Dimensionality reduction using an edge finite element method for periodic magnetostatic fields in a symmetric domain

C.G. Albert[1] O. Biro[2] M.F. Heyn[1] W. Kernbichler[1] S.V. Kasilov[1,3] P. Lainer[1]

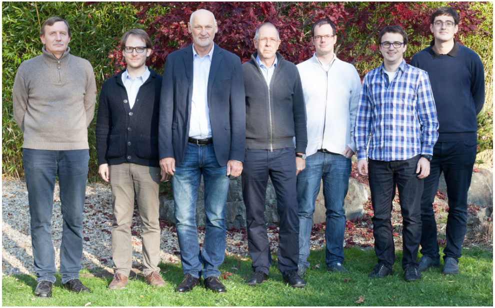
[1]Fusion@ÖAW, Institute of Theoretical and Computational Physics
[2]Institute of Fundamentals and Theory in Electrical Engineering
Graz University of Technology

[3]Institute of Plasma Physics, National Science Center
Kharkov Institute of Physics and Technology

8th FreeFEM++ workshop, Dec 8th 2016

Who are we?

- Theoretical plasma physics group at TU Graz

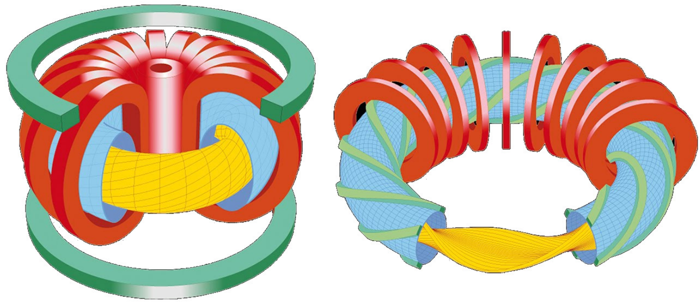


- General topic: **magnetic confinement fusion**
  - Trap a hot plasma to allow for nuclear fusion
  - Work within the **EUROfusion** framework (**ITER**, **W7-X**, ...)

What do we do?

- Our tasks include:
  - Understand **non-axisymmetric perturbations** in tokamaks
  - Compute **transport** and **3D equilibria** in stellarators
- Our strategy:
  - Use a **kinetic Monte Carlo** model for the plasma
  - Couple to **Maxwell's equations** solved by **FEM**
- More complete but slower than magnetohydrodynamics
  - **optimisations needed**

Tokamak and stellarator geometry



- make use of axisymmetry / periodicity

About today's talk

- Most things are well-known
- **Goal**: calculate **3D magnetic field** from known **currents**
- Systematic way of "2.5D" reduction of **curl curl** equation
  - Starting from Maxwell's equations
  - **symmetric** and **oscillatory** part (Fourier series)
- Generalisation to **curvilinear** coordinates
- Efficient realisation with edge elements in **FreeFEM++**

Maxwell's equations of electrodynamics

$$\operatorname{div} \varepsilon \boldsymbol{E} = \rho \qquad (1)$$
$$\mathbf{curl}\, \boldsymbol{E} + \partial_t \boldsymbol{B} = 0 \qquad (2)$$
$$\mathbf{curl}\, \nu \boldsymbol{B} \text{-} \partial_t(\varepsilon \boldsymbol{E}) = \boldsymbol{J} \qquad (3)$$
$$\operatorname{div} \boldsymbol{B} = 0 \qquad (4)$$

- Unknowns: Electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{B}$
- Source terms: **Free** charge density ρ, currents density $\boldsymbol{J}$
- Material parameters: Permittivity ε, **inverse** permeability $\nu = \mu^{-1}$
  - Can lead to discontinous (weak) solutions for $\boldsymbol{E}$ and $\boldsymbol{B}$
- **Continuity equation** for charges as a **concequence**:

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \boldsymbol{J} = 0$$

Scalar and vector potential

$$
\begin{aligned}
\operatorname{div} \varepsilon \boldsymbol{E} &= \rho \\
\mathbf{curl}\, \boldsymbol{E} + \partial_t \boldsymbol{B} &= 0 \\
\mathbf{curl}\, \nu \boldsymbol{B} - \partial_t(\varepsilon \boldsymbol{E}) &= \boldsymbol{J} \\
\operatorname{div} \boldsymbol{B} &= 0\,.
\end{aligned}
$$

