Efficient Stellarator Optimization and Analysis with DESC

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APS DPP October 21, 2022

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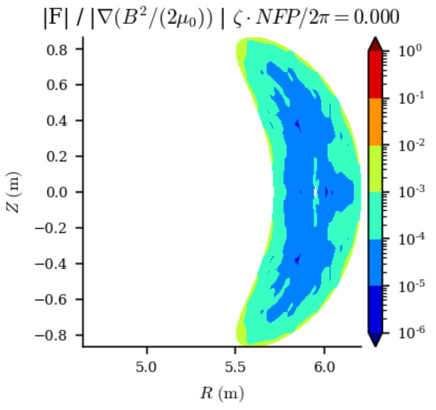
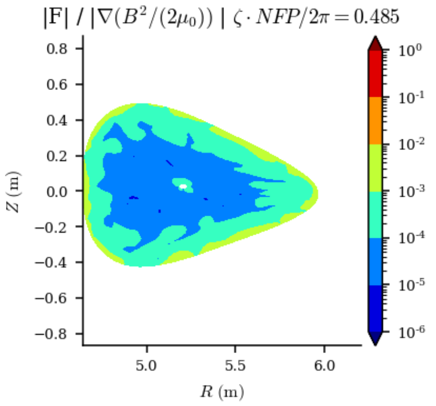
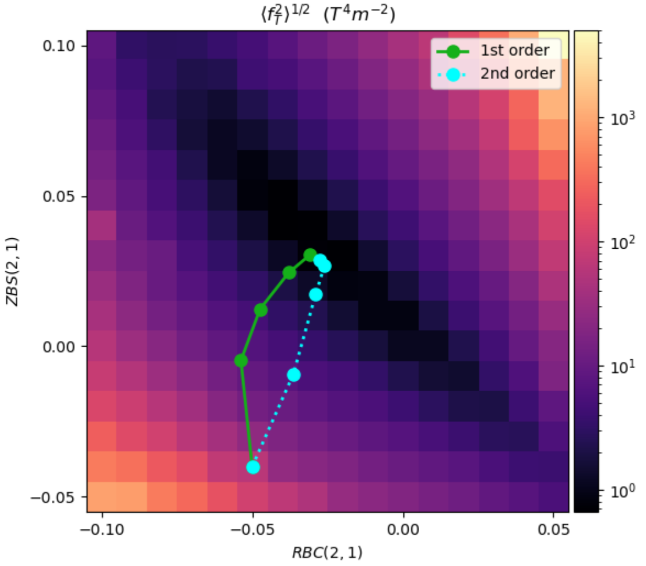
DESC is a new tool for stellarator optimization

Accurate Equilibria

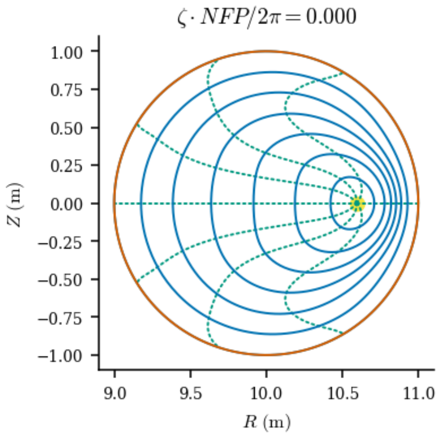


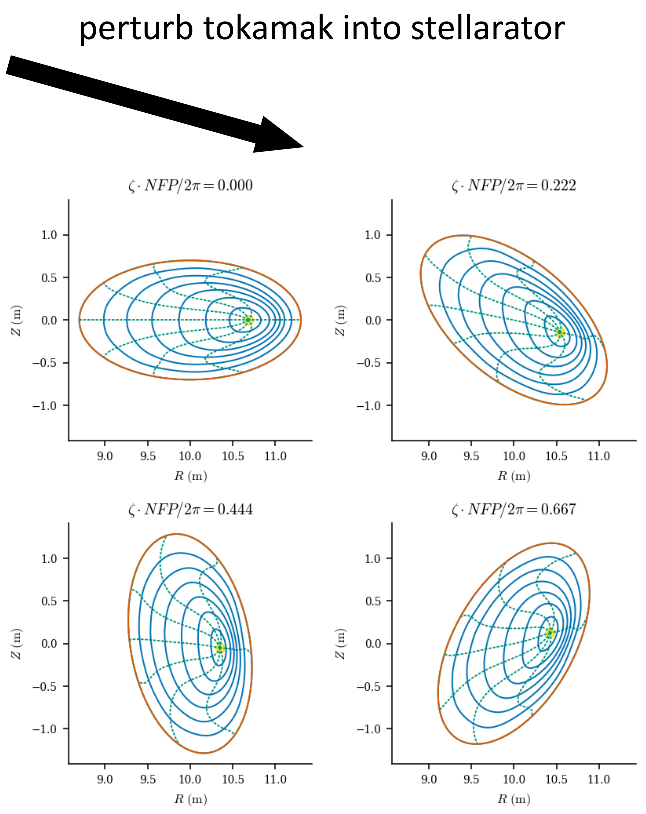


Fast Optimization



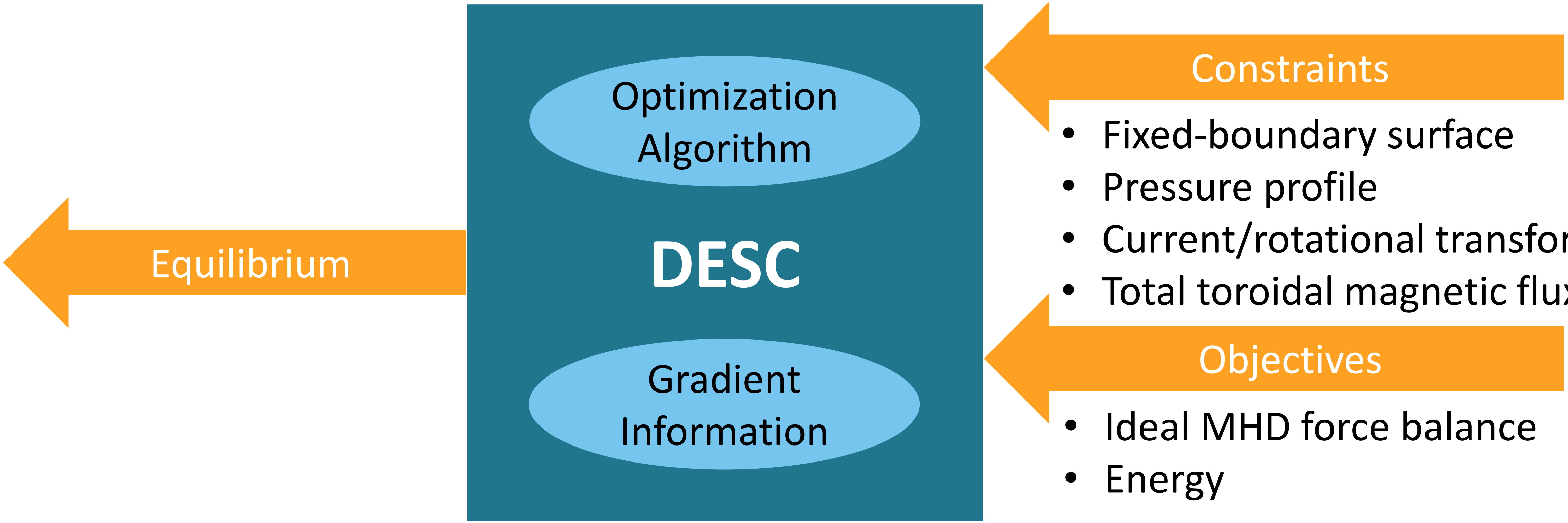
Phase-Space Connections





- Stellarator equilibria are complicated
- Design space is much larger than tokamaks

A flexible stellarator optimization suite



Constraints
- Fixed-boundary surface
- Pressure profile
- Current/rotational transform
- Total toroidal magnetic flux

Objectives
- Ideal MHD force balance
- Energy

A flexible stellarator optimization suite

DESC

Optimization Algorithm

Gradient Information

Optimized Stellarator

Constraints

- Ideal MHD force balance
- Equilibrium profiles
- Some boundary modes

Objectives

- Quasi-symmetry
- Mercier stability
- Aspect ratio
- etc.

Why do we need *another* stellarator code?

Equilibrium solvers: VMEC, NEAR, PIES, HINT, SPEC, GVEC, etc.

Optimization codes: STELLOPT, ROSE, WISTELL, SIMSOPT, etc.

1. Better understand the solution space of stellarator equilibria
2. Integrate the equilibrium solver with optimization tools
3. Avoid Jacobian approximations, near-axis expansions, low-β expansions, etc.
4. Use modern numerical methods and scientific computing practices

Developed with the following design principles:

1. **Simple user interface**
   - Open-source Python code
   - Well documented
   - High test coverage
   - Easy to install
2. **Local error quantification**
   - Pseudo-spectral (collocation) methods
3. **Properly resolve the magnetic axis**
   - Global basis functions
   - Zernike polynomials
4. **Exact derivatives of all objectives**
   - Automatic differentiation
5. **Hardware agnostic**
   - Run on CPUs, GPUs, and TPUs
6. **Extendable to new applications**
   - Modular & flexible code structure

Zernike spectral basis inherently satisfies boundary conditions at the magnetic axis

spectral coefficients

Zernike polynomials

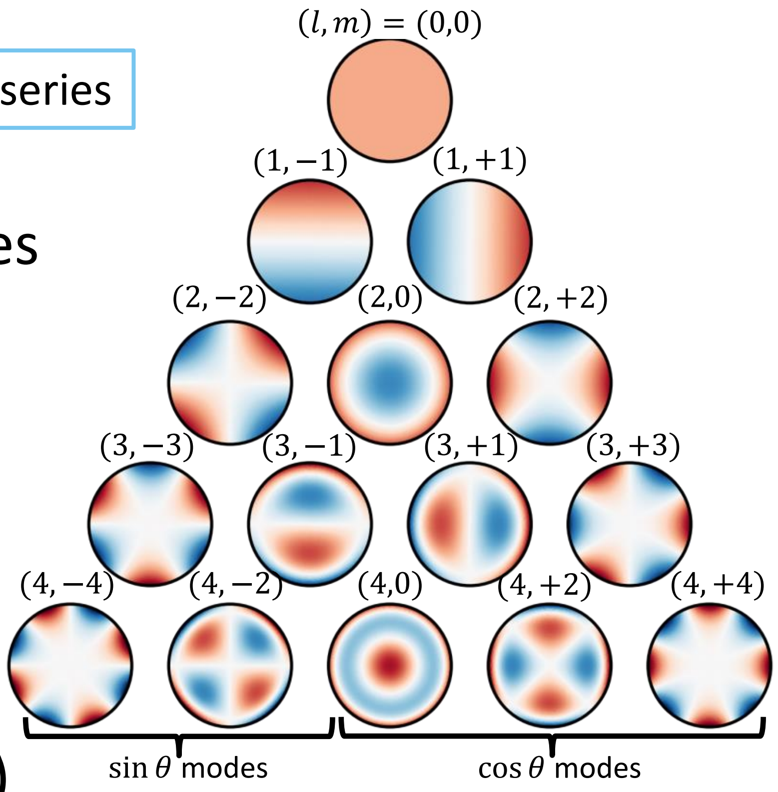
$$X(\rho,\theta,\zeta) = \sum_{lmn} X_{lmn} \mathcal{Z}_l^m(\rho,\theta)\mathcal{F}^n(\zeta)$$

