DESC:
An Efficient Stellarator Equilibrium Code

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Overview & Motivation

DESC[1] is a pseudo-spectral stellarator equilibrium solver that:

1. Uses global spectral methods with Fourier & Zernike basis functions
    - Properly resolves the magnetic axis
    - Minimizes the system dimensionality
    - Gives a global solution (no interpolation between flux surfaces)
2. Solves force balance directly in real space (instead of the energy principle)
    - Avoids numerical issues at rational surfaces
    - Allows for perturbations to easily search the equilibrium solution space
3. Is written modern Python with high-level structure
    - Easy to use and extend the code for individual applications
    - Designed for stellarator optimization: automatic differentiation, GPUs, etc.
4. Currently solves fixed-boundary equilibria with nested flux surfaces

[1] D. W. Dudt, and E. Kolemen, Phys. Plasmas **27** 102513 (2020).

“Inverse” Equilibrium Problem

- Computation domain is the straight field-line coordinate system

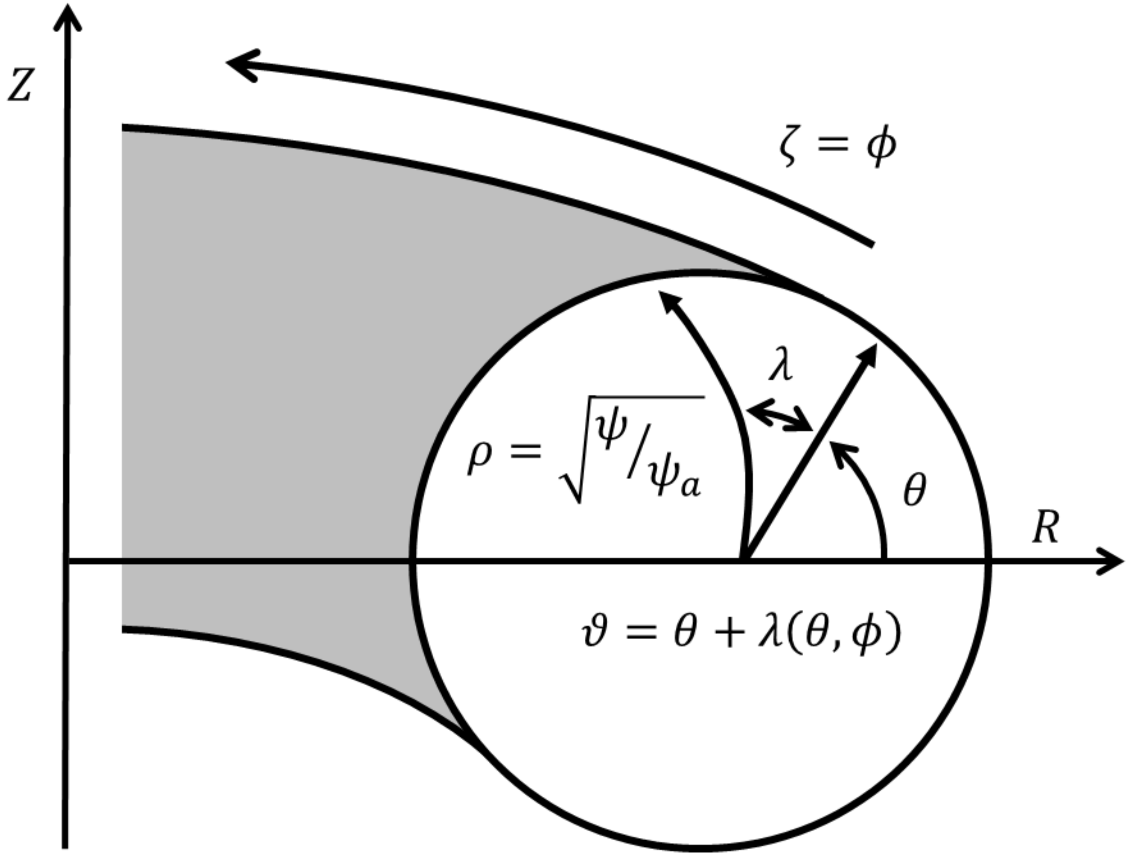
$$(\rho, \vartheta, \zeta)$$

- Free variables are the flux surface shapes

$$R(\rho, \vartheta, \zeta) \;\&\; Z(\rho, \vartheta, \zeta)$$

- Problem is to find the flux surfaces that satisfy the equilibrium conditions:

$$\boldsymbol{J} \times \boldsymbol{B} = \boldsymbol{\nabla} p$$
$$\boldsymbol{\nabla} \times \boldsymbol{B} = \mu_0 \boldsymbol{J}$$
$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$$



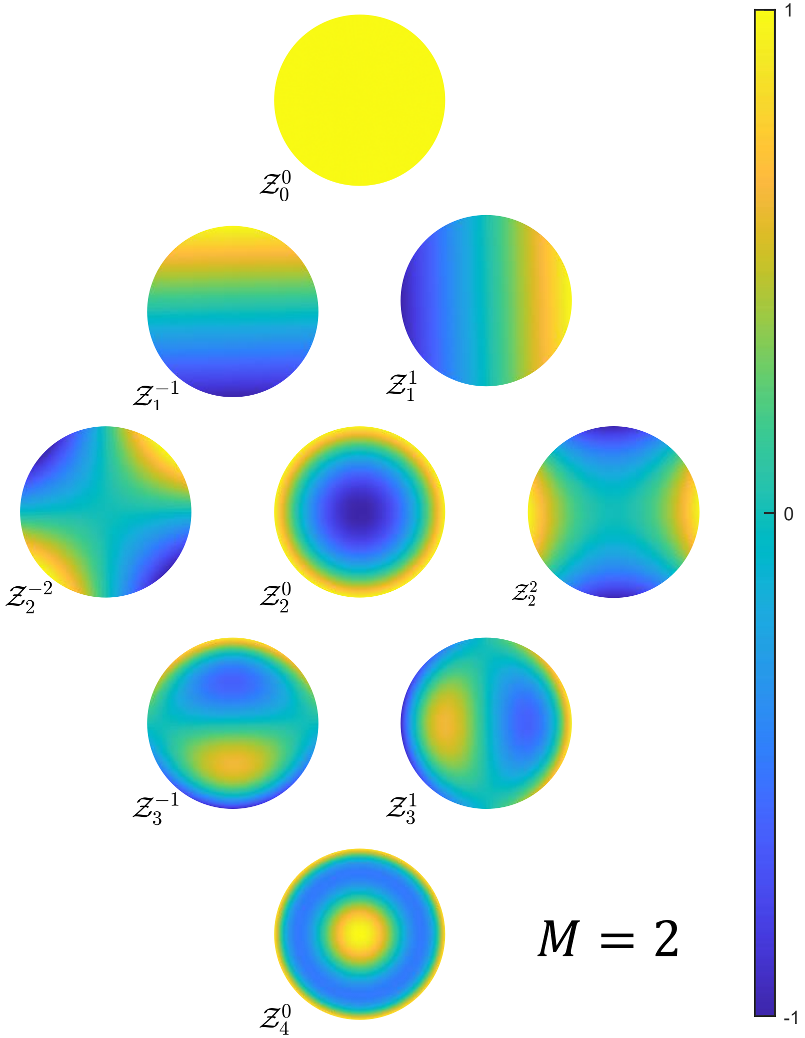
Fourier-Zernike Basis Set

- Discretize flux surfaces with global Fourier-Zernike[2] spectral basis functions:

$$R(\rho,\vartheta,\zeta) = \sum R_{lmn}\mathcal{Z}_l^m(\rho,\vartheta)\mathcal{F}^n(\zeta)$$

$$\mathrm{Z}(\rho,\vartheta,\zeta) = \sum Z_{lmn}\mathcal{Z}_l^m(\rho,\vartheta)\mathcal{F}^n(\zeta)$$

- Inherently satisfies analytic boundary conditions at the magnetic axis
- Number of basis functions scales as $M^2N/2$ (about half as many terms as other methods)



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[2] F. Zernike, Mon. Not. R. Astron. Soc. **94**, 377–384 (1934).