- Simply connected domains: can find potentials Φ and $\boldsymbol{A}$ with

$$\boxed{\boldsymbol{E} = -\mathbf{grad}\,\Phi - \partial_t \boldsymbol{A}, \qquad \boldsymbol{B} = \mathbf{curl}\,\boldsymbol{A} \quad (5)}$$

- Equations fulfiled since $\mathbf{curl}\,\mathbf{grad}\,\Phi = \mathbf{0}$ and $\operatorname{div}\mathbf{curl}\,\boldsymbol{A} = 0\ \forall\, \Phi,\ \boldsymbol{A}$
- Proof: special case of Poincaré lemma

Potential equations

$$-\mathrm{div}\,\varepsilon\,\mathbf{grad}\,\Phi - \mathrm{div}\,\varepsilon\partial_t \boldsymbol{A} = \rho \tag{6}$$

$$\mathbf{curl}\,\nu\,\mathbf{curl}\,\boldsymbol{A} - \partial_t\,\varepsilon\,\mathbf{grad}\,\Phi + \partial_t\,\varepsilon\partial_t \boldsymbol{A} = \boldsymbol{J} \tag{7}$$

$$\text{with } \boldsymbol{E} = -\mathbf{grad}\,\Phi - \frac{\partial \boldsymbol{A}}{\partial t}\,, \qquad \boldsymbol{B} = \mathbf{curl}\,\boldsymbol{A}$$

- **Singular** (non-unique solution) due to gauge freedom

$$\boldsymbol{A} = \boldsymbol{A}' + \mathbf{grad}\,\chi\,, \qquad \Phi = \Phi' + \frac{\partial \chi}{\partial t}$$

since $\mathbf{curl}\,\mathbf{grad}\,\chi = \mathbf{0}$

Textbook example: Lorenz gauge

- For constant ε, ν, $c^2 := \nu/\varepsilon$ **decouple** equations by gauge

$$\operatorname{div} \boldsymbol{A} + \partial_t \Phi / c^2 = 0$$

- **Wave equations** follow with Laplacian $\Delta\Phi := \operatorname{div} \mathbf{grad}\, \Phi$ and Vector Laplacian $\boldsymbol{\Delta A} := \mathbf{grad} \operatorname{div} \boldsymbol{A} - \mathbf{curl}\,\mathbf{curl}\, \boldsymbol{A}$

$$\boxed{\begin{aligned} -\Delta\Phi - \partial_t^2\, \Phi / c^2 &= \rho/\varepsilon && (8) \\ -\boldsymbol{\Delta A} + \partial_t^2 \boldsymbol{A} / c^2 &= \mathbf{J}/\nu && (9) \end{aligned}}$$

- Often better to stay with **curl curl** equation
  - $\boldsymbol{\Delta A} = \Delta A_x \boldsymbol{e}_x + \Delta A_y \boldsymbol{e}_y + \Delta A_z \boldsymbol{e}_z$ **only** in Cartesian coords
  - **Numerical** troubles of (9) in nodal basis (spurious modes)

Static case

$$-\mathrm{div}\,\varepsilon\,\mathbf{grad}\,\Phi - \mathrm{div}\,\varepsilon\partial_t \boldsymbol{A} = \rho \tag{10}$$

$$\mathbf{curl}\,\nu\,\mathbf{curl}\,\boldsymbol{A} - \partial_t\,\varepsilon\,\mathrm{grad}\,\Phi - \partial_t\,\varepsilon\partial_t \boldsymbol{A} = \boldsymbol{J} \tag{11}$$

- Changes of fields over time are neglected
- Relevant to find **equilibrium configurations**
- equations **decouple** into **electrostatics** and **magnetostatics**
- in particular, Eq. (11) leads to

$$\mathrm{div}\,\boldsymbol{J} = \mathbf{0} \tag{12}$$

(continuity equation without sources)