Fourier series

- Periodic boundary conditions for poloidal & toroidal angles
- Satisfies analyticity conditions at the magnetic axis:

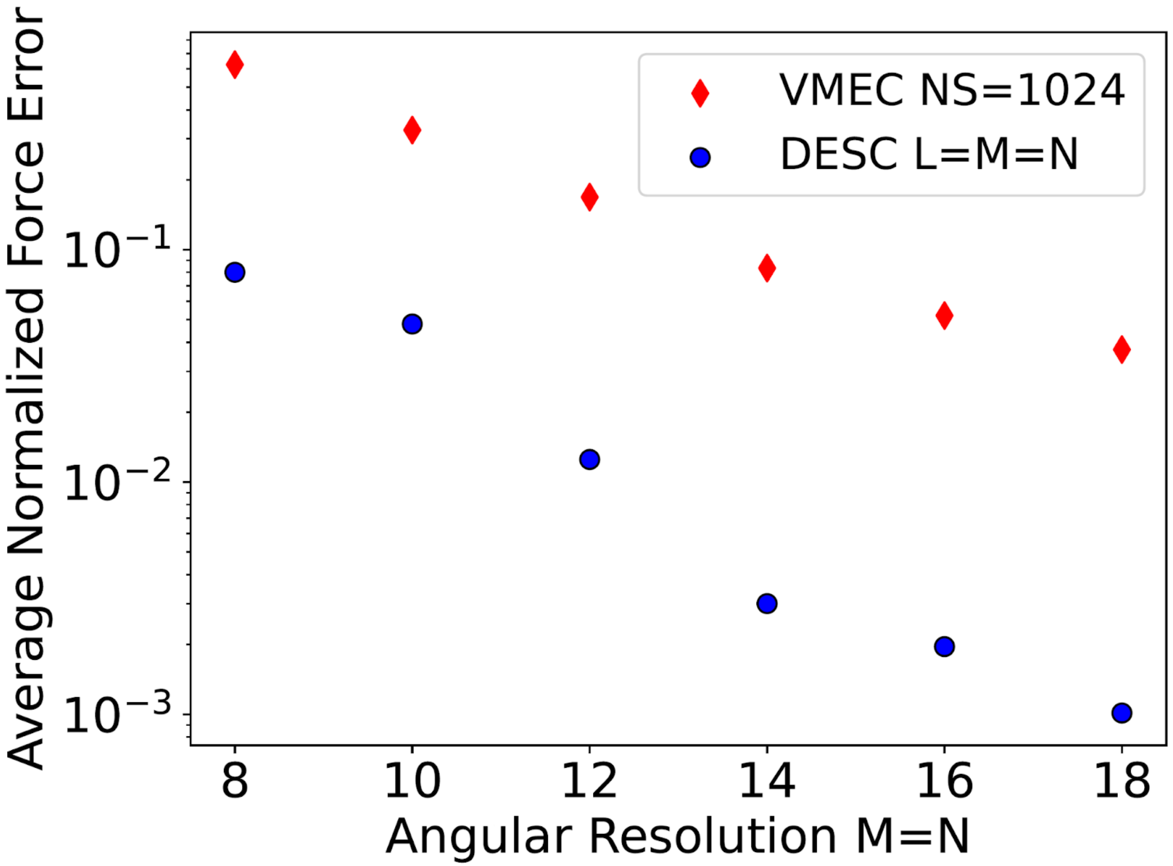
$$f(\rho,\theta) = \sum_m \rho^m\left(a_{m,0} + a_{m,2}\rho^2 + \cdots\right)\cos(m\theta) + \sum_m \rho^m\left(b_{m,0} + b_{m,2}\rho^2 + \cdots\right)\sin(m\theta)$$

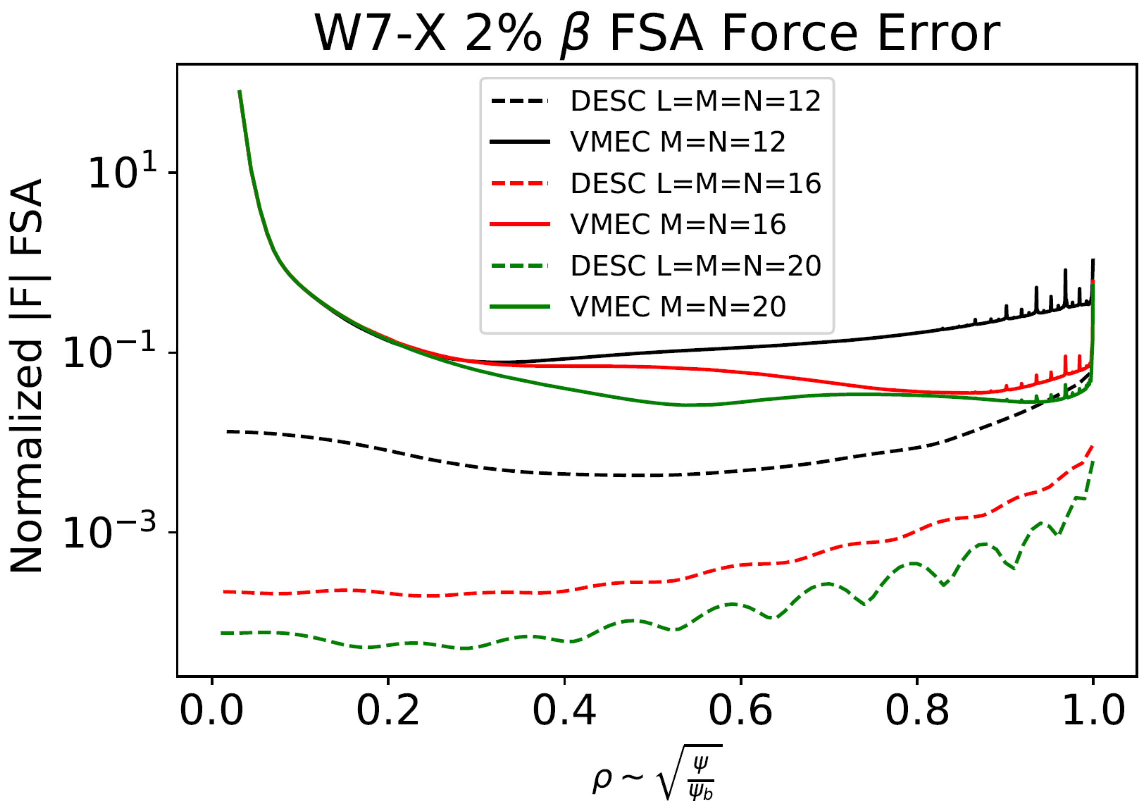
- Exponential convergence (if solution exists and is smooth)



Boyd et al., *J. Comput. Phys.* (2011)
Lewis et al., *J. Math. Phys.* (1990)

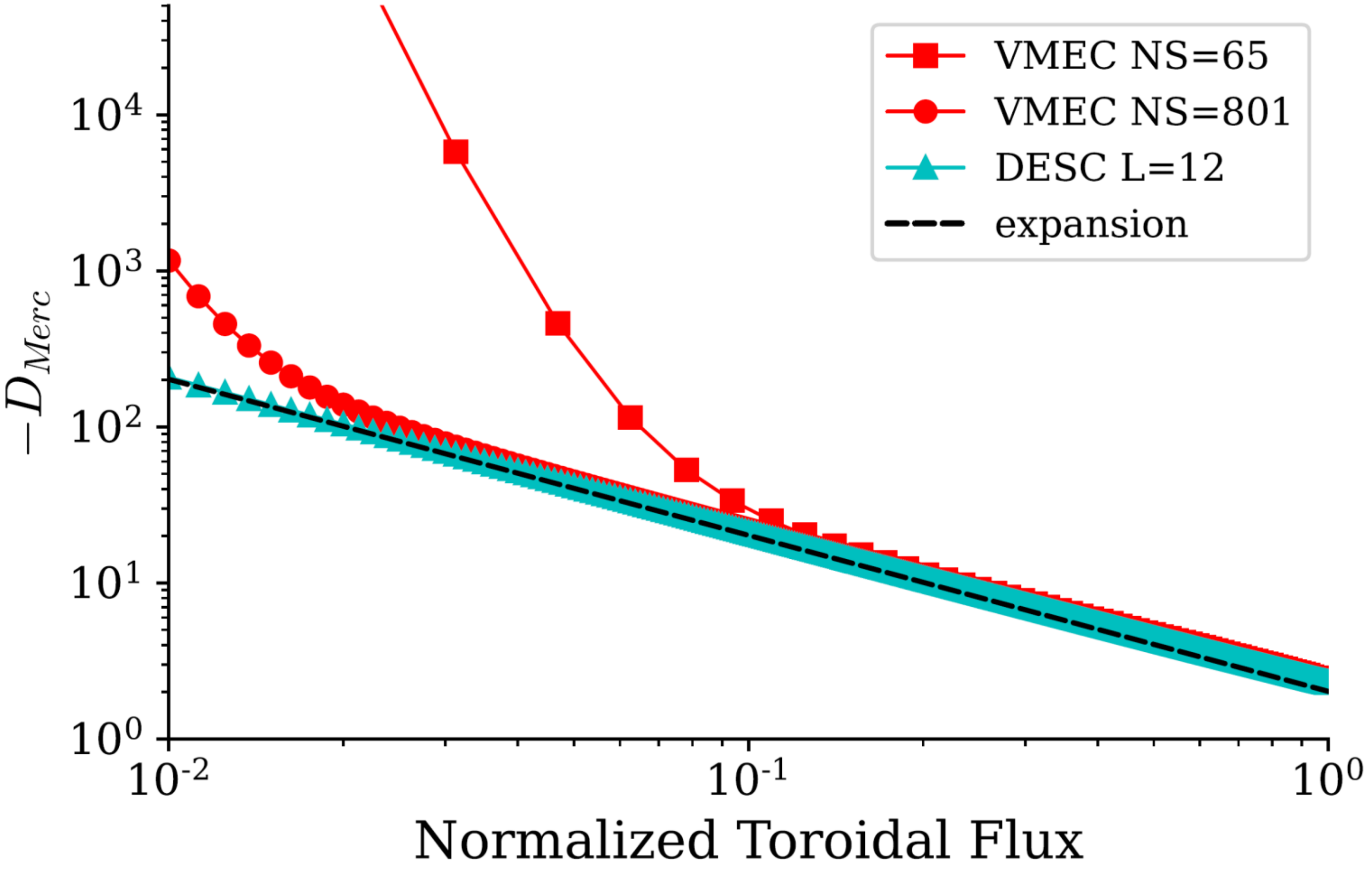
Spectral methods yield more accurate equilibrium solutions