Magnetic Field in Flux Coordinates

- Assume[3] nested flux surfaces: $\boldsymbol{B} \cdot \boldsymbol{\nabla}\rho = 0$, and Gauss's law: $\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$

$$\boldsymbol{B} = \frac{\partial_\rho \psi}{\pi\sqrt{g}}\left(\iota \boldsymbol{e}_\vartheta + \boldsymbol{e}_\zeta\right)$$

$$\boldsymbol{B}(\rho,\vartheta,\zeta) = \boldsymbol{B}(R(\rho,\vartheta,\zeta), Z(\rho,\vartheta,\zeta), \iota(\rho))$$

- Using Ampere's Law: $\boldsymbol{\nabla} \times \boldsymbol{B} = \mu_0 \boldsymbol{J}$

$$J^\rho = \frac{\partial_\vartheta B_\zeta - \partial_\zeta B_\vartheta}{\mu_0\sqrt{g}}, J^\vartheta = \frac{\partial_\zeta B_\rho - \partial_\rho B_\zeta}{\mu_0\sqrt{g}}, J^\zeta = \frac{\partial_\rho B_\vartheta - \partial_\vartheta B_\rho}{\mu_0\sqrt{g}}$$

$$\boldsymbol{J}(\rho,\vartheta,\zeta) = \boldsymbol{J}(R(\rho,\vartheta,\zeta), Z(\rho,\vartheta,\zeta), \iota(\rho))$$

$$\boldsymbol{e}_\rho = \begin{bmatrix} \partial_\rho R \\ 0 \\ \partial_\rho Z \end{bmatrix}$$

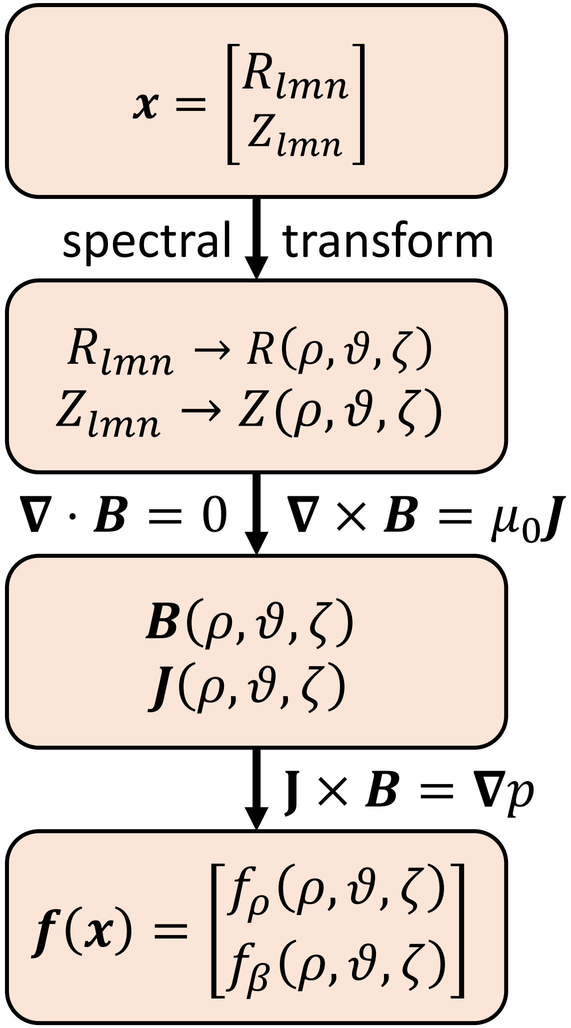
$$\boldsymbol{e}_\vartheta = \begin{bmatrix} \partial_\vartheta R \\ 0 \\ \partial_\vartheta Z \end{bmatrix}$$

$$\boldsymbol{e}_\zeta = \begin{bmatrix} \partial_\zeta R \\ R \\ \partial_\zeta Z \end{bmatrix}$$

[3] W. D. D'haeseleer et al., *Flux Coordinates and Magnetic Field Structure*, (Springer-Verlag, 1991).

Force Balance Equations

- MHD force balance error[4]: $\boldsymbol{F} \equiv \boldsymbol{J} \times \boldsymbol{B} - \boldsymbol{\nabla} p = \boldsymbol{0}$
- Substitute in $\boldsymbol{B}$ and $\boldsymbol{J}$:
$$\begin{aligned} \boldsymbol{F} &= F_\rho \boldsymbol{\nabla}\rho + F_\beta \boldsymbol{\beta} \\ F_\rho &= \sqrt{g}\left(B^\zeta J^\vartheta - B^\vartheta J^\zeta\right) - p' \\ F_\beta &= \sqrt{g} J^\rho \\ \boldsymbol{\beta} &= B^\zeta \boldsymbol{\nabla}\vartheta - B^\vartheta \boldsymbol{\nabla}\zeta \end{aligned}$$
- Form scalar equations:
$$\begin{aligned} f_\rho &= F_\rho \|\boldsymbol{\nabla}\rho\| \\ f_\beta &= F_\beta \|\boldsymbol{\beta}\| \end{aligned}$$
- An equilibrium is a solution to the system of equations $\boldsymbol{f}(\boldsymbol{x}) \approx \boldsymbol{0}$, solved at a given set of collocation points



$\boldsymbol{x} = \begin{bmatrix} R_{lmn} \\ Z_{lmn} \end{bmatrix}$

spectral transform

$R_{lmn} \rightarrow R(\rho, \vartheta, \zeta)$

$Z_{lmn} \rightarrow Z(\rho, \vartheta, \zeta)$

$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$ $\boldsymbol{\nabla} \times \boldsymbol{B} = \mu_0 \boldsymbol{J}$

$\boldsymbol{B}(\rho, \vartheta, \zeta)$

$\boldsymbol{J}(\rho, \vartheta, \zeta)$

$\mathbf{J} \times \boldsymbol{B} = \boldsymbol{\nabla} p$

$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} f_\rho(\rho, \vartheta, \zeta) \\ f_\beta(\rho, \vartheta, \zeta) \end{bmatrix}$