FEM for the 3D curl-curl equation – weak form

$$\boxed{\mathbf{curl}\,\nu\mathbf{curl}\,\boldsymbol{A} = \boldsymbol{J} \qquad (13)}$$

- Standard procedure: domain Ω with Neumann data $\boldsymbol{A}_\mathrm{N} \times \boldsymbol{n}$ on Γ_N

1. Scalar multiplication by test function $\boldsymbol{W}$
2. Do partial integration $\Rightarrow$ weak form

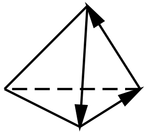
$$\int_\Omega \mathbf{curl}\,\boldsymbol{W} \cdot \nu\,\mathbf{curl}\,\boldsymbol{A}\,\mathrm{d}\Omega = \int \boldsymbol{W} \cdot \boldsymbol{J}\,\mathrm{d}\Omega - \int_{\Gamma_\mathrm{N}} \nu\,\boldsymbol{W} \cdot \mathbf{curl}\,\boldsymbol{A}_\mathrm{N} \times \boldsymbol{n}\,\mathrm{d}\Omega \tag{14}$$

3. Discretise locally on mesh by Galerkin method

FEM for the 3D curl-curl equation – discretisation

$$\boxed{\int_\Omega \mathbf{curl}\, \boldsymbol{W} \cdot \nu\, \mathbf{curl}\, \boldsymbol{A} \,\mathrm{d}\Omega = \int \boldsymbol{W} \cdot \boldsymbol{J} \,\mathrm{d}\Omega - \int_{\Gamma_\mathrm{N}} \nu\, \boldsymbol{W} \cdot \mathbf{curl}\, \boldsymbol{A}_\mathrm{N} \times \boldsymbol{n} \,\mathrm{d}\Gamma_\mathrm{N}}$$

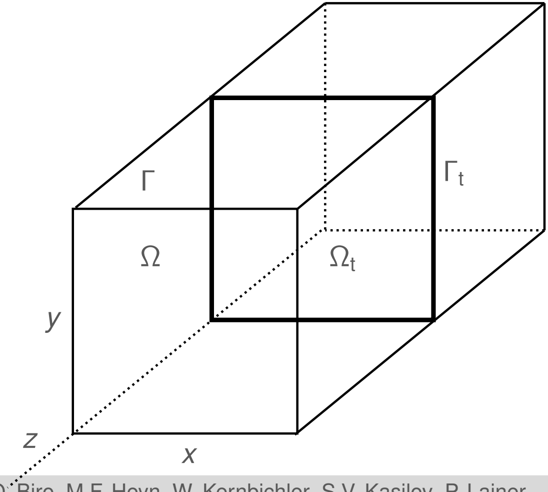
- **Edge** (Nédélec) elements for $\boldsymbol{A}$, $\boldsymbol{W} \in H_{\mathbf{curl}}$
  - DOFs: integral of vector along edges
  - Stokes' law $\oint \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{l} = \int \mathbf{curl}\, \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{S}$ given directly



- **Face** (Raviart-Thomas) elements for $\boldsymbol{B} = \mathbf{curl}\, \boldsymbol{A} \in H_{\mathrm{div}}$
  - DOFs: integral of vector across faces
  - Gauss' law $\oint \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{S} = \int \mathrm{div}\, \boldsymbol{A} \,\mathrm{d}V$ given directly
- Either gauged (tree-cotree) or ungauged (iterative solver)

Example: Cartesian coordinates

- Prism with BCs and parameters 2π-periodic in z



Reduction to 2D - symmetric part (z-independent)

- Curl splits into independent transversal $\boldsymbol{b}$ and longitudinal $B_z \boldsymbol{e}_z$

$$\boldsymbol{B} = \mathbf{curl}\, \boldsymbol{A} = \underbrace{\partial_y A_z\, \boldsymbol{e}_x - \partial_x A_z\, \boldsymbol{e}_y}_{\boldsymbol{b} = \mathbf{curl}_\mathrm{t} A_z} + \underbrace{(\partial_x A_y - \partial_y A_x)}_{B_z = \mathrm{curl}_\mathrm{t}\, \boldsymbol{a}} \boldsymbol{e}_z$$

