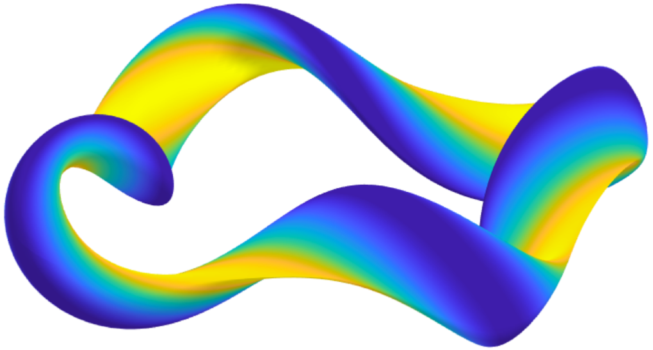
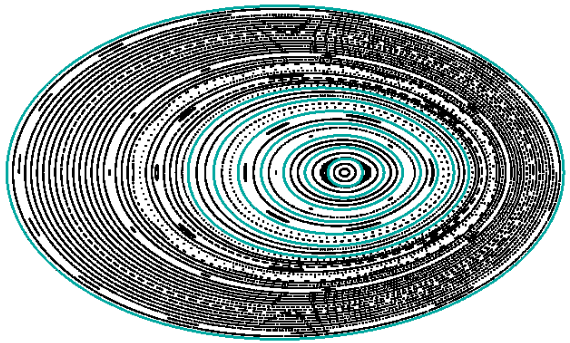
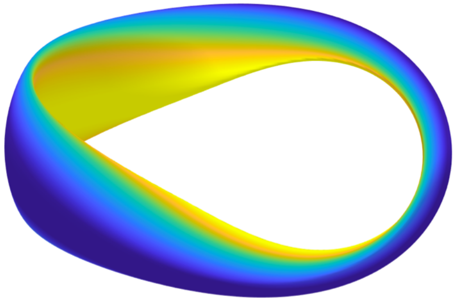
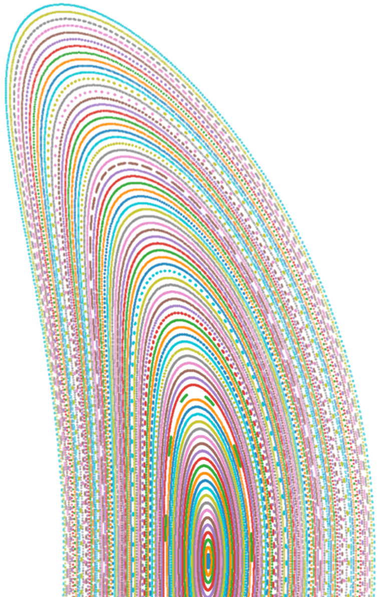
SIMSOPT: New software tools for stellarator optimization



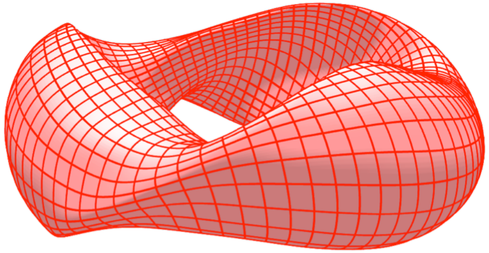


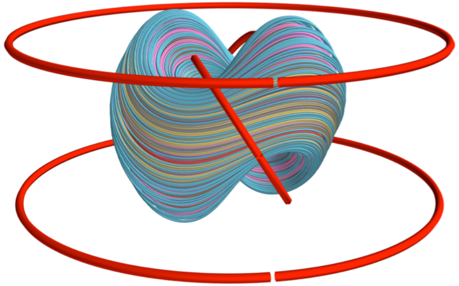




Matt Landreman, University of Maryland

Australian National University: Zhisong Qu
Cornell: David Bindel, Misha Padidar
EPFL: Antoine Baillod, Joaquim Loizu
IPP: Jonathan Schilling
Maryland: Rogerio Jorge
NYU: Andrew Giuliani, Florian Wechsung
PPPL: Stuart Hudson, Bharat Medasani, Caoxiang Zhu
Wisconsin: Aaron Bader, Ben Faber, Thomas Kruger





SIMONS FOUNDATION

- Vision
- Examples
- Design
- Next steps

Simsopt vision

- Extensibility: It should be possible to add new codes and terms to an objective function without editing the core infrastructure or build system. Any edits to working code can potentially introduce bugs.