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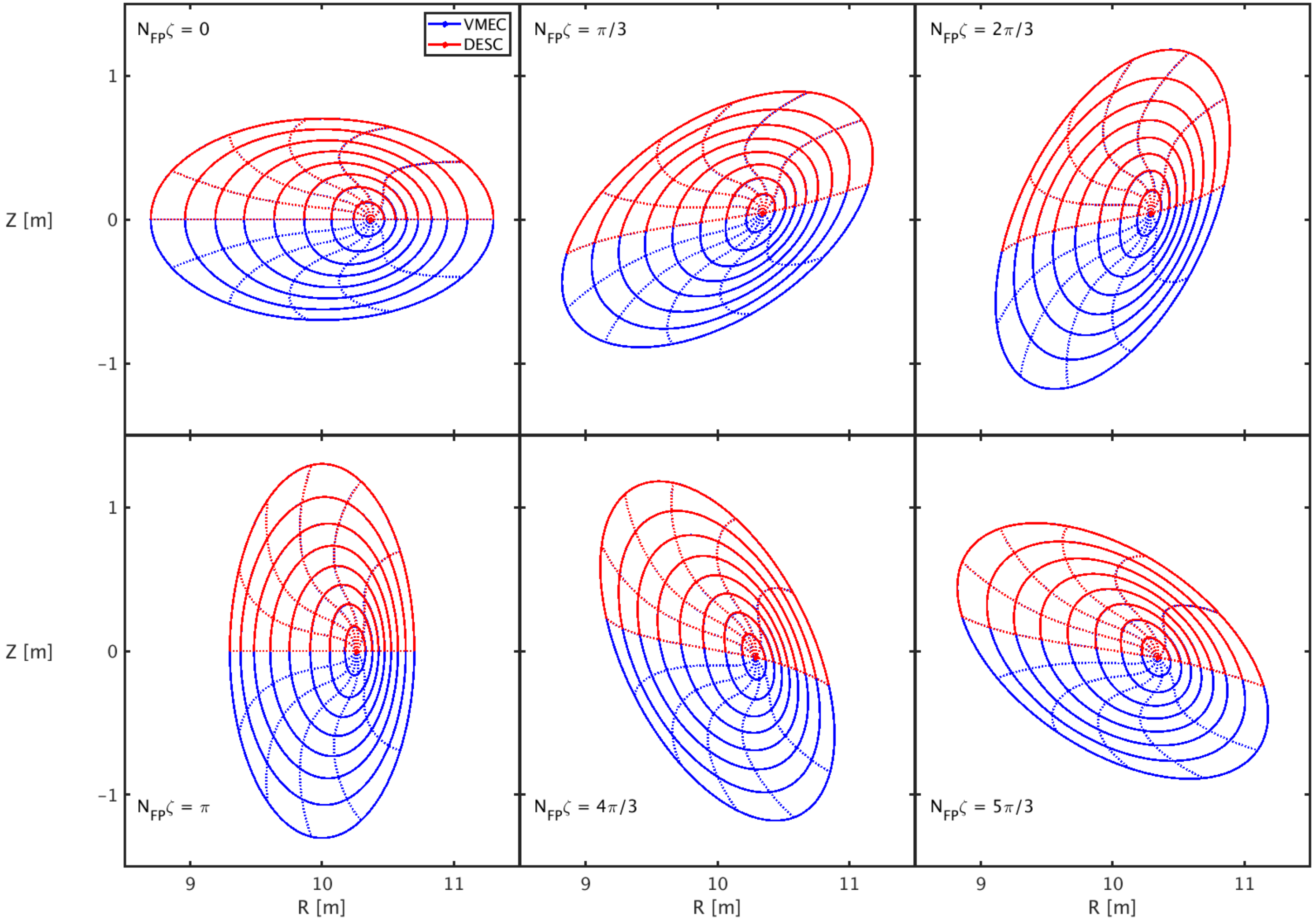
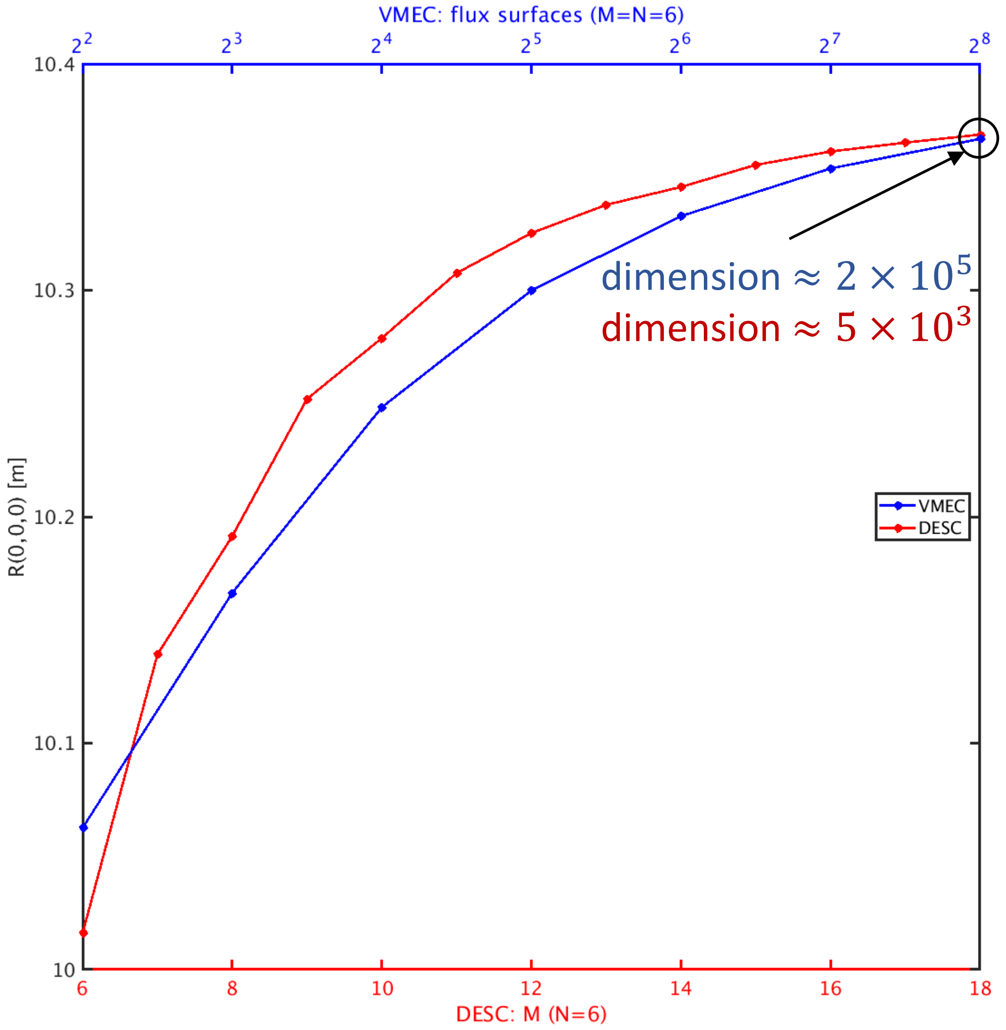
[4] S. P. Hirshman and J. C. Whitson, Phys. Fluids **26**, 3553–3568 (1983).