- Two distinct equations follow from **curl curl** Eq. (13)

$$\boxed{\begin{aligned} \mathbf{curl}_\mathrm{t} \nu \mathrm{curl}_\mathrm{t} \boldsymbol{a} &= \boldsymbol{j} && (15) \\ \mathrm{curl}_\mathrm{t}\, \nu \mathbf{curl}_\mathrm{t} A_z &= J_z && (16) \end{aligned}}$$

- Weak forms of homogenous Neumann problems:

$$\int_\Omega \mathrm{curl}_\mathrm{t}\, \boldsymbol{w}\, \nu\, \mathrm{curl}_\mathrm{t}\, \boldsymbol{a}\, \mathrm{d}\Omega_\mathrm{t} = \int \boldsymbol{w} \cdot \boldsymbol{j}\, \mathrm{d}\Omega_\mathrm{t} \qquad (\rightarrow \text{ edge elements})$$

$$\int_\Omega \mathbf{curl}_\mathrm{t}\, W \cdot \nu\, \mathbf{curl}_\mathrm{t}\, A_z\, \mathrm{d}\Omega_\mathrm{t} = \int W\, J_z\, \mathrm{d}\Omega_\mathrm{t} \qquad (\rightarrow \text{ nodal elements})$$

Reduction to 2D - oscillatory part

- All quantities oscillatory in symmetry direction, e.g. z

$$f(x,y,z) = \mathrm{Re} \sum_{n\neq 0} f_n(x,y)\, \exp(\mathrm{i}nz)$$

- Curl also contains extra terms with $\partial_z = \mathrm{i}n$

$$\boldsymbol{B} = (\partial_y A_z - \mathrm{i}nA_y)\boldsymbol{e}_x + (\mathrm{i}nA_x - \partial_x A_z)\boldsymbol{e}_y + (\partial_x A_y - \partial_y A_x)\boldsymbol{e}_z$$

- $n \neq 0$ – why not eliminate A_z by gauge transformation?

$$\begin{aligned} &\boldsymbol{A} \rightarrow \boldsymbol{A} + \mathbf{grad}\,\chi, \\ &\chi = -\int A_z \mathrm{d}z = -\frac{A_z}{\mathrm{i}n} \qquad \text{(single harmonic)} \end{aligned}$$

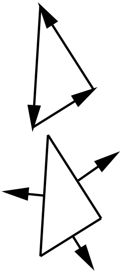
Reduction to 2D - oscillatory part

- Now only transversal $\boldsymbol{a} \perp \boldsymbol{b}$ remains

$$\boldsymbol{B} = -\mathrm{i}n a_y \boldsymbol{e}_x + \mathrm{i}n a_x \boldsymbol{e}_y + (\partial_x a_y - \partial_y a_x)\boldsymbol{e}_z$$

- Splits into "Helmholtz" (+ means decay here) and other

$$\boxed{\begin{aligned} \mathbf{curl}_\mathrm{t}\,\nu\,\mathrm{curl}_\mathrm{t}\,\boldsymbol{a} + n^2\nu\,\boldsymbol{a} &= \boldsymbol{j} \qquad (17) \\ -\mathrm{i}n\,\mathrm{div}_\mathrm{t}\,\nu\boldsymbol{a} &= J_z \qquad (18) \end{aligned}}$$



- Eq. (18) automatically fulfilled with Eq. (17) & div $\boldsymbol{J} \doteq 0$
- Weak form for homogenous Neumann problem

$$\int_\Omega \mathrm{curl}_\mathrm{t}\,\boldsymbol{w}\,\nu\,\mathrm{curl}_\mathrm{t}\,\boldsymbol{a} + n^2\boldsymbol{w}\cdot\nu\boldsymbol{a}\,\mathrm{d}\Omega_\mathrm{t} = \int \boldsymbol{w}\cdot\boldsymbol{j}\,\mathrm{d}\Omega_\mathrm{t} \qquad (\rightarrow \text{ edge elements})$$

Comparison symmetric – oscillatory

- Symmetric part 2D transversal equation ("Poisson")

$$\mathbf{curl}_\mathrm{t}\,\nu\,\mathrm{curl}_\mathrm{t}\,\boldsymbol{a} = \boldsymbol{j}$$

