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Solving the Quasi-Neutrality Equation on Surfaces

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Quasi-neutrality equation

We want to solve the following problem in the domain Ω:

$$\begin{aligned} -\operatorname{div}(\nu \nabla_\perp \phi) &= \rho \text{ in } \Omega \\ \phi &= g \text{ on } \partial\Omega \end{aligned}$$

where ν, g and ρ are scalar functions and $\nabla_\perp \phi = \nabla\phi - (\mathbf{b} \cdot \nabla\phi)\mathbf{b}$ and $\mathbf{b} = \mathbf{B}/|\mathbf{B}|$

Decoupling into 2D problems in ideal situation

Assume we have curvilinear coordinates y^1, y^2, y^3 s.t. for the basis vectors $\mathbf{e}_i = \partial \mathbf{x}/\partial y^i$ we have

$$\mathbf{e}_1, \mathbf{e}_2 \perp \mathbf{b} \text{ and } \mathbf{e}_3 = \mu \mathbf{b}$$

for some non-vanishing scalar field μ. Then the problem becomes w.r.t. these variables

$$-\frac{1}{\mu} \operatorname{div}_{(1,2)}(\nu\mu\nabla_{(1,2)}\phi) = \rho$$

where $\operatorname{div}_{(1,2)}$ is the divergence w.r.t. the first two variables and analogous for $\nabla_{(1,2)}$.

Decoupling of the 2D problems in ideal situation

IDEA: Deal with the problem on the isosurfaces of the third variable $y^3 \to$ the problems decouple

Assume for the surfaces $\{y^3 = \text{const}\} \cap \partial\Omega \neq \varnothing$, so Dirichlet boundary conditions can be imposed

Problem

These surfaces do not exist for general vector fields

Existence of orthogonal surfaces

- Conditions for existence of these surfaces are given by the Frobenius theorem
- There are multiple formulations of it. The most suited one for our purpose is:

Frobenius Theorem (for codimension 1)

Assume **B** is sufficiently regular and non-vanishing. Then the curvilinear coordinates as above exist, iff there are scalar fields α and β s.t. $\mathbf{B} = \alpha \nabla \beta$.

Another equivalent condition for the existence is

$$\mathbf{B} \cdot \operatorname{curl} \mathbf{B} = 0.$$

Question

How large is $\mathbf{B} \cdot \operatorname{curl} \mathbf{B}$ in practice?

Example: Nonexistence of orthogonal surfaces

Counter-example from Omar Maj: **Cylindrically symmetric equilibrium**

$$\mathbf{B} = B_0\mathbf{e}_z + \nabla\psi \times \mathbf{e}_z = \begin{pmatrix} \partial_y\psi \\ -\partial_x\psi \\ B_0 \end{pmatrix}$$

with a constant $B_0 > 0$ and scalar function $\psi = \psi(x, y)$. We choose

$$\psi(x, y) = \frac{a_0}{2}(x^2 + \kappa y^2).$$

- Omar showed that this defines orthogonal surfaces iff $\kappa = -1$
- For the imporant case $\kappa > 0$ (confined field lines), orthogonal surfaces do not exist, not even locally.

Surfaces given by the Dommaschk potential

Let χ be the Dommaschk potential which is of the form [1]

$$\chi(R, \varphi, Z) = F_0\varphi + \sum_{n,m} \chi_{n,m}(R, \varphi, Z), \quad \text{with } \Delta\chi_{n,m} = 0$$

φ is the toroidal angle and F_0 is a constant.

If $\nabla\chi \approx \mathbf{B}$, we can take the isosurfaces of χ.

[1] W. Dommaschk (1986) - "Representations for vacuum potentials in stellarators", Computer Physics Communications 40

Angle between field from VMEC and Dommaschk potential

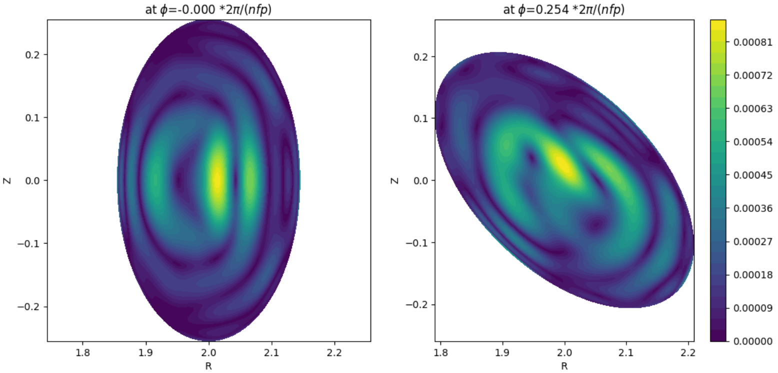
- As a test, Florian Hindenlang took Dommaschk potential fitted to **B**-field from VMEC for W7A with zero toroidal current and zero pressure [2].
- Angle between **B** and $\nabla\chi$ less than 10^{-3}