Convergence: Heliotron $\langle\beta\rangle \approx 2\%$

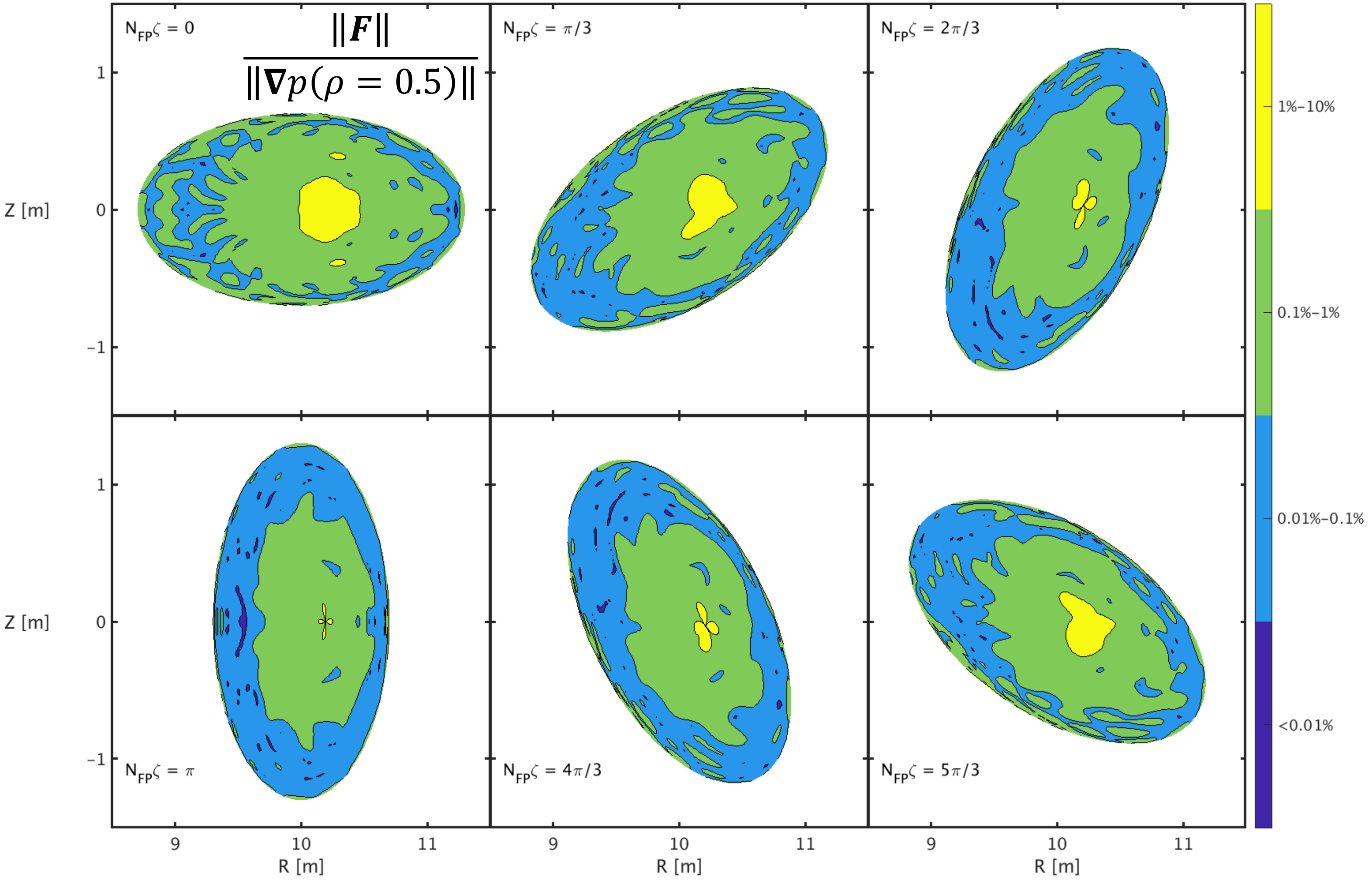




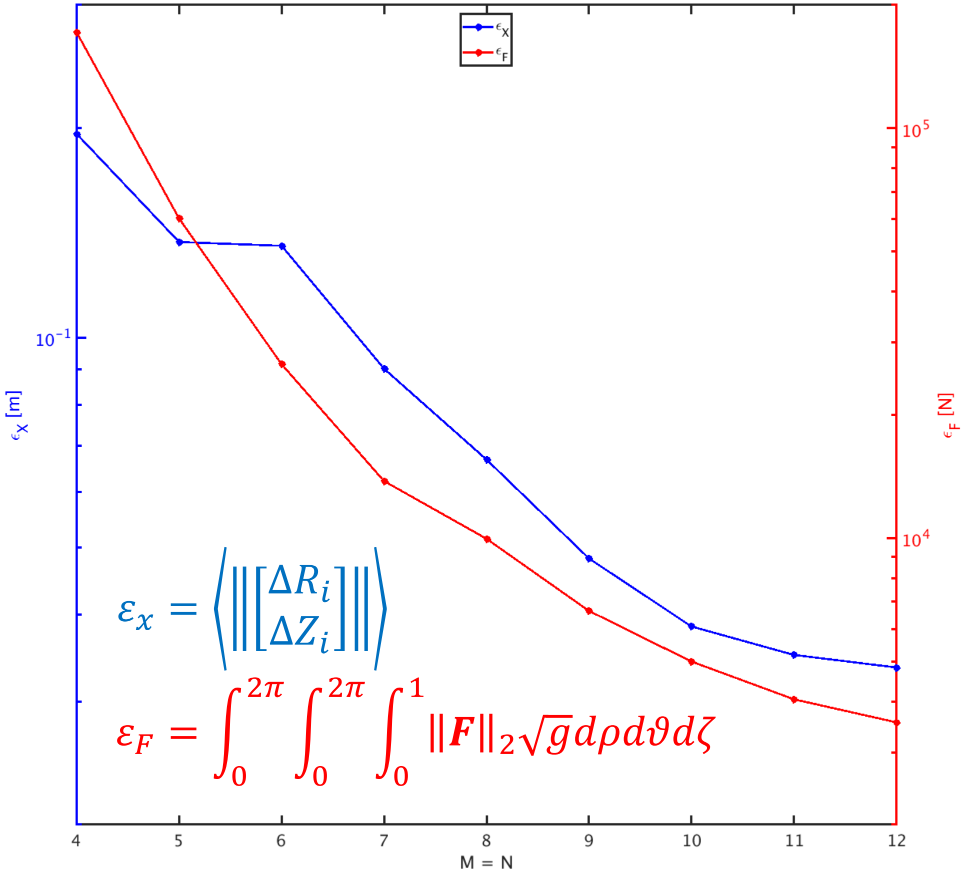
dimension ≈ 2×10^5

dimension ≈ 5×10^3

Error: Heliotron $\langle\beta\rangle \approx 2\%$



$$\frac{\|\boldsymbol{F}\|}{\|\boldsymbol{\nabla} p(\rho = 0.5)\|}$$



$$\varepsilon_x = \left\langle \left\| \begin{bmatrix} \Delta R_i \\ \Delta Z_i \end{bmatrix} \right\| \right\rangle$$

$$\varepsilon_F = \int_0^{2\pi} \int_0^{2\pi} \int_0^{1} \|\boldsymbol{F}\|_2 \sqrt{g}\, d\rho\, d\vartheta\, d\zeta$$

Equilibrium Perturbations

- 1^{st}–order Taylor expansion about an equilibrium solution:

$$\cancelto{0}{\boldsymbol{f}(\boldsymbol{x}+\Delta\boldsymbol{x},\boldsymbol{c}+\Delta\boldsymbol{c})} = \cancelto{0}{\boldsymbol{f}(\boldsymbol{x},\boldsymbol{c})} + \frac{\partial\boldsymbol{f}}{\partial\boldsymbol{x}}\Delta\boldsymbol{x} + \frac{\partial\boldsymbol{f}}{\partial\boldsymbol{c}}\Delta\boldsymbol{c}$$

$$\Delta\boldsymbol{x} = -\left(\frac{\partial\boldsymbol{f}}{\partial\boldsymbol{x}}\right)^{-1}\frac{\partial\boldsymbol{f}}{\partial\boldsymbol{c}}\Delta\mathbf{c}$$

$\boldsymbol{c}$ = input parameters:
- pressure profile
- boundary modes
- etc.

- The new equilibrium solution for any perturbation $\Delta\mathbf{c}$ is trivial to approximate:

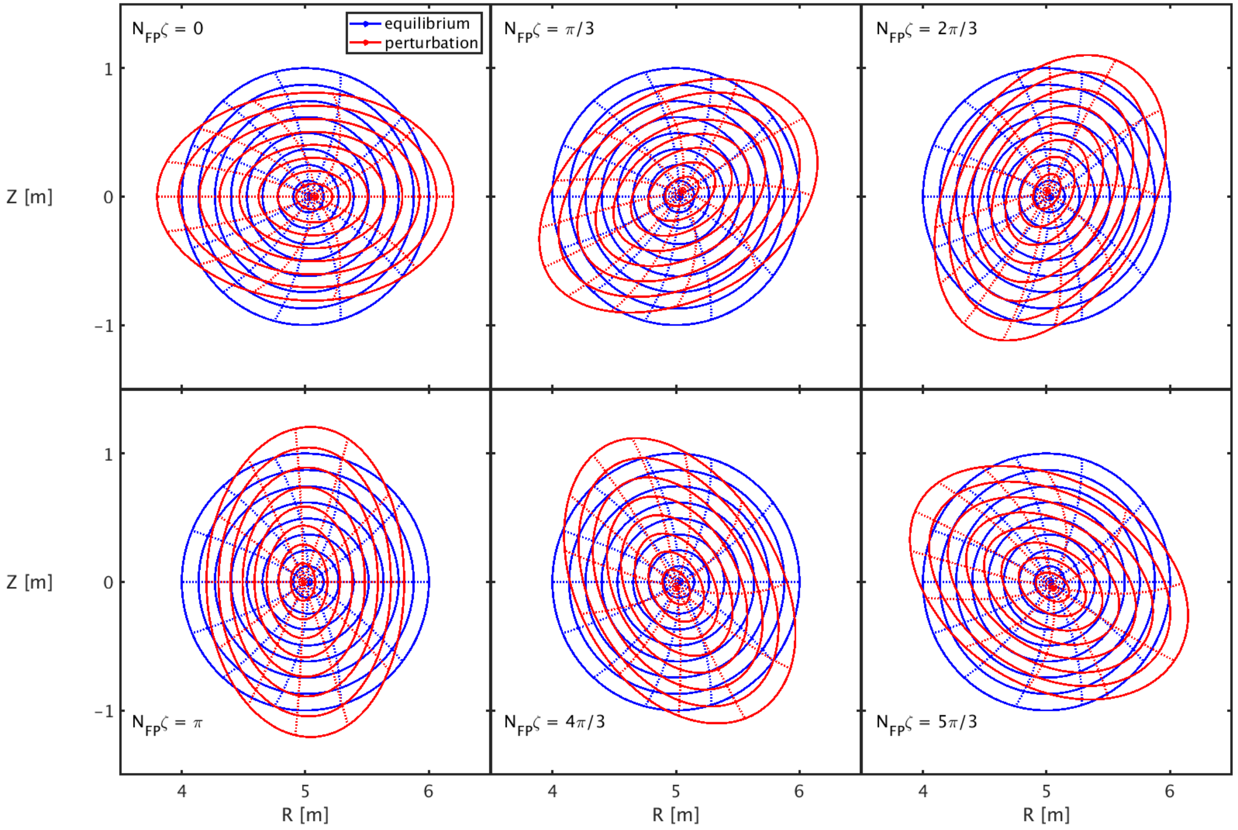
$$\boldsymbol{x}^* = \boldsymbol{x} + \Delta\boldsymbol{x}$$