  - Still singular (ungauged), can add $\mathbf{grad}_\mathrm{t}\chi$ to $\boldsymbol{a}$
  - Only describes B_z component, need also other equation

- Oscillatory part 2D transversal equation ("Helmholtz")

$$\mathbf{curl}_\mathrm{t}\,\nu\,\mathrm{curl}_\mathrm{t}\,\boldsymbol{a} + n^2\nu\,\boldsymbol{a} = \boldsymbol{j}$$

  - Uniquely solvable
  - Describes full $\boldsymbol{B}$ solution using $\mathrm{div}\boldsymbol{B} = \mathrm{div}_\mathrm{t}\boldsymbol{b} + inB_z = 0$

Some basics about curvilinear coordinates

- Coordinates x^k parametrize space: $\boldsymbol{r}(x^1, x^2, x^3) \to$ inverse $x^k(\boldsymbol{r})$
- (Non-orthonormal) covariant and its dual (contravariant) basis

$$\boldsymbol{e}_k = \partial_k \mathbf{r} \qquad \boldsymbol{e}^k = \mathbf{grad}\, x^k$$

- Representation of vectors in contra- and covariant components

$$\boldsymbol{A} = \sum_k A^k \boldsymbol{e}_k = \sum_k A_k \boldsymbol{e}^k, \qquad A^k = \boldsymbol{A} \cdot \boldsymbol{e}^k,\ A_k = \boldsymbol{A} \cdot \boldsymbol{e}_k$$

- Jacobian is the square-root of determinant of metric tensor

$$J = \sqrt{g}, \qquad g_{ij} = \partial_i \boldsymbol{r} \cdot \partial_j \boldsymbol{r}, \qquad A_k = \sum_i g_{ik} A^k$$

- Differential operators (ε^{ijk}=1: ijk=123,231,312 / -1: 321,213,132)

$$\mathrm{div}\boldsymbol{A} = \frac{1}{\sqrt{g}} \sum_k \partial_k \sqrt{g} A^k \qquad \mathbf{curl}\boldsymbol{A} = \boldsymbol{e}_i \sum_{j,k} \frac{\varepsilon^{ijk}}{\sqrt{g}} \partial_j A_k$$

Oscillatory part in 2D coordinate space

- Careful with Fourier in curved coordinates! Assumptions:
  - Orthogonal system (g_{ij} has only diagonal elements)
  - g_{ij} depends only on x^1 and x^2, not on x^3
- Expand **co**variant $\boldsymbol{A}$ and **contra**variant $\boldsymbol{J}$ components

$$A_k(x^1, x^2, x^3) = \sum_{n=-\infty}^{\infty} A_{k,n}(x^1, x^2) e^{inx^3}, \tag{19}$$

$$J^k(x^1, x^2, x^3) = \sum_{n=-\infty}^{\infty} J_n^k(x^1, x^2) e^{inx^3}, \tag{20}$$

- 2D curl in coordinate space

$$\mathrm{curl}_2 \boldsymbol{a} := \frac{\partial a_2}{\partial x^1} - \frac{\partial a_1}{\partial x^2} = \sqrt{g}\,\mathrm{curl}_{\mathrm{t}} \boldsymbol{a}$$

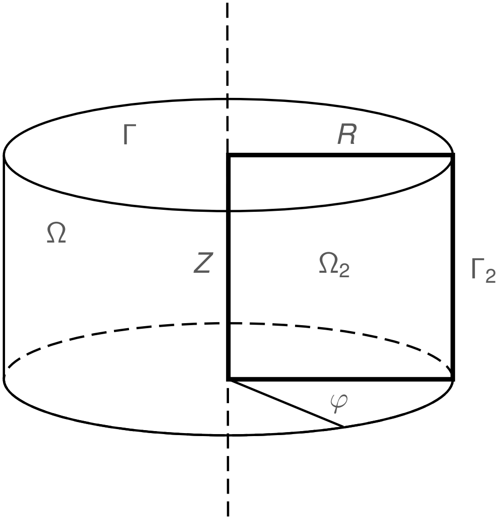
Weak form in 2D coordinate space

- Coordinate space volume element: $d\Omega_2 := dx^1 dx^2$
- Coordinate space line element: $d\Gamma_2 = \sqrt{(dx^1)^2 + (dx^2)^2}$
- Weak form of Eq. (17) homogenous Neumann problem