- Modularity: Physics modules that are not needed for your optimization problem do not need to be downloaded.

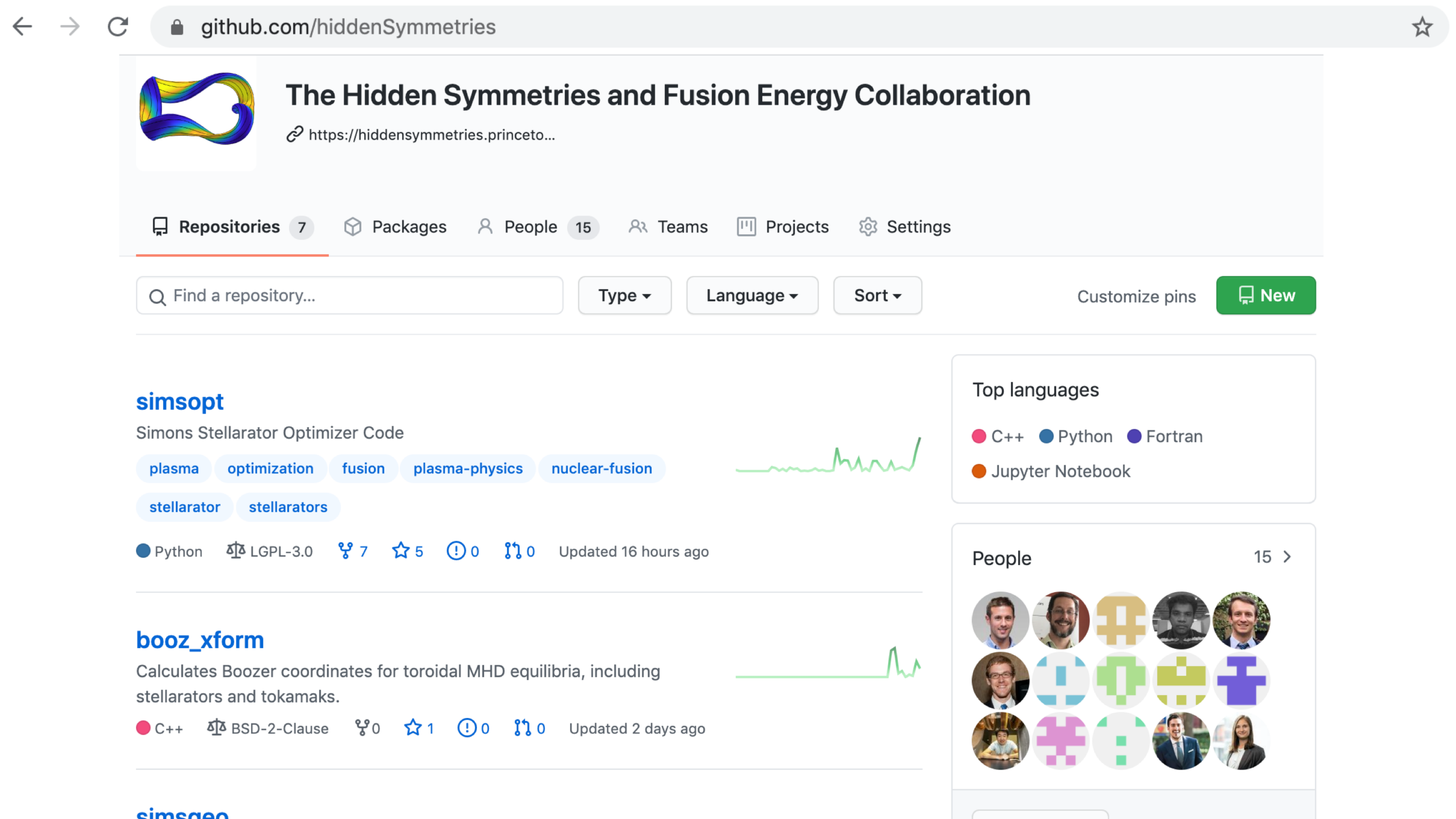
- Flexibility: Components can be used for many purposes, not just standard optimization.

- Thorough unit testing, regression testing, and continuous integration.

Projects with similar goals: Plasma Equilibrium Toolkit & LASSO (Wisconsin), DESC (Princeton).

