + \Delta t \theta \frac{\eta_w}{d_w} \hat{M}_{k,k}^{yy} & \hat{D}_{k,j} &= \xi \hat{M}_{k,j}^{ye} / \hat{S}_{k,k} & \hat{H}_{i,j} &= \hat{M}_{i,j}^{ee} \\
\hat{A}_{k,j} &= -(1 + \xi) \hat{M}_{k,j}^{ye} / \hat{S}_{k,k} & \hat{E}_{i,j} &= \hat{M}_{i,j}^{ee} + \sum_k \hat{M}_{i,k}^{ey} \hat{A}_{k,j} & \hat{J}_{i,j} &= \sum_k \hat{M}_{i,k}^{ey} \hat{D}_{k,j} \\
\hat{B}_{k,k} &= -\Delta t \frac{\eta_w}{d_w} \hat{M}_{k,k}^{yy} / \hat{S}_{k,k} & \hat{F}_{i,k} &= \hat{M}_{i,k}^{ey} (1 + \hat{B}_{k,k}) \\
\hat{C}_{k,k} &= \xi / \hat{S}_{k,k} & \hat{G}_{i,k} &= \hat{M}_{i,k}^{ey} \hat{C}_{k,k}
\end{aligned}$$

and

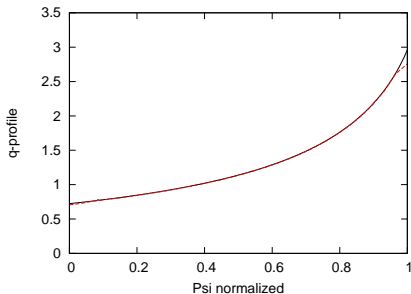
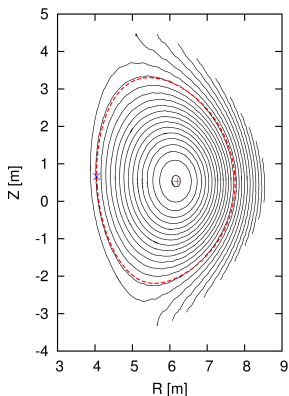
$$\int dV = \sum_{i_{\text{elem}}} \int ds dt d\phi J_2 R \qquad \oint dA = \sum_{i_{\text{bnd}}} \int dt d\phi R \sqrt{\left(\frac{\partial R}{\partial t}\right)^2 + \left(\frac{\partial Z}{\partial t}\right)^2}$$

# 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

JOREK — CEDRES - - - limiter point ×

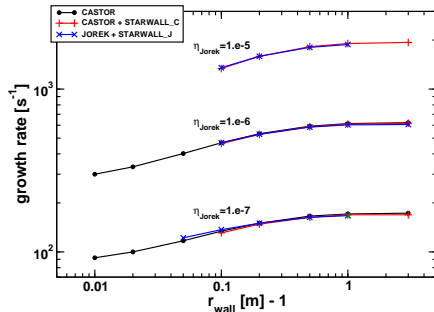


- Flux-surfaces and q-profile agree very well with CEDRES++

# Resistive Wall Model

## Tearing Mode

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

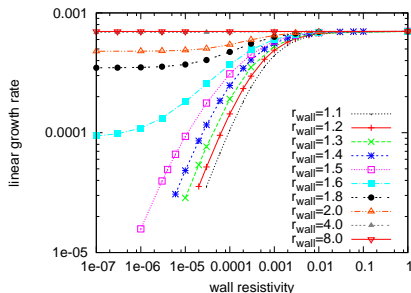


- Excellent agreement with linear CASTOR code for a variety of plasma resistivities and wall distances
- Resistive wall with zero resistivity is consistent

# 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. . .



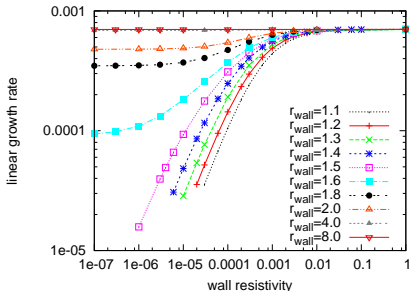
Linear growth rates for different wall radii  
and wall resistivities