$$\int_\Omega \frac{g_{33}}{\sqrt{g}} \nu \, \mathrm{curl}_2 \mathbf{w} \, \mathrm{curl}_2 \mathbf{a}$$

$$+ n^2 \nu \left(\frac{g_{22}}{\sqrt{g}} w_1 a_1 + \frac{g_{11}}{\sqrt{g}} w_2 a_2 \right) \mathrm{d}\Omega_2 = \int_\Omega \mathbf{w} \cdot \mathbf{j} \sqrt{g} \mathrm{d}\Omega_2$$

Example: Cylindrical coordinates



Example: Cylindrical coordinates

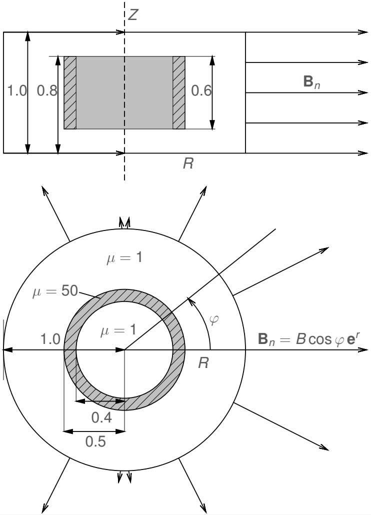
- Coordinates (R, φ, Z) symmetry coordinate: angle φ (ordering!)
- Weak form of Eq. (17) homogenous Neumann problem

$$\int_{\Omega_2} R\nu\, \mathrm{curl}_2 \mathbf{a}\, \mathrm{curl}_2 \mathbf{w} + \frac{n^2}{R}\nu\,(w_R a_R + w_Z a_Z)\,\mathrm{d}R\mathrm{d}Z = \int_{\Omega_2} R\,\mathbf{w}\cdot\mathbf{j}\,\mathrm{d}R\mathrm{d}Z$$

- Weighting factor follows automatically from Jacobian $\sqrt{g}$
- Magnetic field

$$B^R = \frac{in}{R}a_R, \qquad B^Z = -\frac{in}{R}a_Z, \qquad B^\varphi = -\frac{\mathrm{div}_t \boldsymbol{b}}{in},.$$

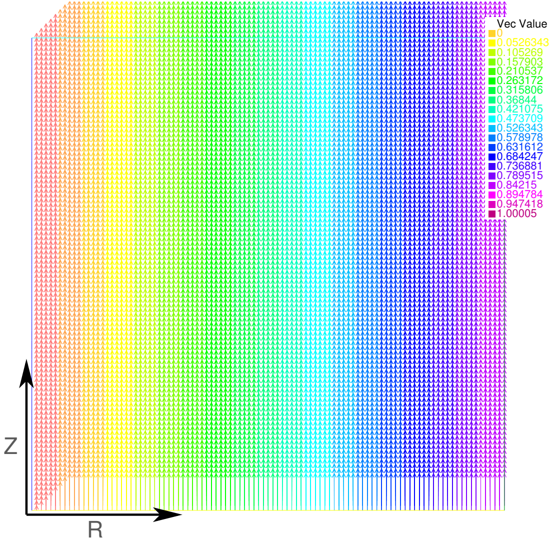
Example: Shielding by cylinder shell with $\mu > 1$