The equilibrium field **B** is almost orthogonal to the isosurfaces of χ

[2] Data provided by Nikita Nikulsin and Rohan Ramasamy, see Nikulsin et al (2022) - "JOREK3D: An extension of the JOREK nonlinear MHD code to stellarators"

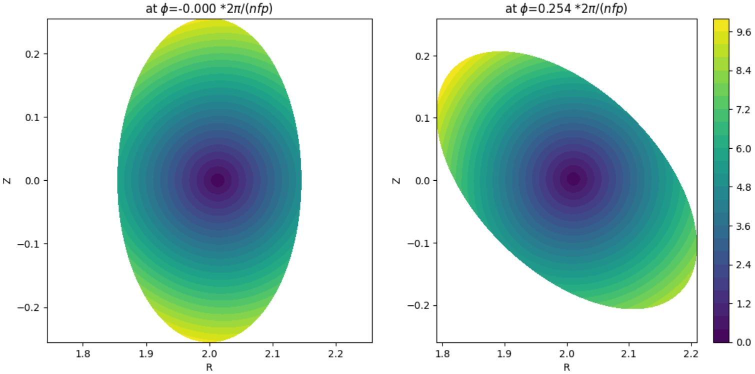
Plot of angle between B and $\nabla\chi$

Plots show the angle between **B** and $\nabla\chi$ in degrees on two poloidal cuts



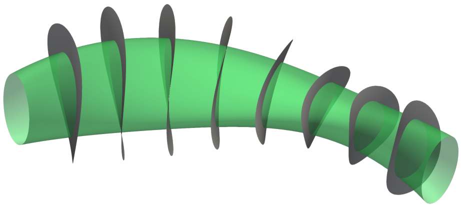
Comparison with taking only φ direction

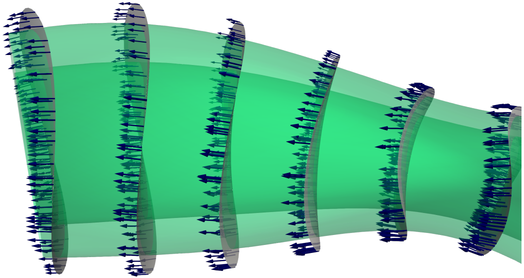
- Plots show the angle between $\mathbf{e}_\varphi$ and $\mathbf{B}$ on the same poloidal cuts
- The angle is larger by 4 orders of magnitude in our example