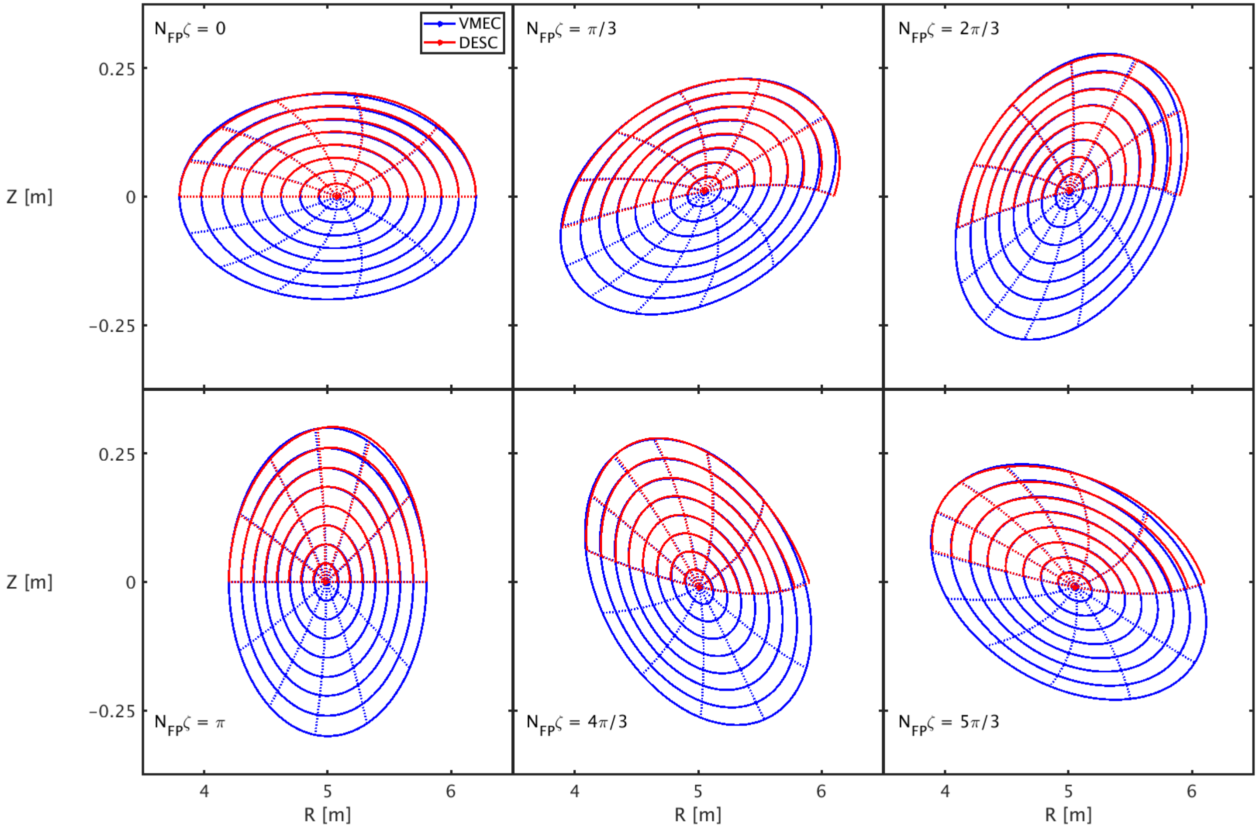
- Can be used to find solution branches in parameter space
- Has been extended to 2^{nd}–order approximations

Jacobian matrix $\left(\frac{\partial\boldsymbol{f}}{\partial\boldsymbol{x}}\right)^{-1}$ was already computed to solve equilibrium

3D Boundary Perturbation

- Perturbing an axisymmetric solution gives an accurate stellarator equilibrium!





Quasi-Symmetric Perturbations

- Define a measure of quasi-symmetry (no Boozer coordinate transform needed!)

$$\boldsymbol{g}(\boldsymbol{x},\boldsymbol{c}) \equiv \boldsymbol{\nabla}\psi \times \boldsymbol{\nabla}B \cdot \boldsymbol{\nabla}(\boldsymbol{B}\cdot\boldsymbol{\nabla}B)$$

- 1st –order Taylor expansion about an equilibrium QS solution:

$$\boldsymbol{g}(\boldsymbol{x} + \cancelto{0}{\Delta\boldsymbol{x}, \boldsymbol{c} + \Delta\boldsymbol{c})} = \boldsymbol{g}\cancelto{0}{(\boldsymbol{x},\boldsymbol{c})} + \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{x}}\Delta\boldsymbol{x} + \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{c}}\Delta\boldsymbol{c}$$

$$= \left[-\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{x}}\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^{-1}\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{c}} + \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{c}}\right]\Delta\boldsymbol{c}$$

- Resulting eigenvalue problem: $\boldsymbol{G}\Delta\boldsymbol{c} = \boldsymbol{0}$
- Eigenvectors of $\boldsymbol{G}$ corresponding to $\lambda = 0$ are perturbations that preserve QS

Summary

DESC is a stellarator equilibrium solver with the following advantages:

- Properly resolves the magnetic axis
- Minimizes the system dimensionality
- Gives a global solution (no interpolation between flux surfaces)
- Avoids numerical issues at rational surfaces
- Allows for perturbations to easily search the equilibrium solution space
- Easy to use and extend the code for individual applications
- Designed for stellarator optimization: automatic differentiation, GPUs, etc.

Future Development

- Improved performance, user interface, documentation
- Quasi-symmetry optimization
- Ideal MHD stability calculations
- Free-boundary equilibria
- Magnetic islands & stochastic regions

Repository: https://github.com/ddudt/DESC

Publication: D. W. Dudt, and E. Kolemen, Phys. Plasmas **27** 102513 (2020)

References

[1] D. W. Dudt, and E. Kolemen, Phys. Plasmas **27** 102513 (2020).

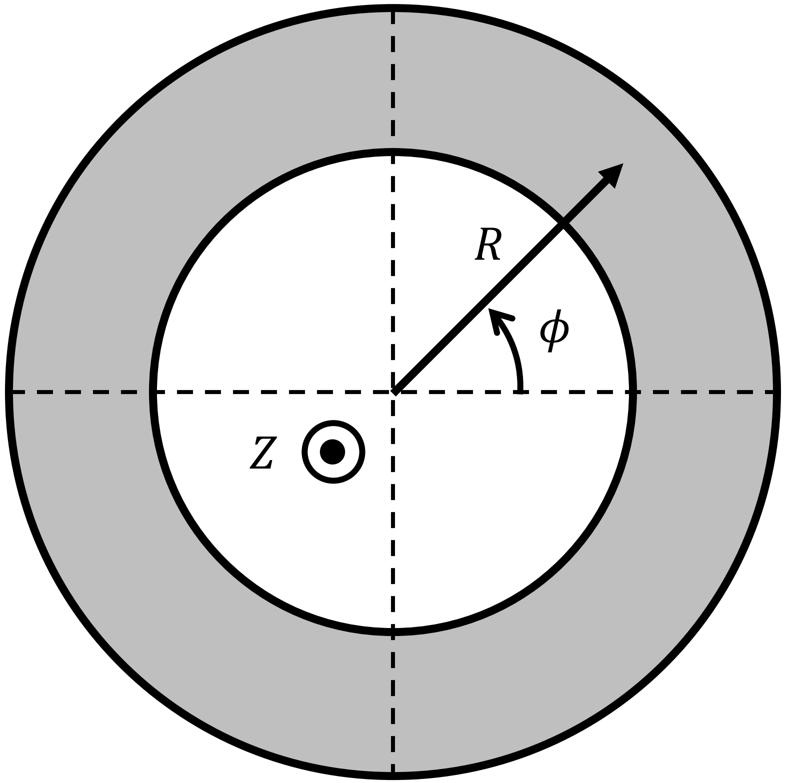
[2] F. Zernike, Mon. Not. R. Astron. Soc. **94**, 377–384 (1934).