Hirshman & Whitson, *Phys. Fluids* (1983)

Accurately resolving the magnetic axis is important for stability calculations



VMEC requires high radial resolution to resolve axis

<u>Run times:</u>

- DESC = 0.2 GPU-hours (NVIDIA A100)
- VMEC = 5.2 CPU-hours (AMD Opteron 6276)

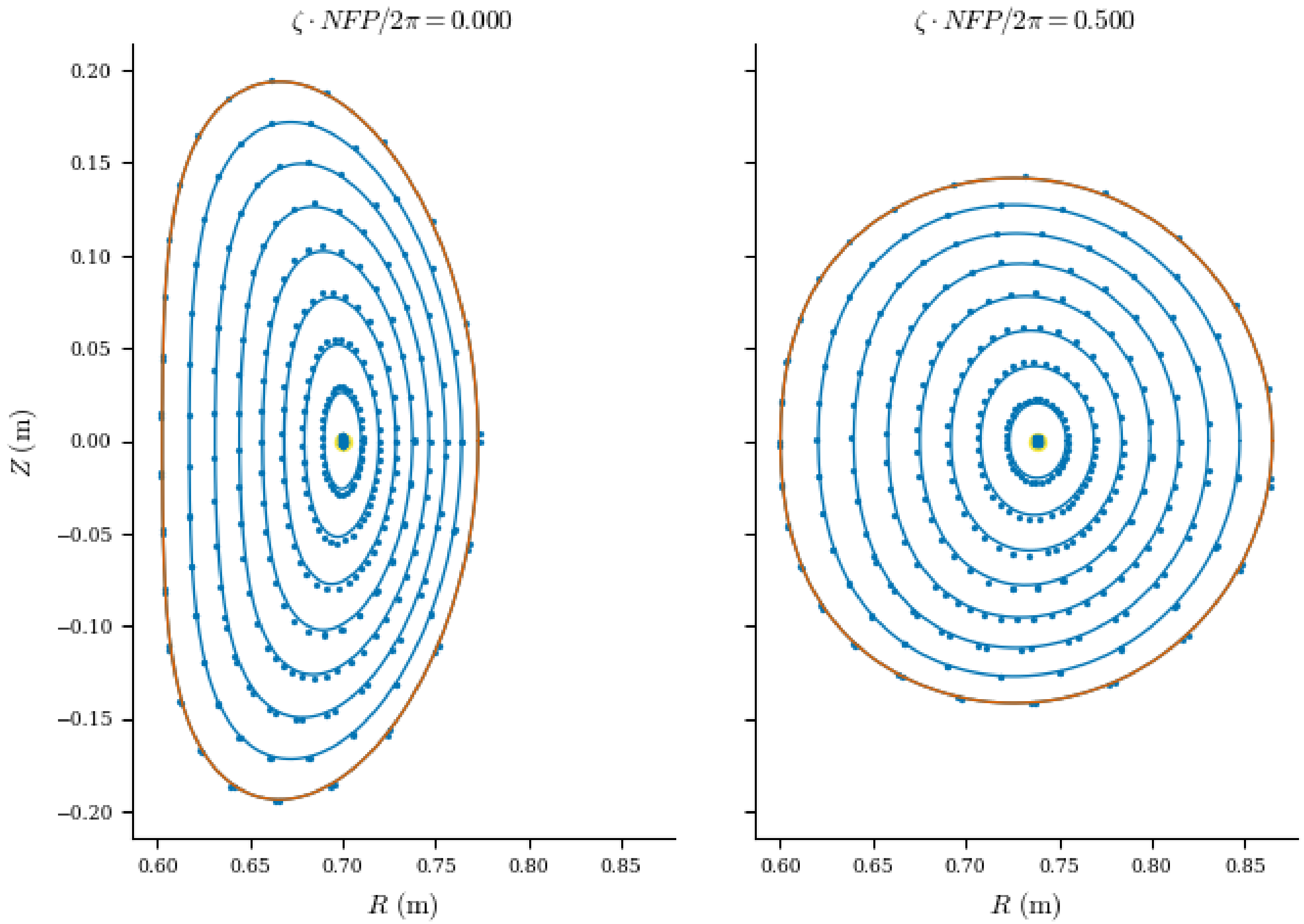
Landreman & Sengupta, *J. Plasma Phys.* (2019)

Extended to free-boundary equilibria

<u>Algorithms:</u>

- NESTOR implemented
- BIEST in progress
- Testing other methods

- Vacuum solution agrees with field-line tracing
- Benchmarked against VMEC



Merkel, *J. Comp. Phys.* (1986)
Malhotra et al., *J. Comp. Phys.* (2019)

Novel boundary conditions to better parameterize stellarator design space

<u>Conventional boundary condition:</u>

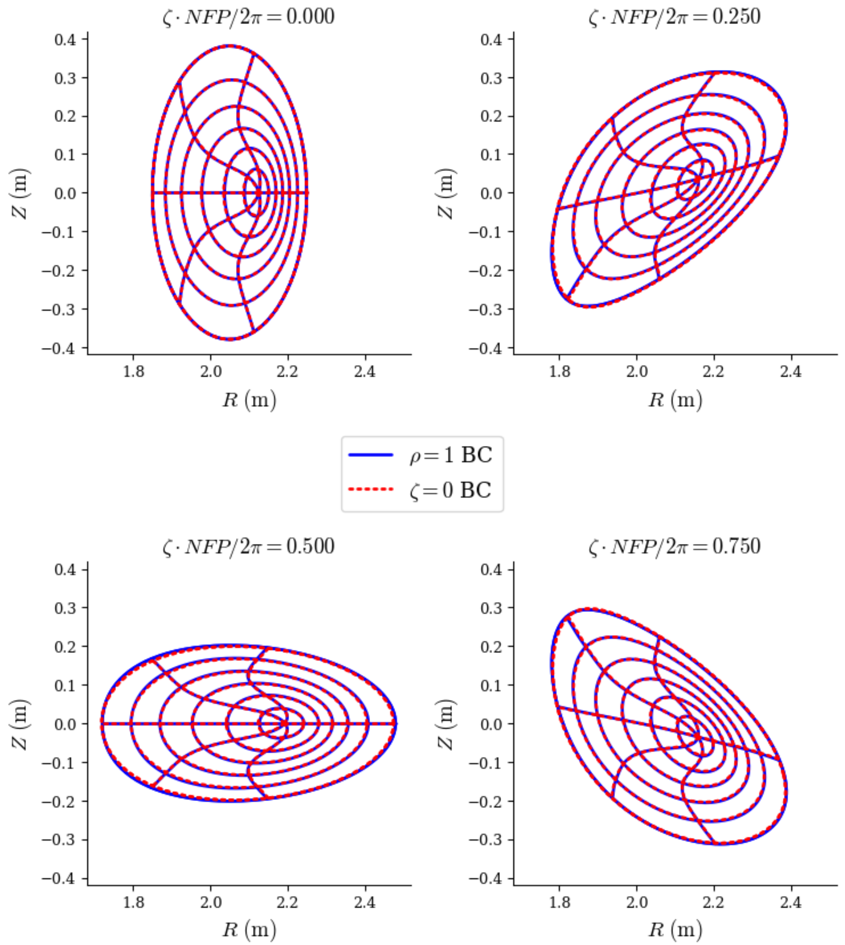
Specify shape of the last closed flux surface at $\rho = 1$

- Do equilibria with nested flux surfaces exist?

<u>Poincarè boundary condition:</u>

Specify surfaces in the cross-section at $\phi = 0$

- Restrict solution space to nested flux surfaces
- Connects tokamaks and stellarators in phase space



Gradient computations are the bottleneck of traditional stellarator optimization

- $g(\boldsymbol{c})$ = cost function to be minimized; $\boldsymbol{c}$ = optimization variables
- Gradient descent optimization:

$$\boldsymbol{c}_{n+1} = \boldsymbol{c}_n - \gamma \nabla g(\boldsymbol{c}_n)$$

Finite Differences:

- Requires $\geq \dim(\boldsymbol{c})$ equilibrium solves
- Inaccurate and sensitive to step size

Adjoint methods:

- Not applicable to all objectives
- Laborious to implement

Efficient computing with the ease of Python

Automatic Differentiation (AD)

- Optimization requires derivative information
- Exact derivatives of arbitrary functions to any order

Just-In-Time (JIT) Compilation

- Comparable speed to C or Fortran compiled languages
- Hardware agnostic (CPU, GPU, TPU)

Requires specific code structure, but easy to implement: **`import jax.numpy as jnp`**

DESC optimization only requires a single equilibrium solve per iteration

1. Newton optimization step with equilibrium constraint

$$\boldsymbol{c}_{n+1} = \boldsymbol{c}_n + \Delta\boldsymbol{c}$$

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

Exact Jacobians known from automatic differentiation!