Angle between $\mathbf{B}$ and $\mathbf{e}_\varphi$ in degrees

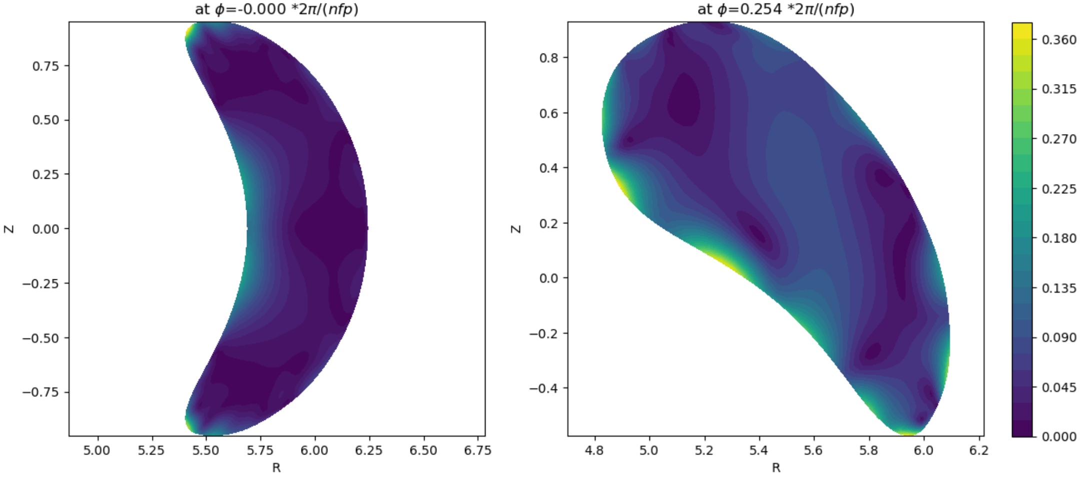
Isosurfaces of the Dommaschk potential



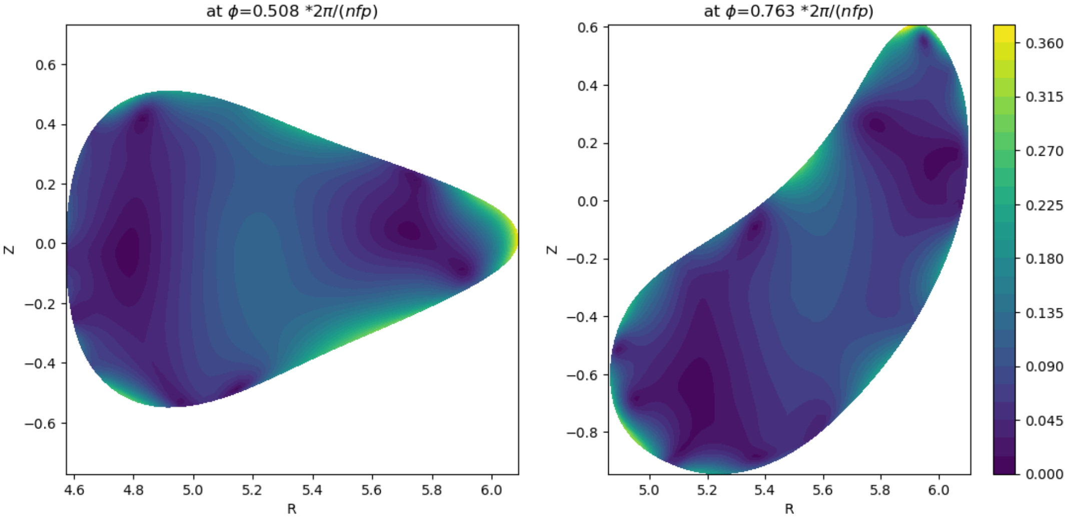


- Grey surfaces: Isosurfaces of the Dommaschk potential
- Green surfaces: Isosurfaces of an approximate flux surface invariant computed from the Dommaschk potential
- Dark blue glyphs: Magnetic field from VMEC

Comparison on W7-X



Comparison on W7-X



Computing generalized potentials

B defines orthogonal surfaces iff $\mathbf{B} = \alpha\nabla\beta$, but there exist no such α and β in general.

Idea: Approximate **B** with vector fields of the form $\alpha\nabla\beta$

Define the error functional

$$J(\alpha,\beta) = \int_U |\mathbf{B} - \alpha\nabla\beta|^2 \, dx$$

where $U \subseteq \Omega$ is a toroidal cut of the domain of interest and solve the minimization problem

$$\min_{\alpha,\beta} J(\alpha,\beta)$$

Discrete optimization problem

Use splines for the discretization, so the discrete minimization problem reads

$$\min_{\alpha_h, \beta_h \in V_h^0} J(\alpha_h, \beta_h)$$

where V_h^0 is a pushforward tensor product spline space.

Since we are interested in the surfaces only, these spline spaces can be chosen local in the toroidal angle $\zeta \rightarrow$ Well suited for parallelization

Another discretization than splines is also possible.

Gradient descent

The Gateaux derivative of the functional is

$$\delta_\alpha J(\alpha,\beta;\alpha_1) = -2\int_\Omega (\mathbf{B}-\alpha\nabla\beta)\cdot(\alpha_1\nabla\beta)\,dx \text{ and}$$

$$\delta_\beta J(\alpha,\beta;\beta_1) = -2\int_\Omega (\mathbf{B}-\alpha\nabla\beta)\cdot(\alpha\nabla\beta_1)\,dx$$

$$\alpha_h = \sum_{i=1}^{N}\mu_i\Lambda_i, \quad \beta_h = \sum_{i=1}^{N}\lambda_i\Lambda_i.$$

$$\frac{\partial}{\partial\boldsymbol{\mu}}J(\alpha_h,\beta_h) = \left(-2\int_\Omega (\mathbf{B}-\alpha_h\nabla\beta_h)\cdot(\Lambda_i\nabla\beta_h)\right)_{i=1}^{N}$$

$$\frac{\partial}{\partial\boldsymbol{\lambda}}J(\alpha_h,\beta_h) = \left(-2\int_\Omega (\mathbf{B}-\alpha\nabla\beta_h)\cdot(\alpha_h\nabla\Lambda_i)\right)_{i=1}^{N}$$