[3] W. D. D'haeseleer, W. N. G. Hitchon, J. D. Callen, and J. L. Shohet, *Flux Coordinates and Magnetic Field Structure*, Springer Series in Computational Physics, edited by R. Glowinski, M. Holt, P. Hut, H. B. Keller, J. Killeen, S. A. Orszag, and V. V. Rusanov (Springer-Verlag, 1991).

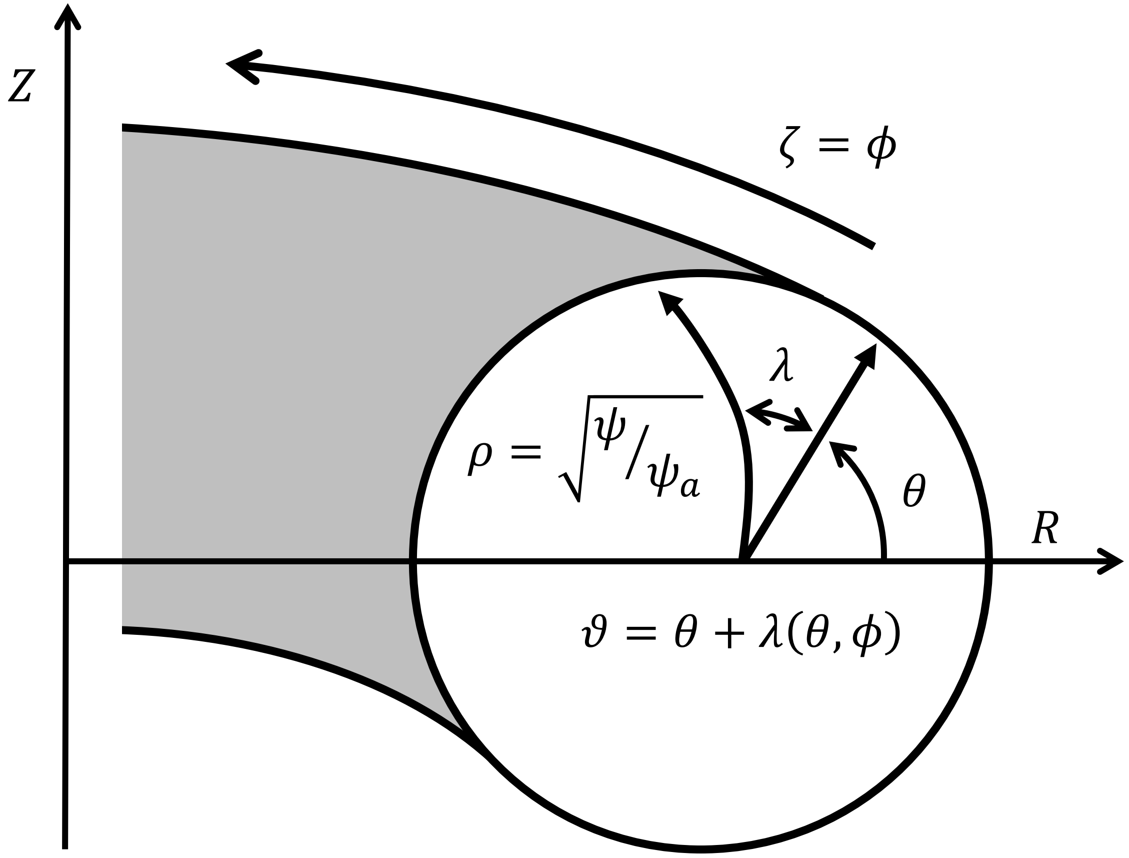
[4] S. P. Hirshman and J. C. Whitson, Phys. Fluids **26**, 3553–3568 (1983).

Bonus Slides

PEST[1] Flux Coordinates



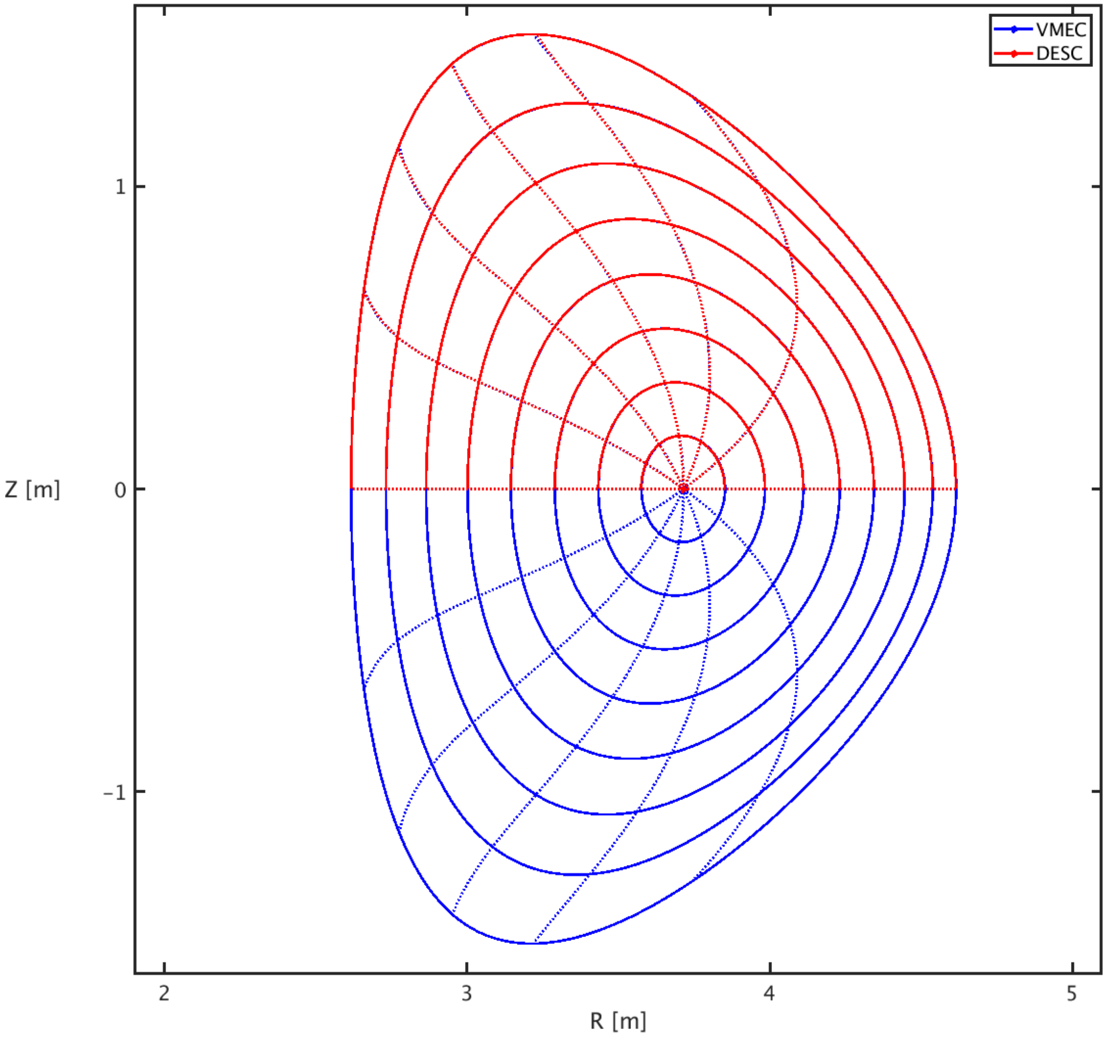
toroidal coordinates: (R, ϕ, Z)