$\boldsymbol{f}$ = equilibrium constraint
$\boldsymbol{g}$ = optimization objective

$\boldsymbol{x}$ = equilibrium solution
$\boldsymbol{c}$ = optimization variables

2. Perturb equilibrium solution to reflect new parameters

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta\boldsymbol{x}$$

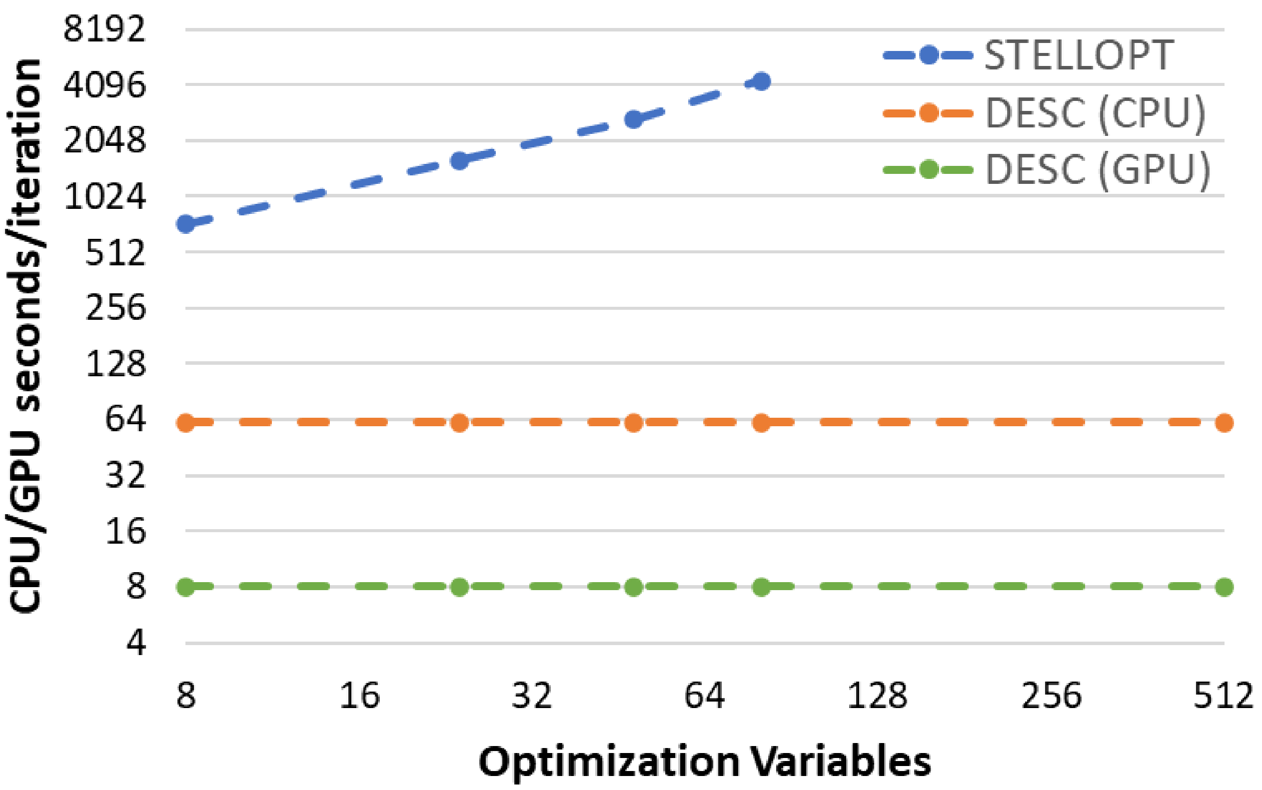
$$\Delta\boldsymbol{x} = -\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}_n}\right)^{-1}\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{c}_n}\Delta\mathbf{c}$$

3. Re-solve equilibrium from this close initial guess

$$\boldsymbol{x}_{n+1} = \text{argmin}_{\boldsymbol{x}}\left(\|\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{c}_{n+1})\|^2\right)$$

Only 1 “warm-start” equilibrium solve per optimization step!

Fast computations enable exploration of the large stellarator design space



- Finite differences scale unfavorably
- Parallelization can help reduce wall time, but not total resources
- GPU hardware is still improving

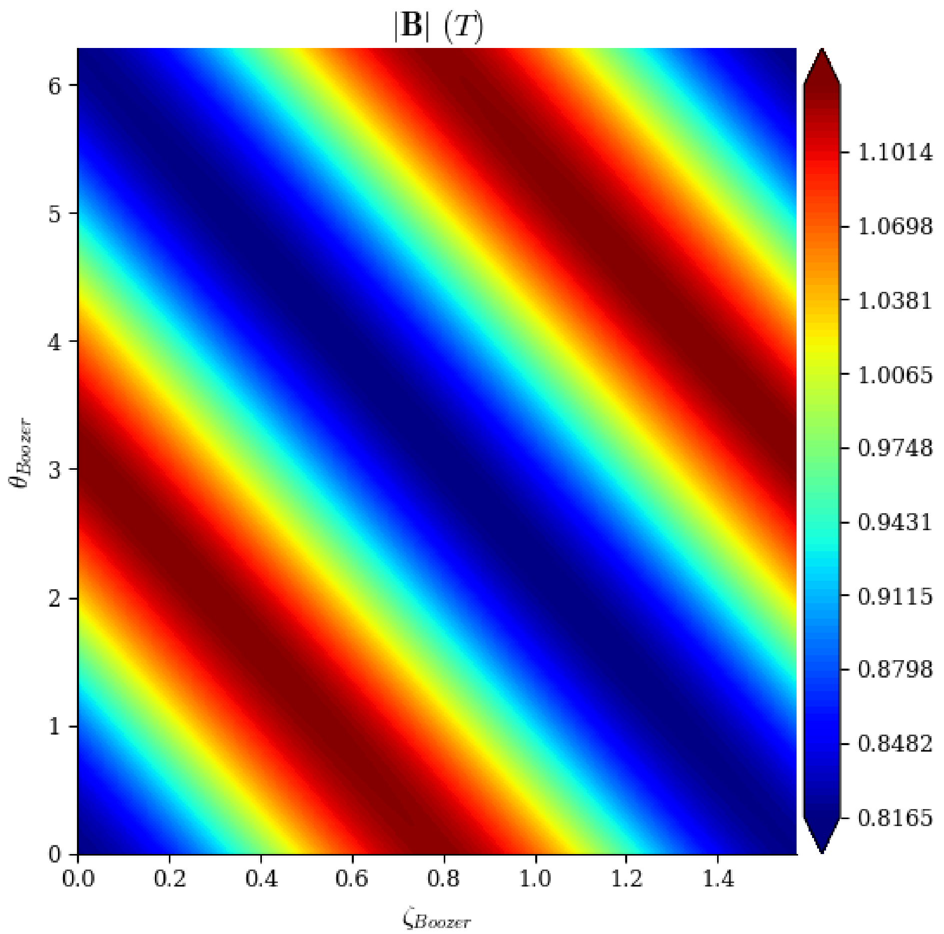
W7-X $\beta = 2\%; L = 24, M = N = 12$

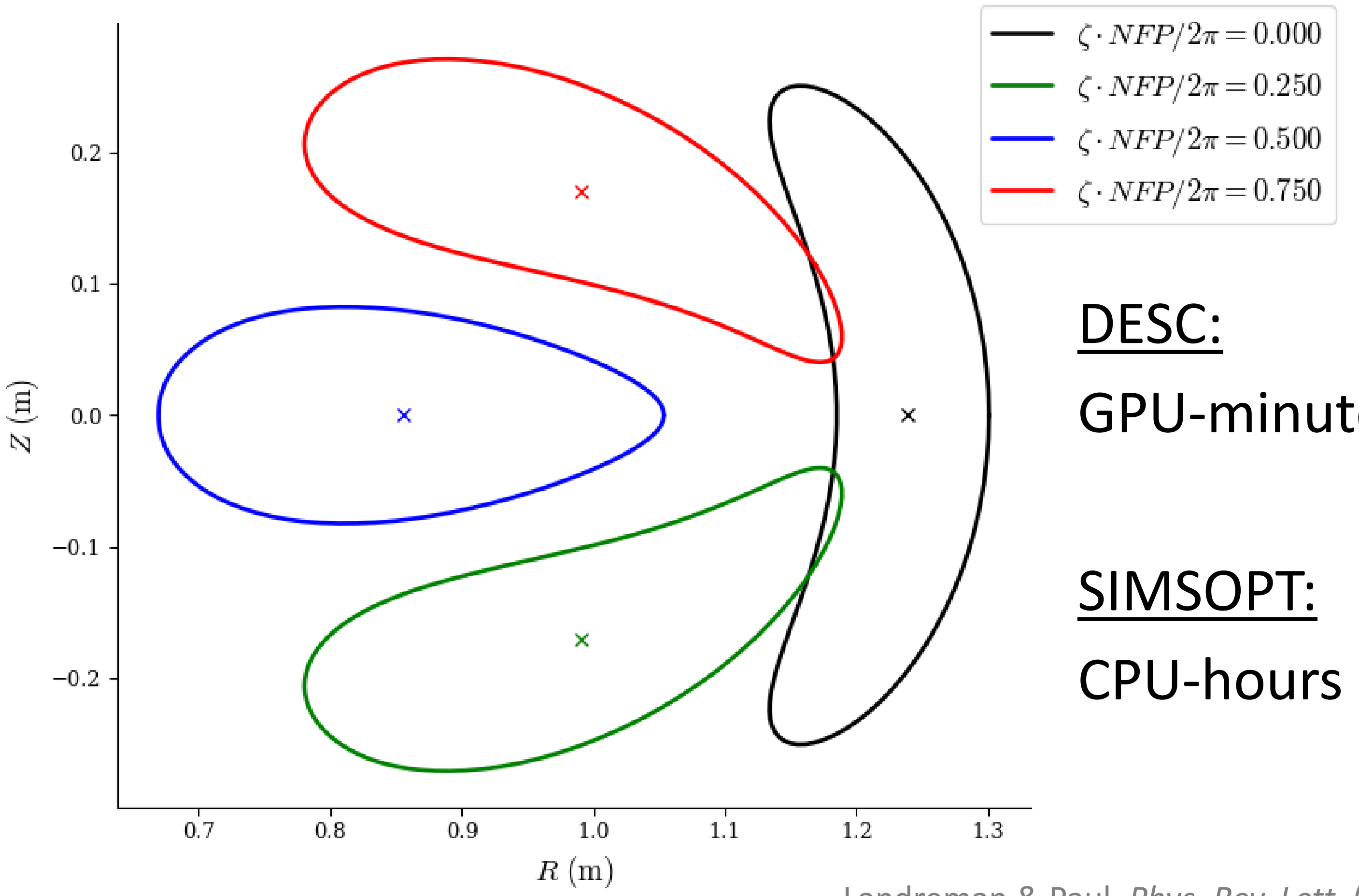
Hardware	Run Time
Intel Cascade Lake CPU	48 min
NVIDIA A100 GPU	20 min