Assembly of the gradients using Psydac library

- Gradients are finite dimensional representations of linear forms $\rightarrow$ can be easily assembled using Psydac [3]
- Acceleration with Pyccel achieves speedup by a factor $\approx$1000 compared to Python

```
expr = -2*(alpha*dot(B, grad(beta1))
          - alpha**2 * dot(grad(beta), grad(beta1)))
lambda_deriv_symbolic = LinearForm(beta1, integral(domain, expr))
lambda_deriv_discrete = discretize(lambda_deriv_symbolic,
                                   domain_h,
                                   derham_h.V0,
                                   backend=PSYDAC_BACKEND_GPYCCEL)
lambda_deriv = lambda_deriv_discrete.assemble(B=B_h,
                                              alpha=alpha_h,
                                              beta=beta_h).toarray()
```

[3] Güçlü, Y., Hadjout, S. and Ratnani, A. PSYDAC: a high-performance IGA library in Python. 2022. (https://github.com/pyccel/psydac)

Gradient descent

Using this the gradient and functional evaluation is feasible for gradient descent.

Outlook

So far, we have only run the algorithm for test examples where the field is given as a gradient. We want to try the following tests:

- Use a magnetic field from GVEC and use the Dommaschk potential as initial guess to see if we can improve the approximation
- Symmetric cylinder geometry from Omar's counterexample
- Analytical Grad-Shafranov geometry

Different approaches to finding the surfaces

Taking poloidal planes

- Captures the dominant part of the field

Isosurfaces of the Dommaschk potential

- Good approximation for vacuum fields
- Improvement by several orders of magnitude possible

Generalized potentials

- Most general approach
- Not current free and thus possibly better for fields with strong current
- Not tested on physically relevant fields yet

Solving the quasi-neutrality equation on the surfaces

This material is taken from the Acta Numerica paper from Dziuk and Elliott [4]. There are three main ideas:

1. Use the potential to solve the PDE on all level sets simultaneously (implicit surface FEM)
2. Solve the PDE locally in a small neighborhood of a surface (Unfitted bulk FEM)
3. Discretize the surface directly (not discussed here)

[4] Dziuk, Elliott (2013), "Finite Element Methods for Surface PDEs", Acta Numerica, pp. 289-396.

Implicit surface FEM

We want to solve the Poisson equation on level sets of β. For a potential β, we get the normal field

$$\mathbf{n} := \frac{\nabla\beta}{|\nabla\beta|}$$

and define

$$\nabla_\beta f := P_\beta \nabla f, \quad P_\beta = I - \mathbf{n} \otimes \mathbf{n}.$$

Then for a equation

$$-\nabla \cdot (P_\beta \nabla\phi |\nabla\beta|) + c\phi|\nabla\beta| = f|\nabla\beta|$$

with some scalar fields f and c with $c > \bar{c} > 0$, the weak formulation reads

$$\int_\Omega \nabla_\beta\phi \cdot \nabla_\beta\eta |\nabla\beta| \, dx + \int_\Omega c\phi\eta|\nabla\beta| \, dx = \int_\Omega f\eta|\nabla\beta| \, dx.$$

where we implicitely used a no flux-boundary condition across $\partial\Omega$.

Implicit surface FEM

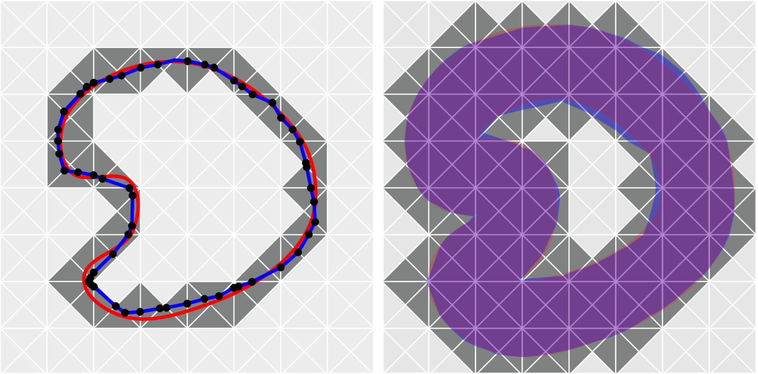
This can be discretized on the domain Ω and we have existence, uniqueness, convergence and regularity results.