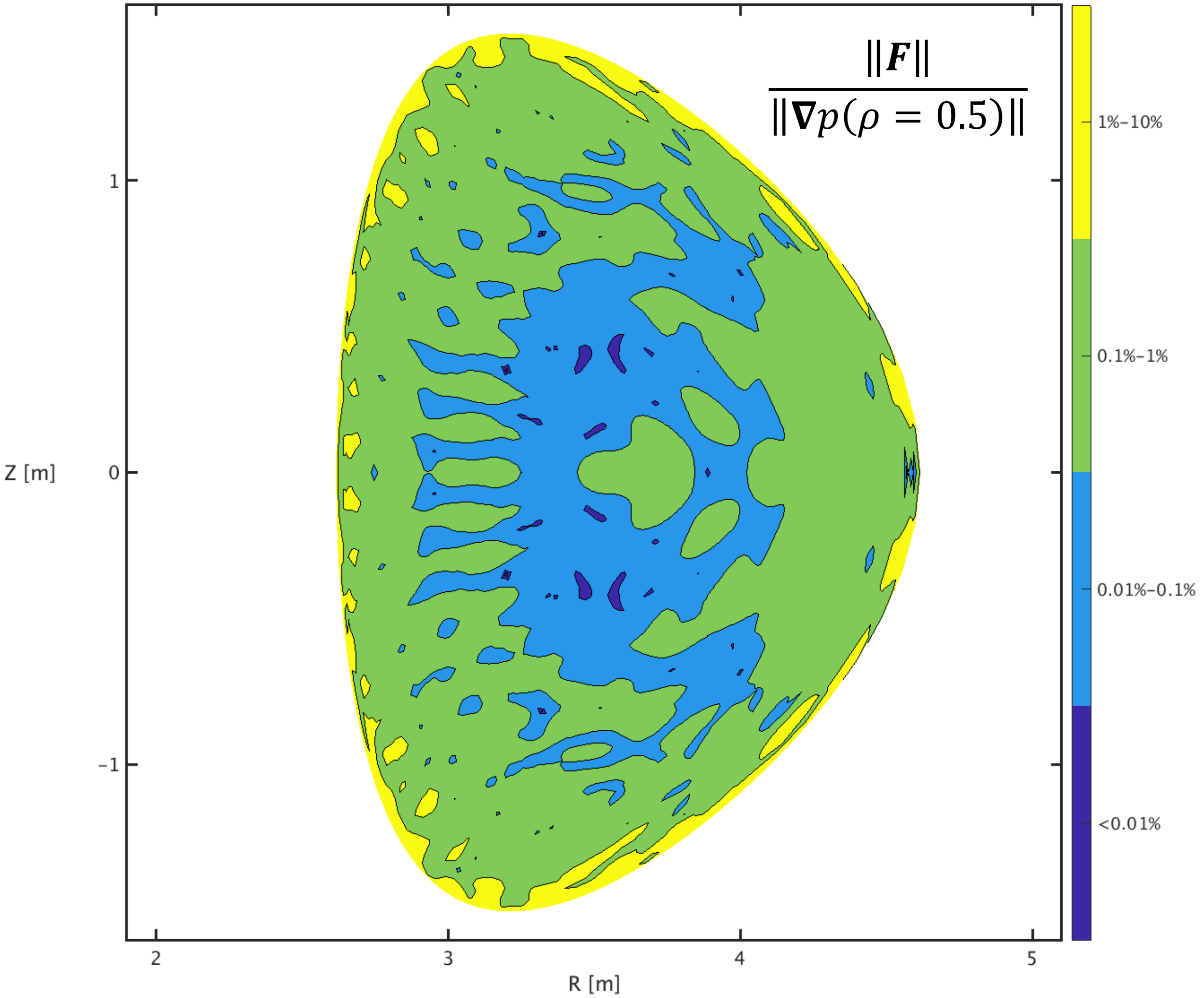


straight field-line coordinates: (ρ, ϑ, ζ)

[1] R. C. Grimm, J. M. Greene, and J. L. Johnson (Academic Press, Inc, New York, 1976) pp. 253–280.

Axisymmetric Results: “D-shape” $\langle\beta\rangle \approx 3\%$



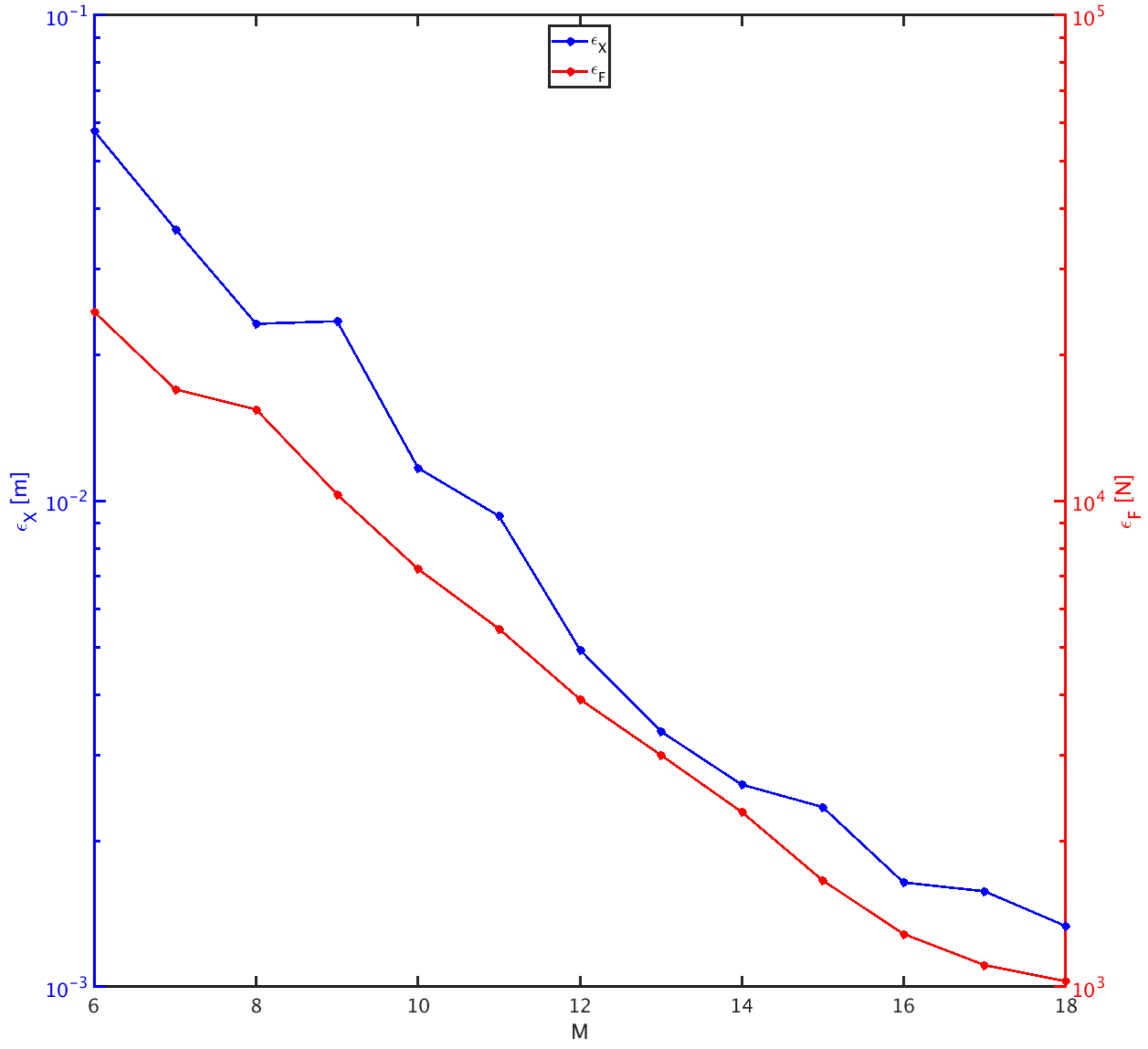


Axisymmetric Results: “D-shape” $\langle\beta\rangle \approx 3\%$

- Accuracy metrics:

$$\varepsilon_x = \left\langle \left\| \begin{bmatrix} \Delta R_i \\ \Delta Z_i \end{bmatrix} \right\| \right\rangle$$

$$\varepsilon_F = \int_0^{2\pi} \int_0^{2\pi} \int_0^{1} \|\boldsymbol{F}\|_2 \sqrt{g}\, d\rho\, d\vartheta\, d\zeta$$



Boundary Condition: Magnetic Axis

- An analytic function expanded near the origin of a disc must have a real Fourier series of the form[1,2]:

$$f(\rho,\vartheta) = \sum_{m} \rho^{m}\left(a_{m,0} + a_{m,2}\rho^{2} + a_{m,4}\rho^{4} + \cdots\right)\cos(m\vartheta) \\ + \sum_{m} \rho^{m}\left(b_{m,0} + b_{m,2}\rho^{2} + b_{m,4}\rho^{4} + \cdots\right)\sin(m\vartheta)$$

- The Zernike polynomials inherently satisfy this condition!
  - Reduces the number of variables by eliminating the unnecessary high-frequency modes near the axis
  - No additional boundary condition equations need to be solved

[1] J. P. Boyd and F. Yu, J. Comput. Phys. **230**, 1408–1438 (2011).