Run optimizations in a few lines of Python code

```python
set_device("gpu")  # run on a GPU
eq = desc.io.load("path/to/initial/equilibrium.h5")
grid = LinearGrid(M=eq.M, N=eq.N, NFP=eq.NFP, rho=np.linspace(0.1, 1, 10))  # computation grid
objective = ObjectiveFunction((AspectRatio(target=8),  # target aspect ratio
    QuasisymmetryTwoTerm(helicity=(1, -eq.NFP), grid=grid, weight=2e-1)))  # optimize for QH
# optimize boundary modes with |m|,|n|<=5 (constrain boundary modes with |m|,|n|>5)
R_modes = np.vstack(([0, 0, 0],  # fix major radius
    eq.surface.R_basis.modes[np.max(np.abs(eq.surface.R_basis.modes), 1) > 5, :]))
Z_modes = eq.surface.Z_basis.modes[np.max(np.abs(eq.surface.Z_basis.modes), 1) > 5, :]
constraints = (ForceBalance(), FixBoundaryR(modes=R_modes), FixBoundaryZ(modes=Z_modes),
    FixPressure(), FixCurrent(), FixPsi())  # fix vacuum profiles
optimizer = Optimizer("lsq-exact")  # least-squares optimization algorithm
eq.optimize(objective, constraints, optimizer)  # run optimization
eq.save("path/to/optimal/solution.h5")
```

Can find “precise quasi-symmetry” & more





<u>DESC:</u>

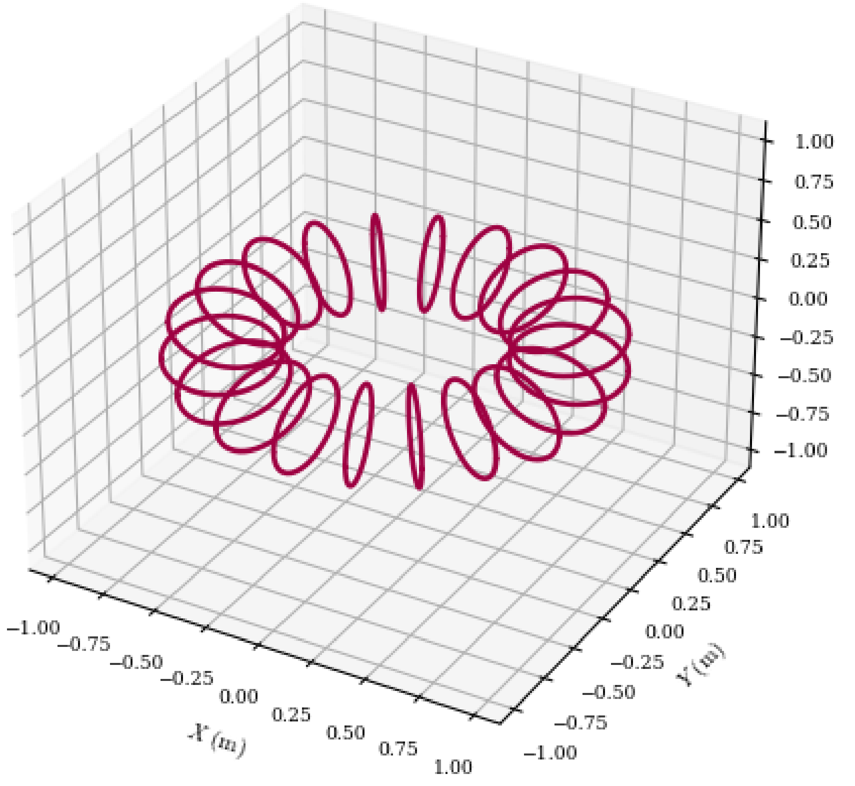
GPU-minutes

<u>SIMSOPT:</u>

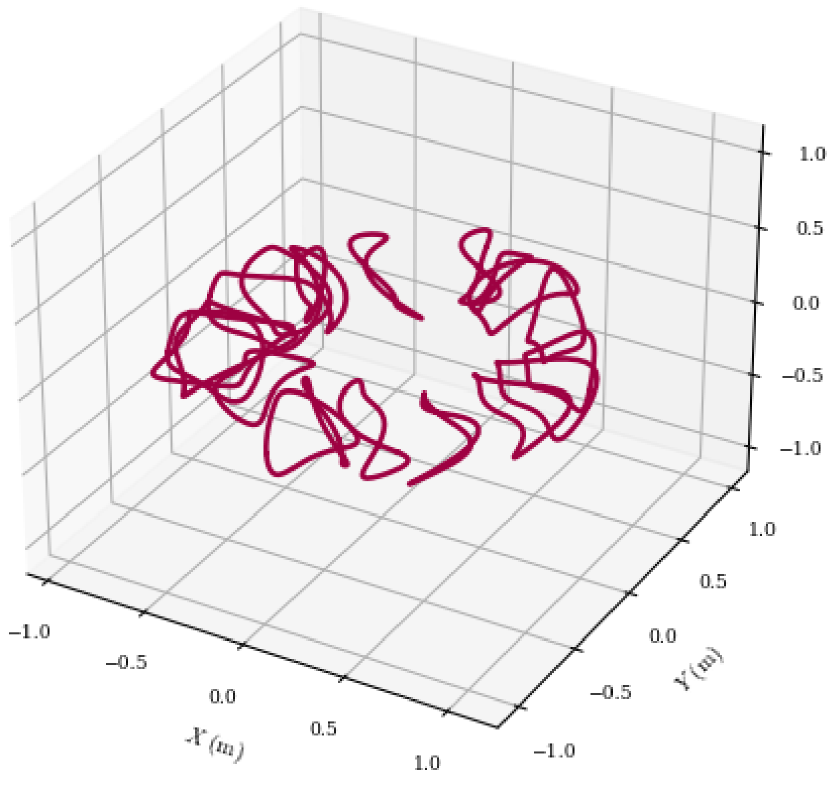
CPU-hours

Landreman & Paul, *Phys. Rev. Lett.* (2022)