Outlook

- In our case, the situation is slightly different due to Dirichlet boundary conditions and $c = 0$
- It is mostly standard elliptic theory for FE being used, which should be applicable
- Instead of the full domain Ω, we can take subdomains $\Omega \cap \{c_1 < \beta < c_2\}$ for parallelization because the boundary conditions on the limiting surfaces $\{\beta = c_i\}$, $i = 1, 2$, vanish.

Unfitted bulk FEM

- Idea: Use already existing 3D mesh and discretize the problem only on the elements intersecting the surface (or a neighborhood of it)
- Approach using implicit surfaces is localized without the need to mesh the surface directly



Appendix: Derivation of the PDE in two variables

Let

$$\mathbf{b} = b^i \mathbf{e}_i$$

so

$$\nabla \phi \cdot \mathbf{b} = \frac{\partial \phi}{\partial x^i} b^i.$$

and so

$$\nabla_\perp \phi = \nabla \phi - (\mathbf{b} \cdot \nabla \phi)\mathbf{b} = \left[\frac{\partial \phi}{\partial x^i} g^{ij} - \left(\frac{\partial \phi}{\partial x^k} b^k \right) b^j \right] \mathbf{e}_j$$

With the given assumptions $b^3 = 1/\mu$, $b^1 = b^2 = 0$, $g^{12} = g^{13} = 0$ and $g^{33} = 1/\mu^2$. This gives

$$\nabla_\perp \phi = \sum_{i,j=1}^{2} g^{ij} \frac{\partial \phi}{\partial x^i} \mathbf{e}_j = \nabla_{(1,2)} \phi.$$

Appendix: Derivation of the PDE in two variables

Let G be the metric tensor and $\tilde{G}$ be the metric tensor of the first two coordinates, g be the metric determinant and $\tilde{g}$ be the metric determinant of the first two coordinates. Then we have $\sqrt{g} = \sqrt{\tilde{g}}\mu$ Taking the general divergence in curvilinear coordinates we have

$$\frac{1}{\sqrt{g}} \sum_{i=1}^{3} \frac{\partial(\sqrt{g}\nu(\nabla_\perp \phi)^i)}{\partial x^i} = \frac{1}{\sqrt{\tilde{g}}\mu} \sum_{i=1}^{2} \frac{\partial(\sqrt{\tilde{g}}\mu\nu(\nabla\phi)^i)}{\partial x^i} = \frac{1}{\mu} \mathrm{div}_{(1,2)}(\nu\mu\nabla_{(1,2)}\phi)$$

Appendix: Proof that orthogonal surfaces exist only for $\kappa = -1$

Let β be the 1-form corresponding to **B**. Then a necessary condition for the surfaces to exist is

$$\beta \wedge d\beta = 0.$$

We have in our case

$$\beta = a_0(\kappa y dx - x dy) + B_0 dz$$

and then

$$\beta \wedge d\beta = -B_0 a_0(\kappa + 1) dx \wedge dy \wedge dz$$

and thus $\beta \wedge d\beta$ iff $\kappa = -1$.

Appendix: Frobenius theorem (vector field formulation)

There are two main formulations of the Frobenius theorem. The first one is for vector fields on manifolds. Let M be a manifold of class C^p, $p \geq 2$. We call a subbundle E of the tangent bundle **locally integrable** at x_0 if for any $x_0 \in M$ there exist a submanifold N s.t. $T_{x_0}N = E_{x_0}$. We call E integrable if it is integrable everywhere.

Frobenius theorem (vector field formulation)

Let E be a subbundle of the tangent bundle. Then E is integrable iff for any two vector fields X, Y with values in E we have $[X, Y] \in E$ where $[\cdot, \cdot]$ is the Lie bracket.

Appendix: Frobenius theorem (differential forms formulation)

The general version of the one mentioned at the beginning is

Frobenius theorem (differential form formulation)

Let M be a smooth manifold. If we have a Pfaffian system $\mathcal{I} = \{\theta^1, ..., \theta^s, d\theta^1, ..., d\theta^s\}$ s.t.

$$d\theta^\sigma \wedge \theta^1 \wedge \cdots \wedge \theta^s = 0 \quad \text{for } 1 \leq \sigma \leq s.$$

Then for every $x \in M$, there exist local coordinates y^1, y^2, ..., y^n s.t.

$$\mathcal{I} = \{dy^1, dy^2, ..., dy^s\}.$$

The other direction is trivially true. Also, the local integral manifold is given by the level sets $\{y^1 = c_1, y^2 = c_2, ..., y^s = c_s\}$ for real constants c_i.

This theorem can be globalized in the sense, that through every $x \in M$ passes a unique maximal integral manifold N. It is maximal in the sense that every other integral manifold going through x is included in N.