[2] H. R. Lewis and P. M. Bellan, J. Math. Phys. **31**, 2592–2596 (1990).

Boundary Condition: Last Closed Flux Surface

- Fixed-boundary surface is given as: $R^b = R^b(\theta, \phi), Z^b = Z^b(\theta, \phi)$
- Last closed flux surface is evaluated as: $R|_{\rho=1} = R(\vartheta, \zeta), Z|_{\rho=1} = Z(\vartheta, \zeta)$
- Introduce $\lambda(\theta, \phi)$ to convert between coordinates: $\vartheta = \theta + \lambda(\theta, \phi), \zeta = \phi$

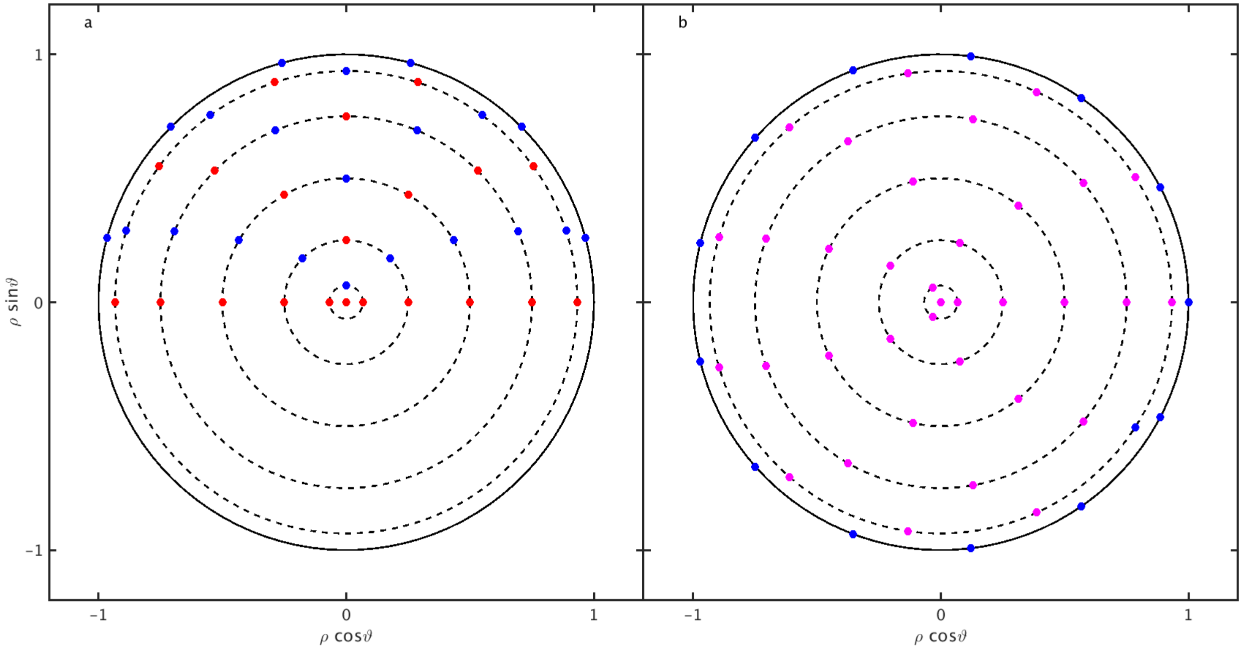
$$R\Big|_{\rho=1} = \sum\nolimits_{m,n} R_{mn} \mathcal{F}(\vartheta, \zeta) \quad \Longrightarrow \quad R\Big|_{\rho=1} = \sum\nolimits_{m,n} \tilde{R}_{mn} \mathcal{F}(\theta, \phi)$$

$$Z\Big|_{\rho=1} = \sum\nolimits_{m,n} Z_{mn} \mathcal{F}(\vartheta, \zeta) \quad \Longrightarrow \quad Z\Big|_{\rho=1} = \sum\nolimits_{m,n} \tilde{Z}_{mn} \mathcal{F}(\theta, \phi)$$

- Boundary condition: $\sum_l \tilde{R}_{lmn} = R^b_{mn}$ $\qquad$ $\sum_l Z_{lmn} = \tilde{Z}^b_{mn}$

Collocation Nodes

- The computational grid is a finite set of discrete points $(\rho_i, \vartheta_i, \zeta_i)$
- The force balance errors $f_\rho(\rho, \vartheta, \zeta)$ & $f_\beta(\rho, \vartheta, \zeta)$ are minimized at these nodes
- The equilibrium solution is still valid everywhere, and spectral collocation theory predicts *global* convergence
- Great flexibility in choosing the nodes
  - Control grid refinement
  - Avoid rational surfaces



Continuation Methods

1. Perturbations to solve for complex equilibria:
   - vacuum solution → *pressure perturbation* → finite-β solution
   - axisymmetric tokamak → *boundary perturbation* → 3D stellarator
2. Perturbations to optimize for quasi-symmetry:
   - axisymmetric tokamak → *boundary perturbation* → QA stellarator
   - non-QS equilibrium → *perturb some inputs* → more-QS equilibrium

Order of ODE to Solve

Order of Derivatives	Variables	Equations
0	R, Z	
1	$\partial_i R, \partial_i Z \rightarrow \boldsymbol{B}$	$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$
2	$\partial_{ij} R, \partial_{ij} Z \rightarrow \boldsymbol{J}$	$\boldsymbol{J} \times \boldsymbol{B} = \boldsymbol{\nabla} p$
3	$\partial_{ijk} R, \partial_{ijk} Z$	$\boldsymbol{\nabla} \cdot \boldsymbol{J} = 0$

- The equilibrium equations are a 2nd-order ODE
- Rational surface issues arise at the next higher level with $\boldsymbol{\nabla} \cdot \boldsymbol{J} = 0$

Equilibrium Example Inputs

Axisymmetric
“D-shaped” Tokamak

$$\begin{aligned} R^b &= 3.51 - \cos\theta + 0.106\cos 2\theta \\ Z^b &= 1.47\sin\theta + 0.16\sin 2\theta \\ \iota &= 1 - 0.67\rho^2 \\ p &= 1.65\times 10^3\left(1-\rho^2\right)^2 \\ \psi_a &= 1 \end{aligned}$$

Non-Axisymmetric
high-β Heliotron

$$\begin{aligned} R^b &= 10 - \cos\theta - 0.3\cos(\theta - 19\phi) \\ Z^b &= \sin\theta - 0.3\sin(\theta - 19\phi) \\ \iota &= 1.5\rho^2 + 0.5 \\ p &= 3.4\times 10^3\left(1-\rho^2\right)^2 \\ \psi_a &= 1 \end{aligned}$$

Perturbation Example Inputs

Axisymmetric

Non-Axisymmetric

$$M = 6, N = 2$$

Axisymmetric:

$$\begin{aligned} R^b &= 5 - \cos\theta \\ Z^b &= \sin\theta \\ \iota &= 1.618 \\ p &= 0 \\ \psi_a &= 1 \end{aligned}$$

Non-Axisymmetric:

$$\begin{aligned} R^b &= 5 - \cos\theta - 0.2\cos(\theta - \phi) \\ Z^b &= \sin\theta - 0.2\sin(\theta - \phi) \\ \iota &= 1.618 \\ p &= 0 \\ \psi_a &= 1 \end{aligned}$$