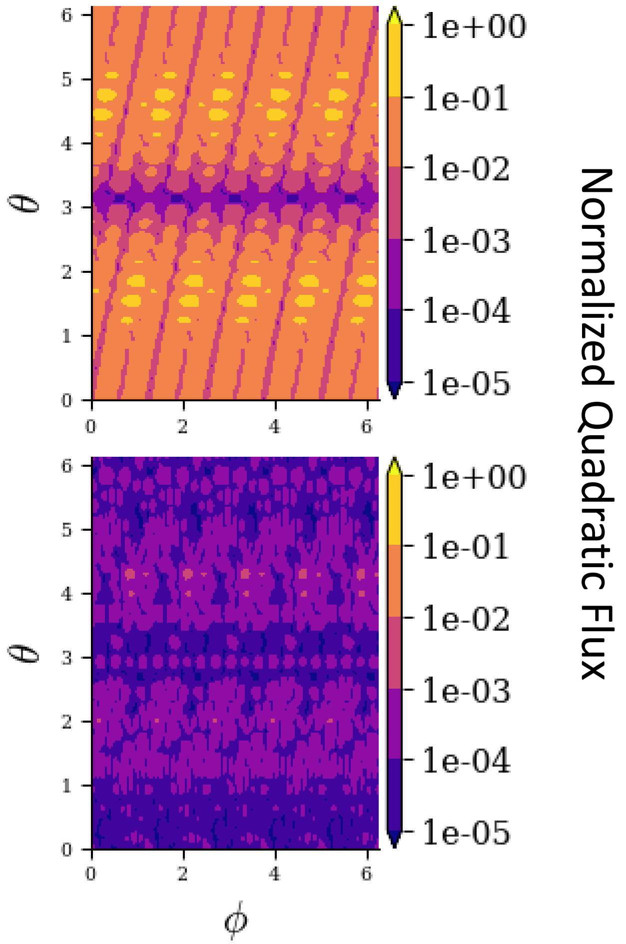
Can perform coil design & optimization



Initial

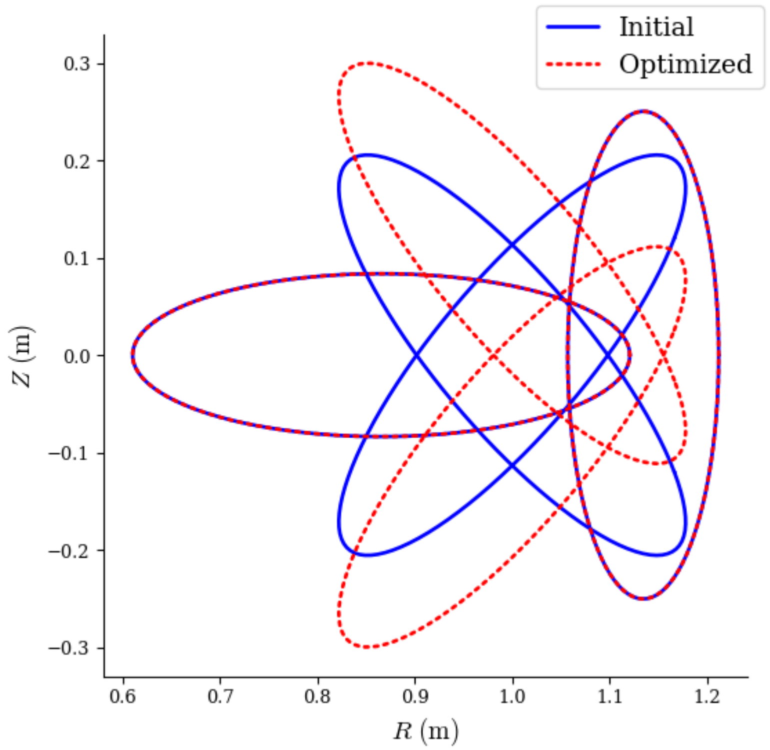


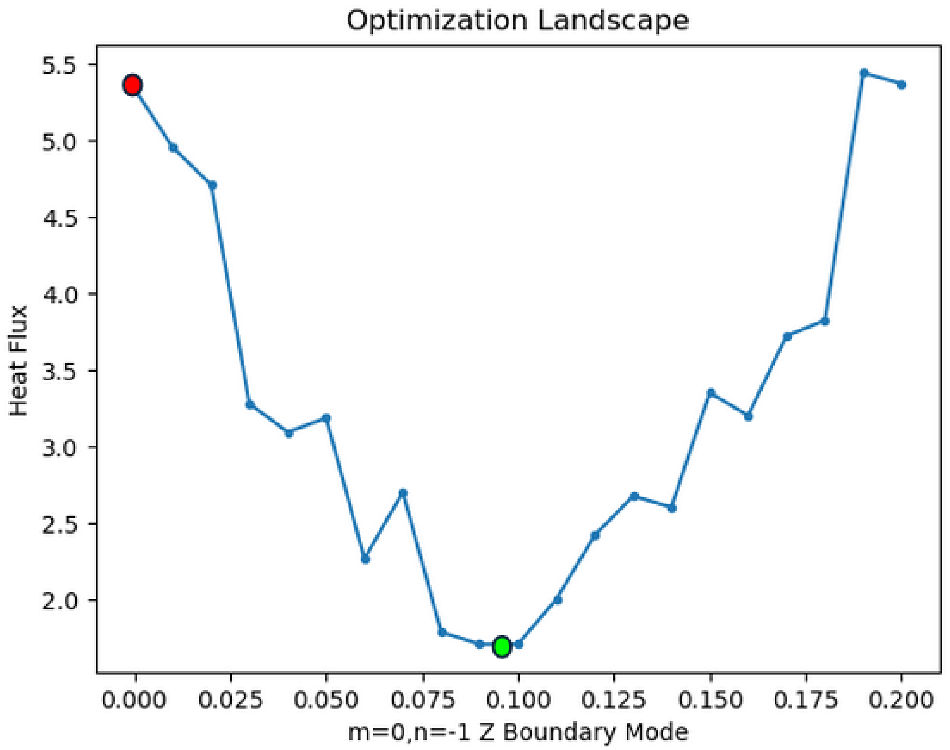
Final



Can wrap other codes with finite differences

- GX is a fast (minutes) pseudo-spectral gyrokinetic code for stellarators



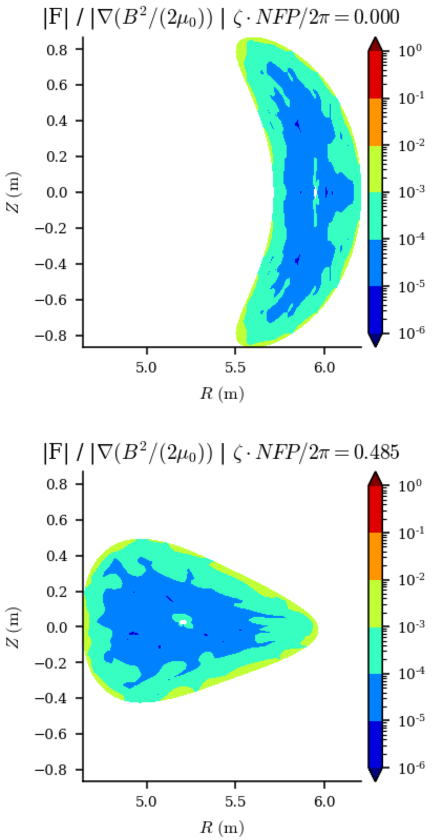


- Also wrapped NEO to optimize for effective ripple ε_{eff}

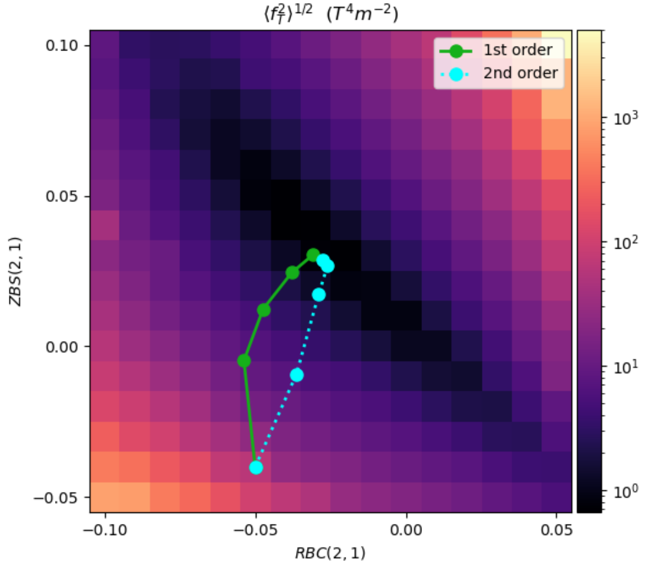
Mandell et al., *J. Plasma Phys.* (2018)
Gonzalez et al., *J. Plasma Phys.* (2022)
Nemov et al., *Phys. Plasmas* (1999)

DESC is a new tool for stellarator optimization

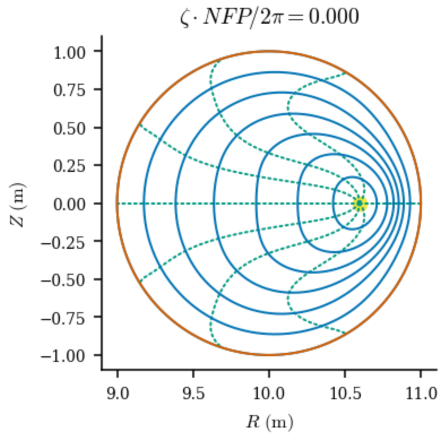
Accurate Equilibria



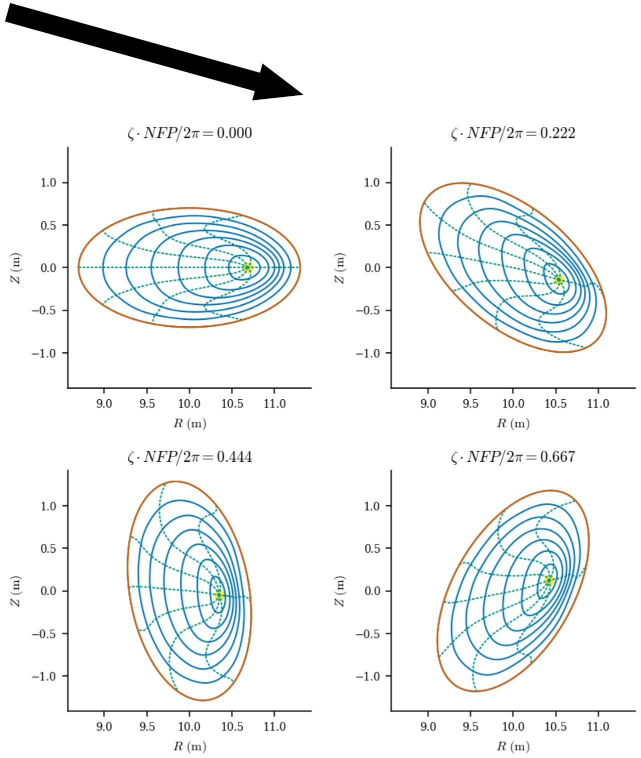
Fast Optimization



Phase-Space Connections



perturb tokamak into stellarator



Better tools = better stellarator reactors!

Additional Resources

Princeton Plasma Control
control.princeton.edu

Software

- Open-source repository: `https://github.com/PlasmaControl/DESC`
- Python package: `pip install desc-opt`

Papers

- The DESC Stellarator Code Suite Part I https://arxiv.org/abs/2203.17173
- The DESC Stellarator Code Suite Part II https://arxiv.org/abs/2203.15927
- The DESC Stellarator Code Suite Part III https://arxiv.org/abs/2204.00078

The Princeton Plasma Control group is recruiting graduate students and post-docs!

Contact Egemen Kolemen: ekolemen@pppl.gov

The MHD equilibrium equations are solved using a pseudo-spectral collocation method

Substituting the spectral expansions into the original PDE

$$\boldsymbol{F} \equiv (\boldsymbol{\nabla} \times \boldsymbol{B}) \times \boldsymbol{B} - \mu_0 \boldsymbol{\nabla} p = \boldsymbol{0}$$

reduces it to a system of nonlinear algebraic equations

equilibrium force balance equations evaluated in real space

$$\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{c}) = \boldsymbol{0}$$

errors evaluated at a set of collocation points

spectral coefficients

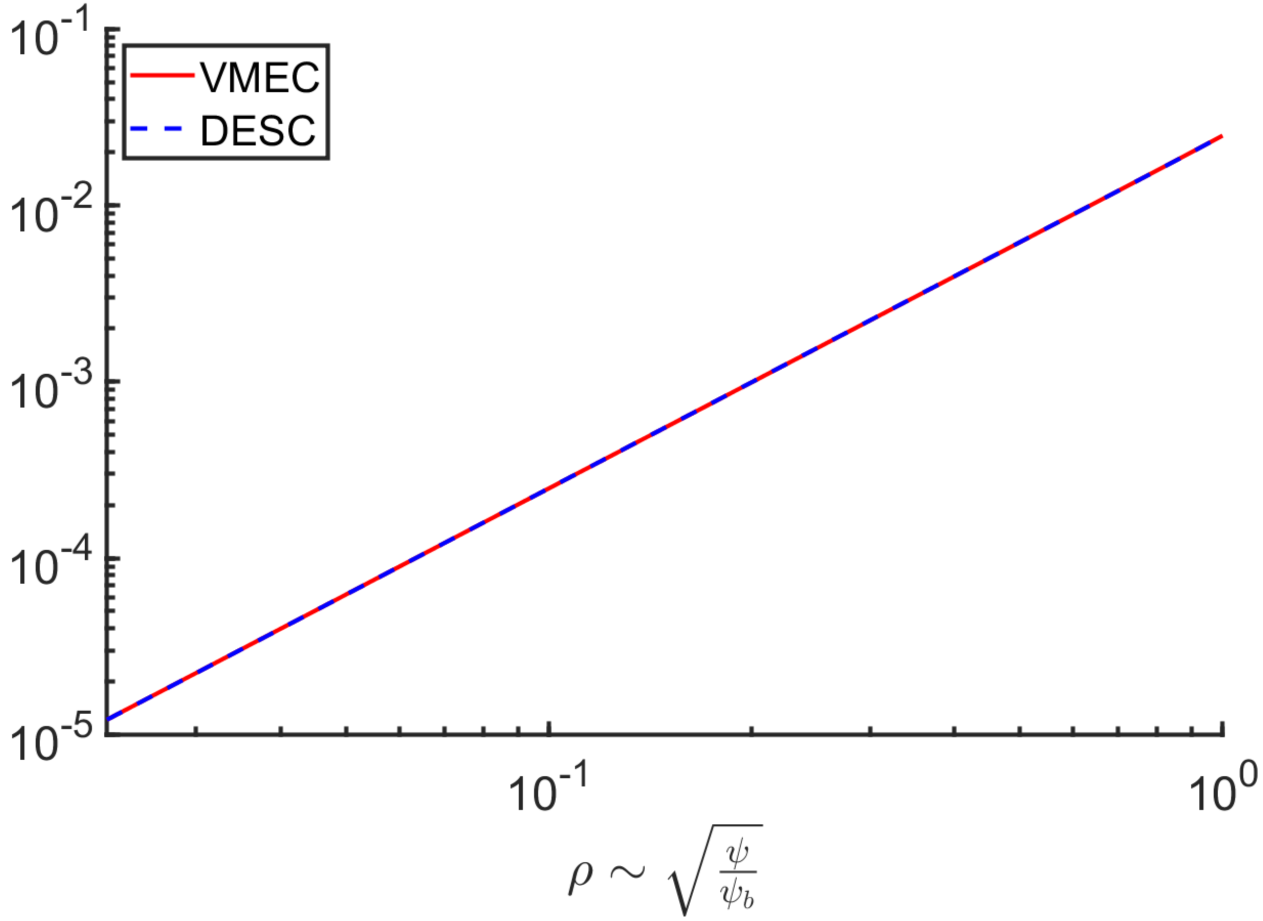
boundary conditions

which is then solved by a Gauss-Newton method (super-linear convergence)