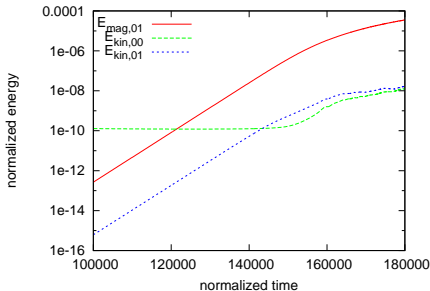
# Resistive Wall Model

## 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



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

# Resistive Wall Model

## Summary for this Part

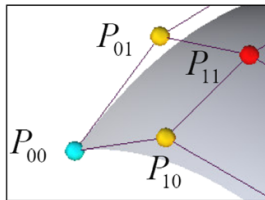
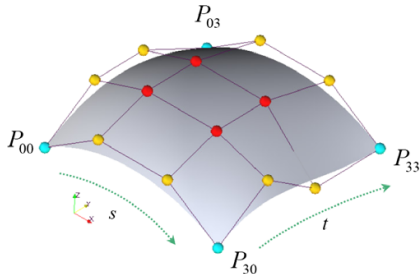
- Plasma instabilities induce mirror currents in conducting structures
- These act back onto the instabilities affecting linear and non-linear behaviour
- Aim: Non-linear investigations
- Coupling JOEREK and STARWALL via natural boundary condition
- Full-implicitness of JOEREK time-integration is kept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

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# Numerical Aspects (non-expert view)

## Spatial Discretization

- Toroidal Fourier-decomposition
- 2D Bezier finite elements [Czarny and Huysmans \[2008\]](#)
  - Bicubic Bezier surfaces: 3<sup>rd</sup> 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  $\mathbf{u}$ :

$$\dot{\mathbf{A}}(\mathbf{u}(t)) = \mathbf{B}(\mathbf{u}(t))$$

- Time-Discretization ( $\mathbf{u}^{n+1} = \mathbf{u}^n + \delta\mathbf{u}^n$ ):

$$\left[ (1 + \xi) \left( \frac{\partial \mathbf{A}}{\partial \mathbf{u}} \right)^n - \Delta t \theta \left( \frac{\partial \mathbf{B}}{\partial \mathbf{u}} \right)^n \right] \delta \mathbf{u}^n = \Delta t \mathbf{B}^n + \xi \left( \frac{\partial \mathbf{A}}{\partial \mathbf{u}} \right)^{n-1} \delta \mathbf{u}^{n-1}$$

- Already involves a linearization  
(can be understood as a Newton iteration stopped after one step)
- Crank-Nicholson:  $\theta = 0.5$ ,  $\xi = 0$  or Gears:  $\theta = 1$ ,  $\xi = 0.5$

⇒ Large sparse system of equations  $\hat{\mathbf{M}} \mathbf{x} = \mathbf{b}$

## Generalized Minimum Residual Method (GMRES)

- $\hat{M} \mathbf{x} = \mathbf{b}$  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  $\mathbf{f} = \hat{P}^{-1} \mathbf{g}$  for some vector  $\mathbf{g}$ , where  $\hat{P}$  is the left preconditioning matrix

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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**



## 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?

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see also: [www.ipp.mpg.de/~mhoelzl](http://www.ipp.mpg.de/~mhoelzl)

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$$\frac{\partial p}{\partial t} = -\mathbf{v} \cdot \nabla p - \gamma p \nabla \cdot \mathbf{v} + \text{Diffusion} + \text{Source}$$
$$\frac{\partial(\rho T)}{\partial t} = -\mathbf{v} \cdot \nabla(\rho T) - \gamma \rho T \nabla \cdot \mathbf{v} + \nabla \cdot (\mathbf{K}_{\perp} \nabla_{\perp} T + \mathbf{K}_{\parallel} \nabla_{\parallel} T) + S_T$$