Simsopt components

- Interfaces to physics codes
- Surface & curve objects, with several parameterizations
- Tools for defining objective function & parameter space, e.g. fixed vs free degrees of freedom
- Biot-Savart and other magnetic field types, with derivatives
- Parallelized finite differences
- Plotting & graphics



github.com/hiddenSymmetries

The Hidden Symmetries and Fusion Energy Collaboration

https://hiddensymmetries.princeto...

Repositories 7 Packages People 15 Teams Projects Settings

Find a repository... Type ▾ Language ▾ Sort ▾ Customize pins New

simsopt

Simons Stellarator Optimizer Code

plasma optimization fusion plasma-physics nuclear-fusion stellarator stellarators

● Python LGPL-3.0 7 5 0 0 Updated 16 hours ago

booz_xform

Calculates Boozer coordinates for toroidal MHD equilibria, including stellarators and tokamaks.

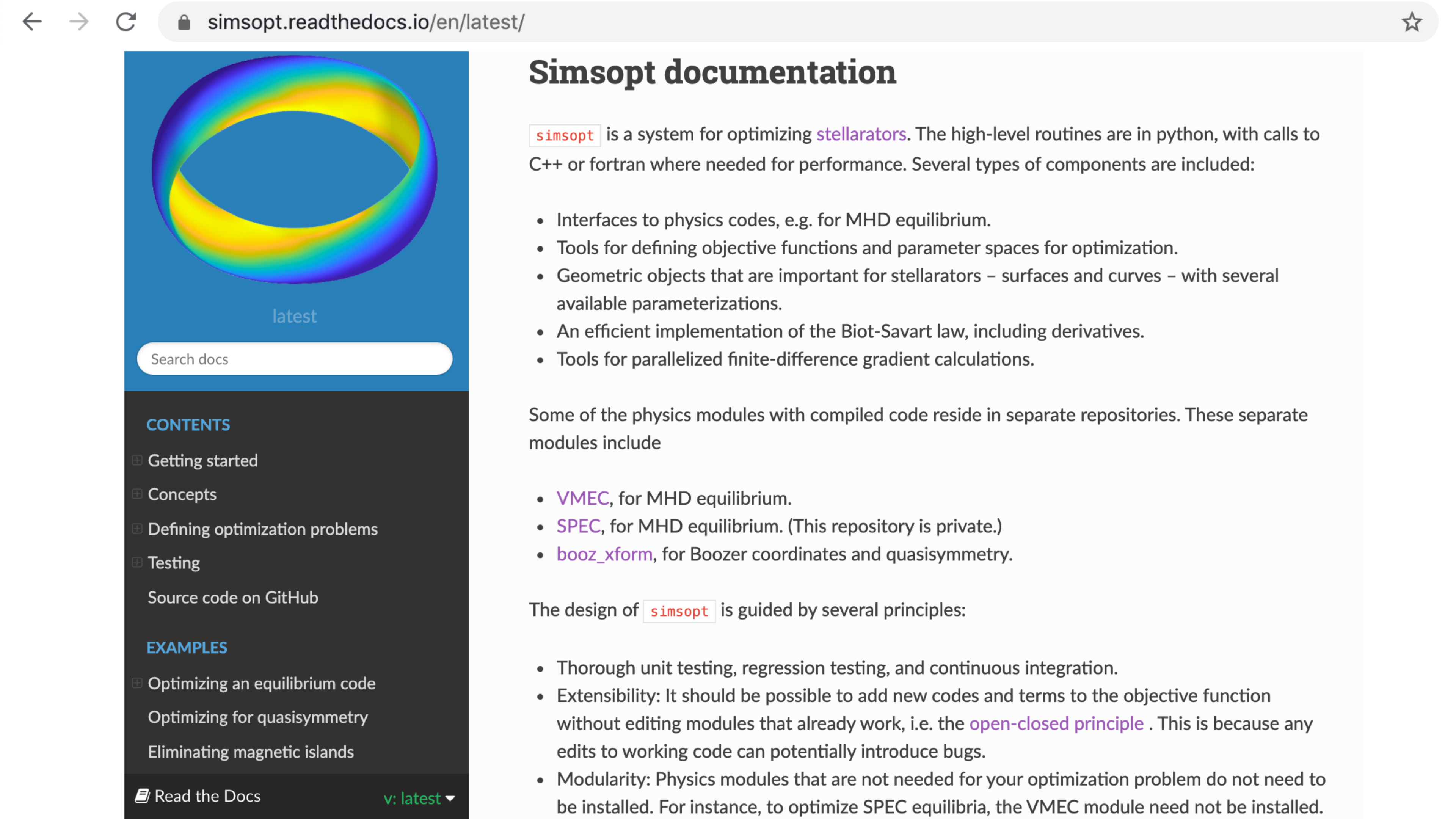
● C++ BSD-2-Clause 0 1 0 0 Updated 2 days ago