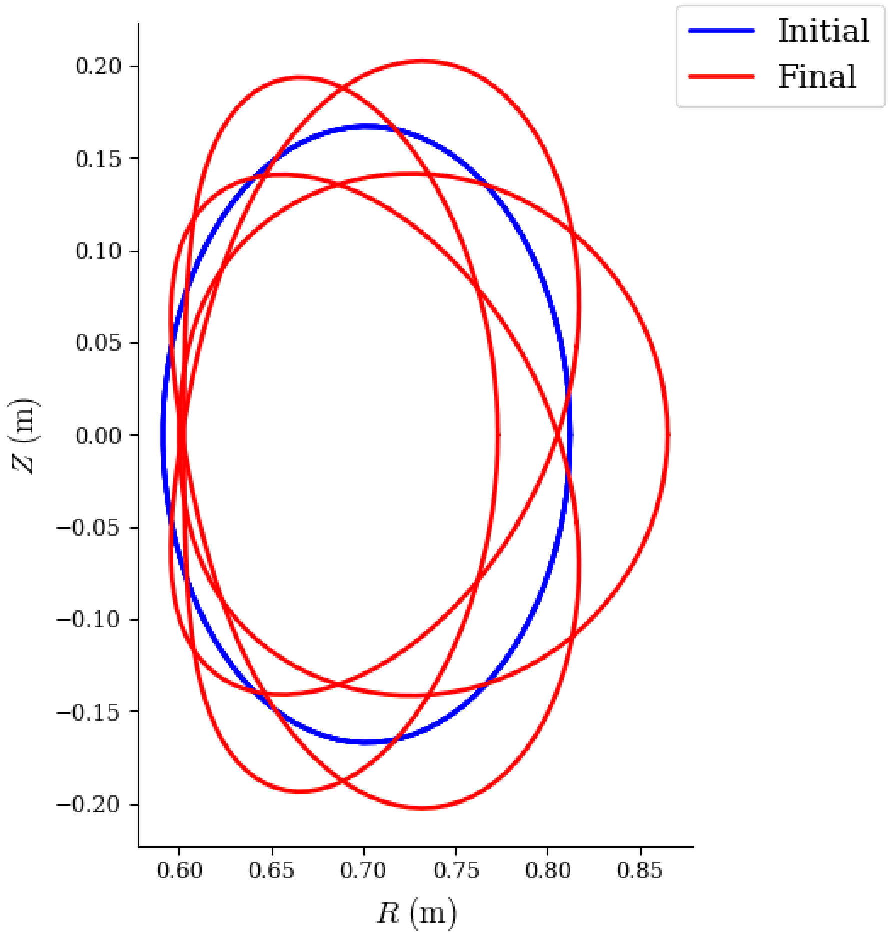
$$\boldsymbol{x}^* = \operatorname{argmin}_{\boldsymbol{x}}\left(\|\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{c})\|^2\right) \qquad \dim(\boldsymbol{f}) \geq \dim(\boldsymbol{x})$$

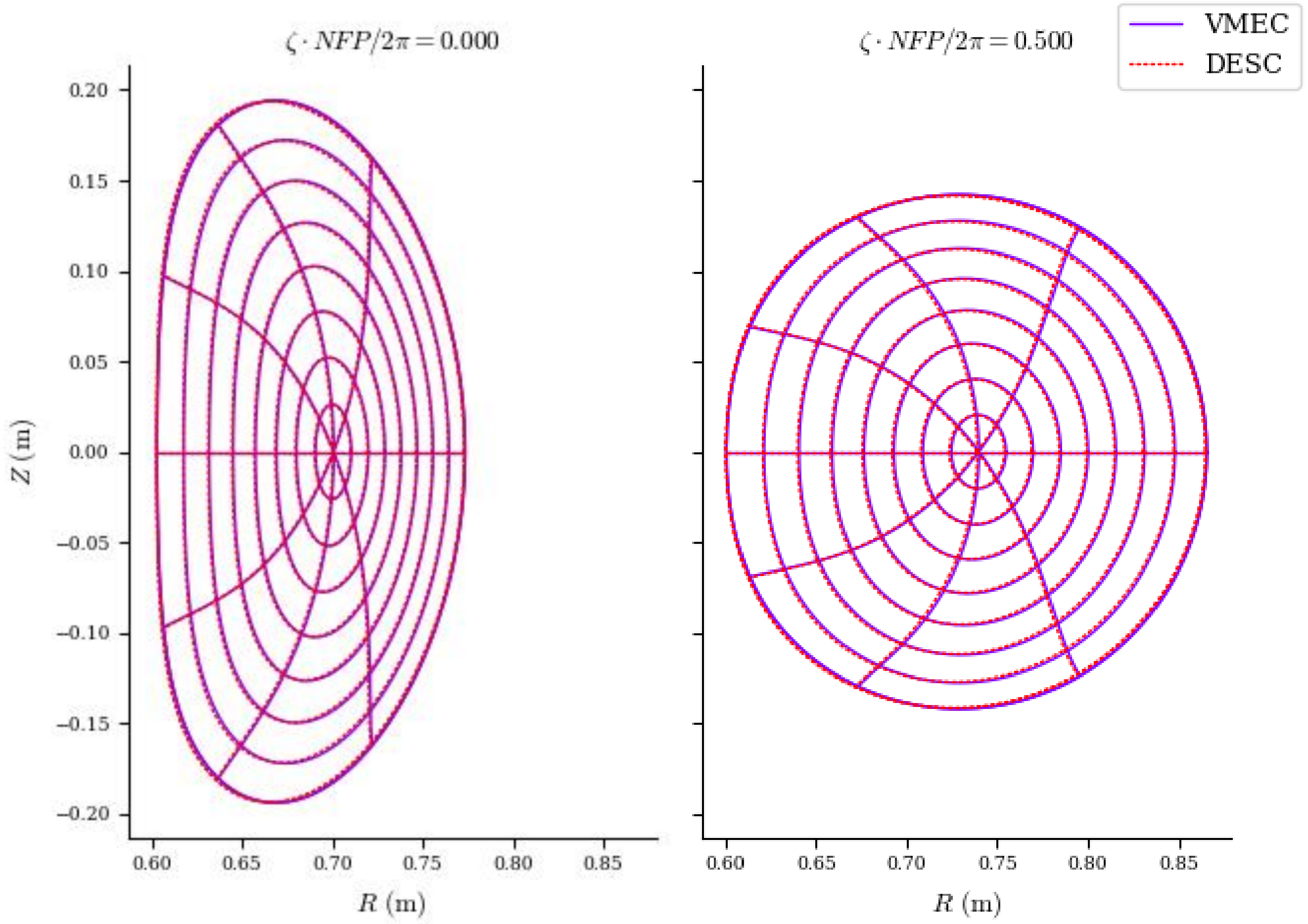
Spectrally condense λ without explicit constraint

$$\frac{\sum_{m,n} m^2\left(R_{mn}^2 + Z_{mn}^2\right)}{\sum_{m,n}\left(R_{mn}^2 + Z_{mn}^2\right)}$$