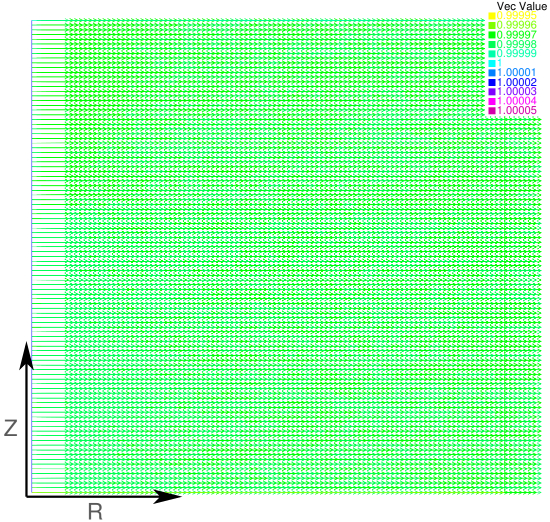
FreeFEM++ implementation

```
load "Element_Mixte"; // for 1st order edge elements
real n = 1.0;  // mode number

mesh Th = square(50,50,[x+1e-31,y]); // cylinder cross-section

fespace Hrot(Th,RT1Ortho); fespace Hdiv(Th,RT1); // 1st order

Hrot [ax,ay], [wx,wy]; Hdiv [jr,jz];

func real nu(real rp, real zp) { // nu = 1/mu
  if((rp>0.4)&&(rp<0.5)&&(zp>0.2&&(zp<0.8))) return 1.0/50.0;
  return 1.0;
}

solve CurlCurl([ax,ay],[wx,wy],solver=UMFPACK) =
  int2d(Th)(nu(x,y)*(x*(dx(wy)-dy(wx))*(dx(ay)-dy(ax))
                   + n^2*1.0/x*(wx*ax+wy*ay)))
  + on(1,ax=0.0,ay=0.0)
  + on(2,3,4,ax=0.0,ay=1.0*x);

plot([ax,ay],wait=true,value=true,ps="a_mu.eps");
```

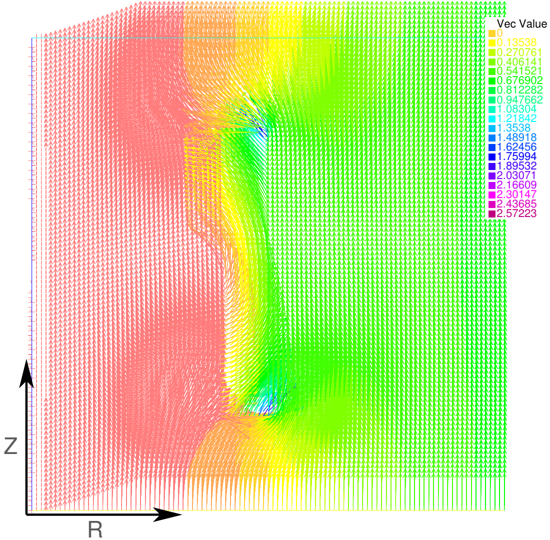
a field: homogenous mag. field, $\mu = 1$ everywhere



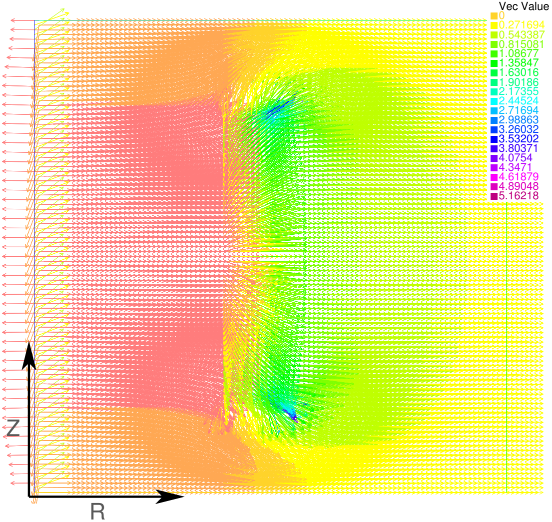
b field: homogenous field, $\mu = 1$ everywhere



a field: shielding by cylinder shell with $\mu > 1$



b field: shielding by cylinder shell with $\mu > 1$



A few technical issues

- Careful with $\frac{1}{R}$ terms near axis (1st order works "well enough")
  - 0th order causes troubles
- Complex numbers "emulated" now
- Find best interface FreeFEM++ $\leftrightarrow$ Fortran