simsgeo

Top languages

● C++ ● Python ● Fortran ● Jupyter Notebook

People 15 >


simsopt.readthedocs.io/en/latest/
latest
Search docs
CONTENTS
Getting started
Concepts
Defining optimization problems
Testing
Source code on GitHub
EXAMPLES
Optimizing an equilibrium code
Optimizing for quasisymmetry
Eliminating magnetic islands
Read the Docs
v: latest

Simsopt documentation

`simsopt` is a system for optimizing stellarators. The high-level routines are in python, with calls to C++ or fortran where needed for performance. Several types of components are included:

- Interfaces to physics codes, e.g. for MHD equilibrium.
- Tools for defining objective functions and parameter spaces for optimization.
- Geometric objects that are important for stellarators – surfaces and curves – with several available parameterizations.
- An efficient implementation of the Biot-Savart law, including derivatives.
- Tools for parallelized finite-difference gradient calculations.

Some of the physics modules with compiled code reside in separate repositories. These separate modules include

- VMEC, for MHD equilibrium.
- SPEC, for MHD equilibrium. (This repository is private.)
- booz_xform, for Boozer coordinates and quasisymmetry.

The design of `simsopt` is guided by several principles:

- Thorough unit testing, regression testing, and continuous integration.
- Extensibility: It should be possible to add new codes and terms to the objective function without editing modules that already work, i.e. the open-closed principle . This is because any edits to working code can potentially introduce bugs.
- Modularity: Physics modules that are not needed for your optimization problem do not need to be installed. For instance, to optimize SPEC equilibria, the VMEC module need not be installed.