Free boundary comparison to VMEC

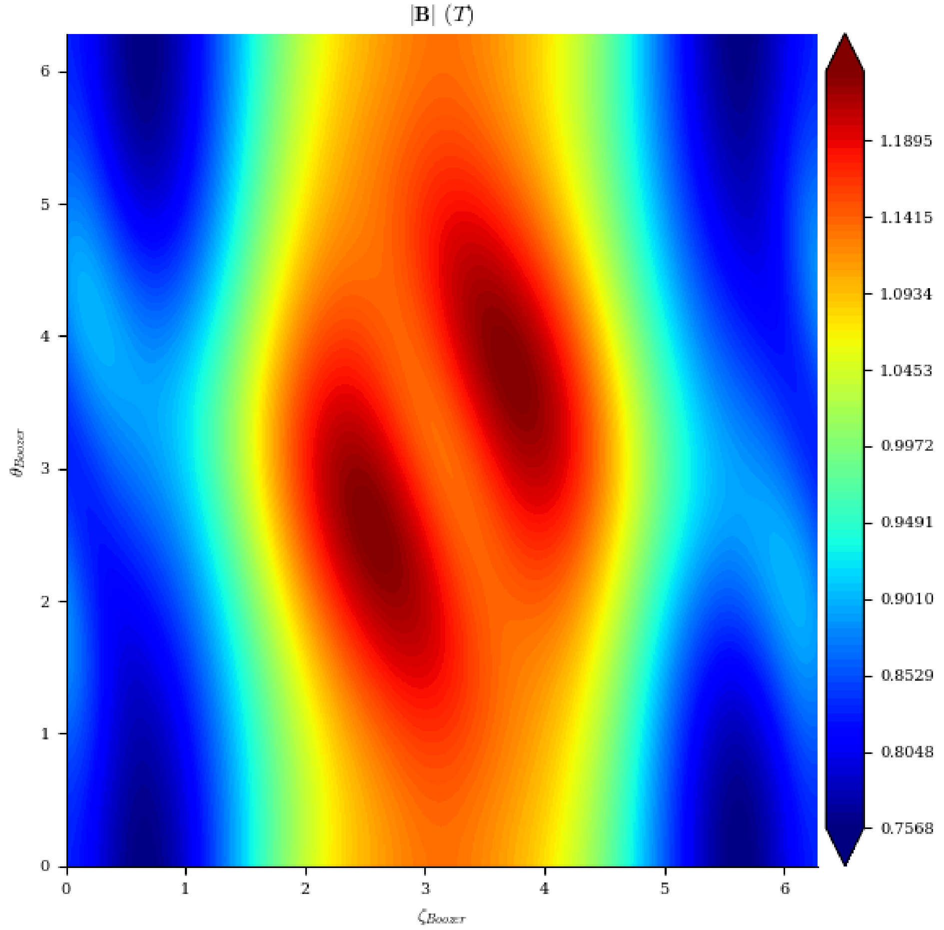




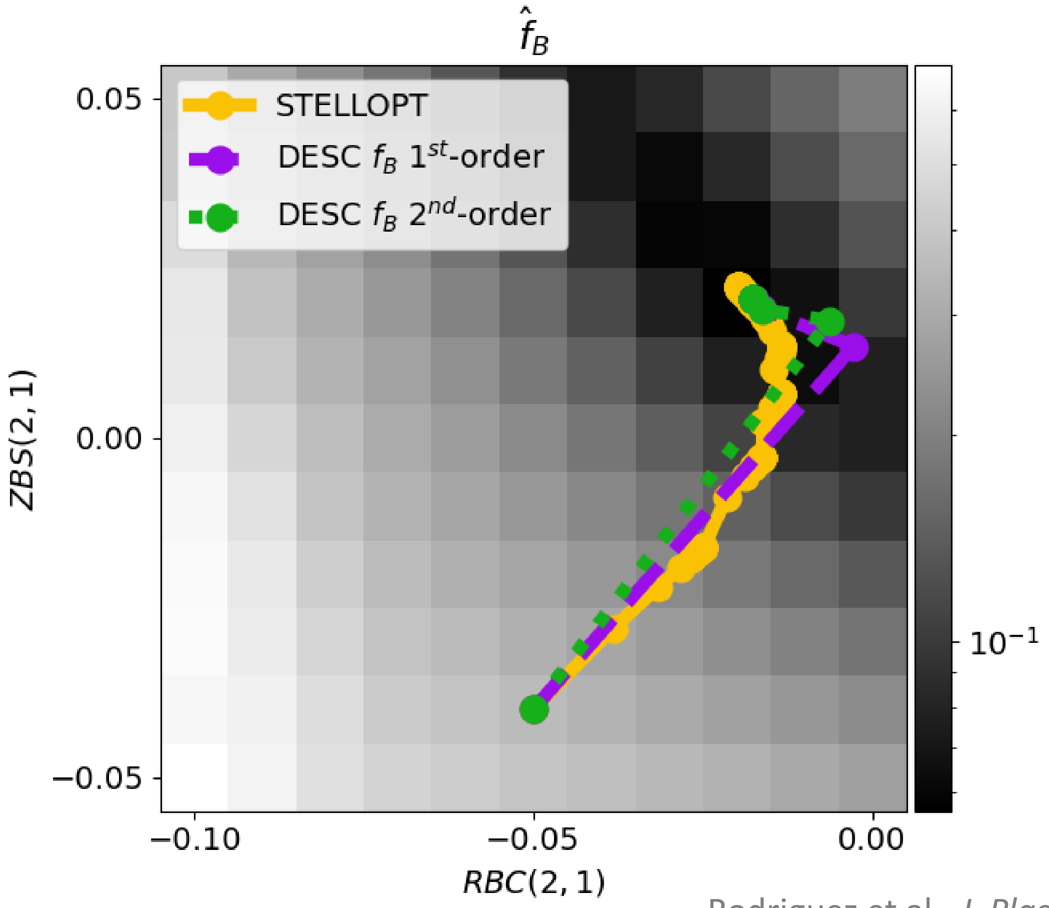
Near-axis expansions can be used as an initial guess for further optimization

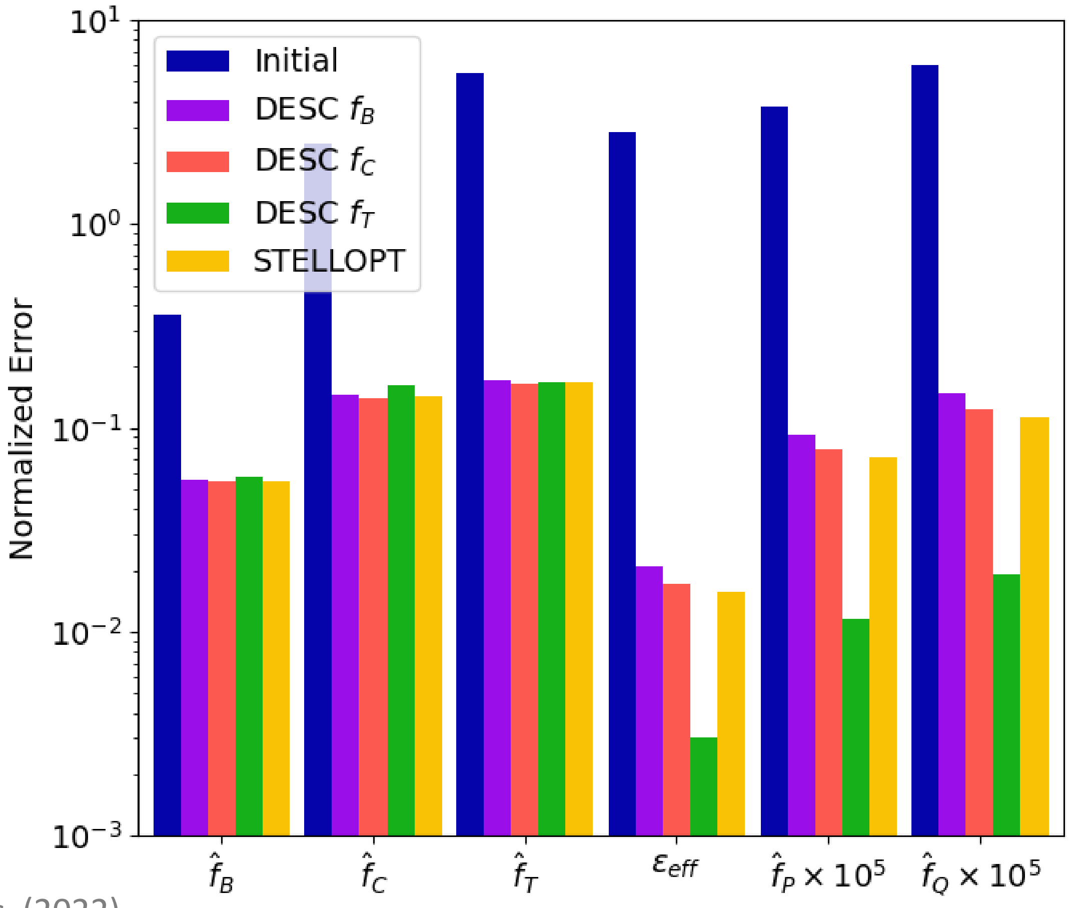
```
# using the pyQSC near-axis expansion code
stel = Qsc.from_paper("r2 section 5.4")
# load QH equilibrium solution
eq = Equilibrium.from_near_axis(stel, r=0.1, M=8, N=8)

# generate QI/QP boundary surface from model
surf = FourierRZToroidalSurface.from_near_axis(
    aspect_ratio=10, elongation=4,
    mirror_ratio=0.3, axis_Z=0.2)
# create vacuum configuration with boundary surface
eq = Equilibrium(M=8, N=8, surface=surf)
eq.solve()  # solve equilibrium force balance
```

Landreman et al., *J. Plasma Phys.* (2019)



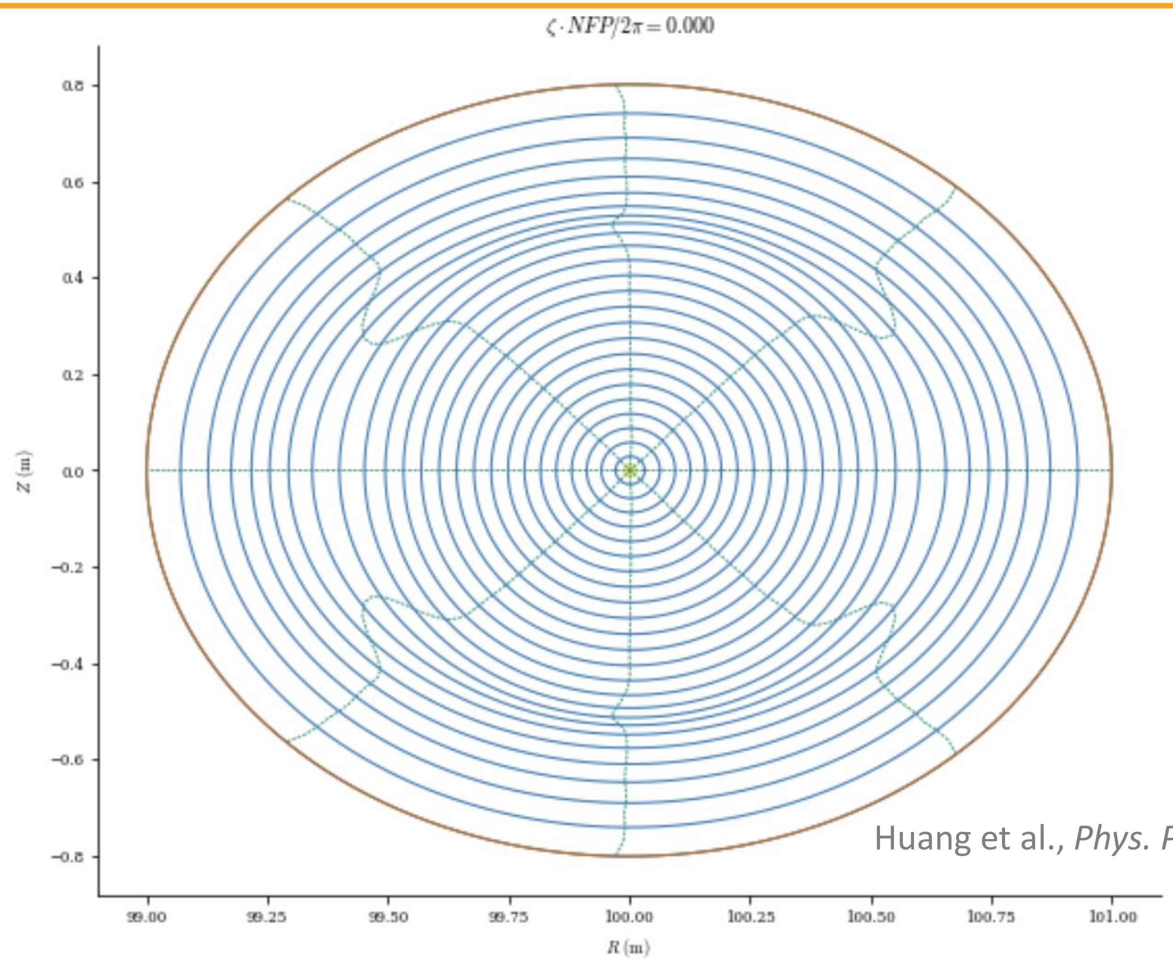
Optimization with various forms of QS





Rodriguez et al., *J. Plasma Phys.* (2022)

Ideal MHD behavior at rational surfaces with Hahm-Kulsrud-Taylor problem



Huang et al., *Phys. Plasmas* (2022)