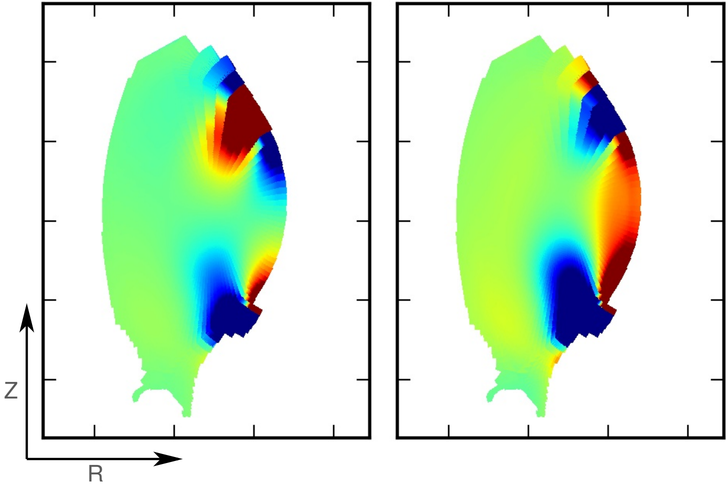
Iterations for kinetic plasma equilibria

- Formally, **curl curl** solver yields $\boldsymbol{B} = \hat{M}\boldsymbol{J}$ with solution operator $\hat{M}$
- Monte Carlo kinetic code yields $\boldsymbol{J} = \hat{K}(\boldsymbol{B}_0 + \boldsymbol{B})$ (noisy)
- Equilibrium field: fixed point $\boldsymbol{B} = \hat{M}\hat{K}(\boldsymbol{B}_0 + \boldsymbol{B})$ or

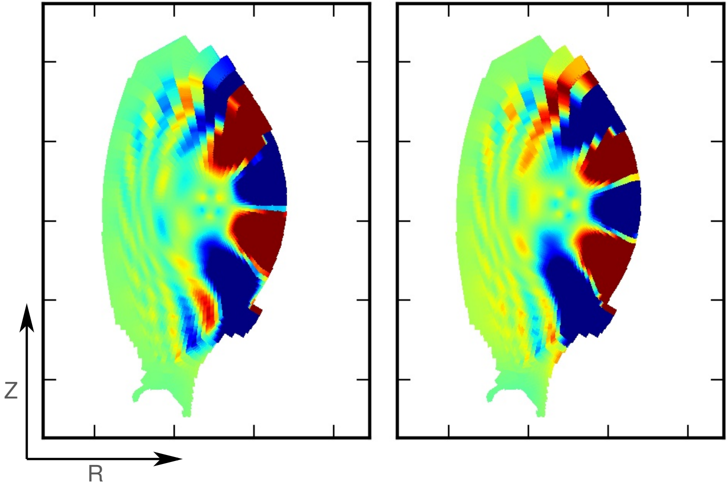
$$(\hat{M}\hat{K} - \hat{I})\boldsymbol{B} = -\hat{M}\hat{K}\boldsymbol{B}_0$$

- Eigenvalues of $\hat{M}\hat{K} > 1$: **relaxed** iterations **do not help**
- Trick: **Arnoldi** method, solve unstable part **separately**
- Challenge: **random noise** from Monte Carlo method

ITER-like tokamak (B_r, vacuum) [4]



ITER-like tokamak (B_r, kinetic equilibrium) [4]



Conclusion

Take-home messages:

- Magnetostatics written as singular **curl curl** equation for ***A***
  - 2D eqs. **ungauged** for symmetric, **gauged** for oscillatory
- **Co-/contravariant** notation useful for easy **generalisation**
- **FreeFEM++ very** useful for fast and easy **solution**
- **Outlook**: Apply to eddy currents, fluid dynamics (Stokes), etc.

References:

[1] A Bossavit, IEEE Trans. Mag. 26, 702 (1990)

[2] O Biro, Comput. Meth. Appl. Mech. Eng. 169, 391 (1999)

[3] Z Belhachmi, C Bernardi, S Deparis, F Hecht,
Math. Models Methods Appl. Sci. 16, 233 (2006)

[4] CG Albert, MF Heyn, SV Kasilov, W Kernbichler, AF Martitsch, AM Runov,
Joint Varenna-Lausanne International Workshop, P.01 (2016)