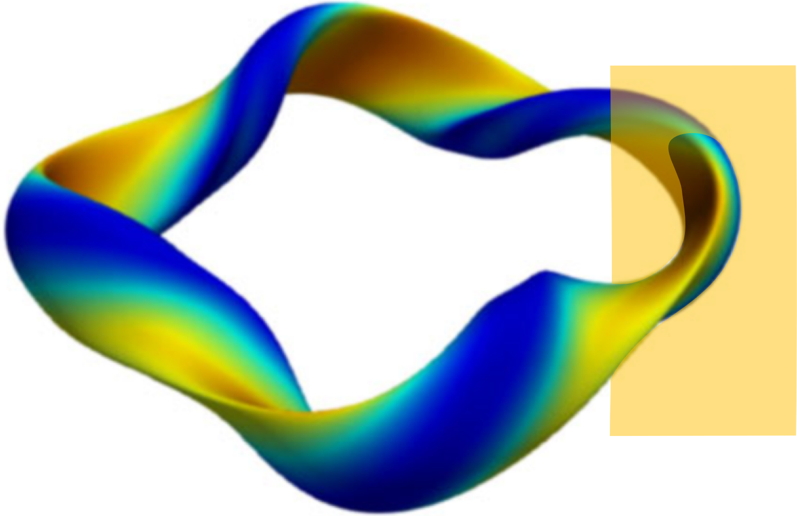
How to get involved

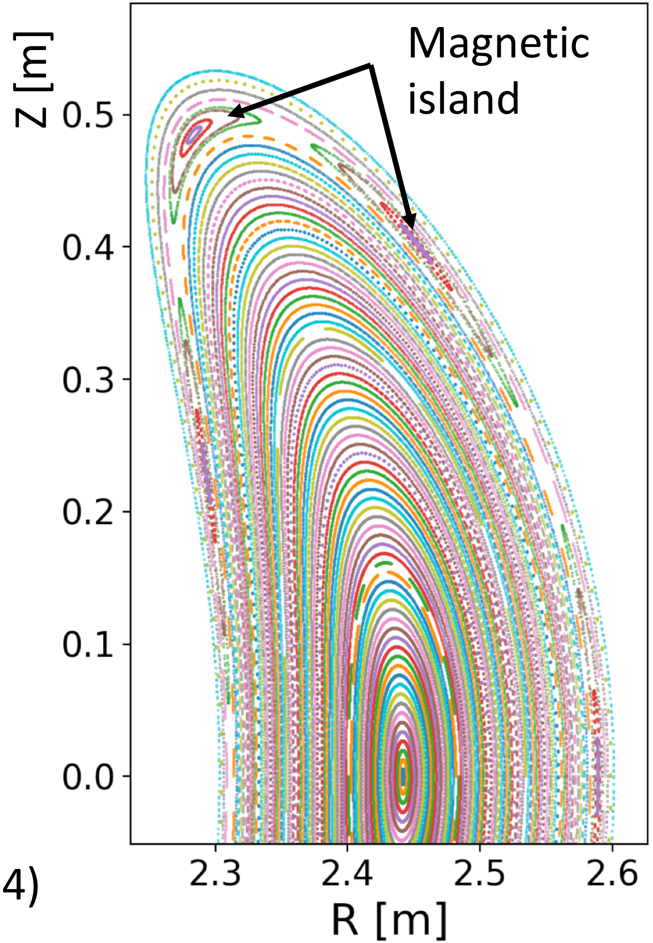
- `https://github.com/hiddenSymmetries/simsopt`
- Everyone is welcome at development meetings: Mondays @ 9am NY, 3pm Europe
- simsopt slack workspace, #developers channel
- Play around with the code and examples
- Try container: `docker run -it --rm hiddensymmetries/simsopt`
- Fork the repository, add a feature, submit pull request

- Vision
- Examples
- Design
- Next steps

Simsopt can optimize SPEC configurations to eliminate magnetic islands

Starting point: a quasi-helically symmetric configuration from Wisconsin [Bader et al (2020)]





We'll minimize Greene's residue, similar to Hanson & Cary (1984)

Islands can be eliminated by optimizing Greene's residue

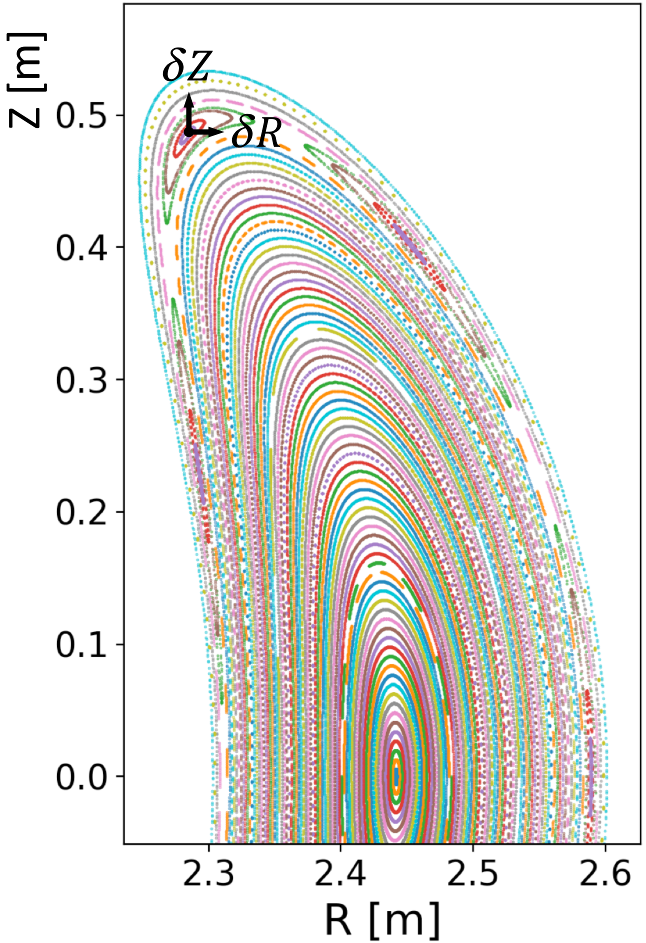
$$\text{residue} = \frac{1}{4}\left(2 - \mathrm{Tr}\,\overleftrightarrow{M}\right)$$

$\overleftrightarrow{M} =$ "full orbit tangent map":

$$\begin{pmatrix} \delta R \\ \delta Z \end{pmatrix}_{\text{final}} = \overleftrightarrow{M} \begin{pmatrix} \delta R \\ \delta Z \end{pmatrix}_{\text{initial}}$$

Residue = 0 for a good surface.

Greene, *J Math Phys* (1979)



Islands can be eliminated by optimizing Greene's residue with simsopt using a high-level python script

$$\text{residue} = \frac{1}{4}\left(2 - \text{Tr}\,\overleftrightarrow{M}\right)$$

$$\overleftrightarrow{M} = \text{"full orbit tangent map":}$$

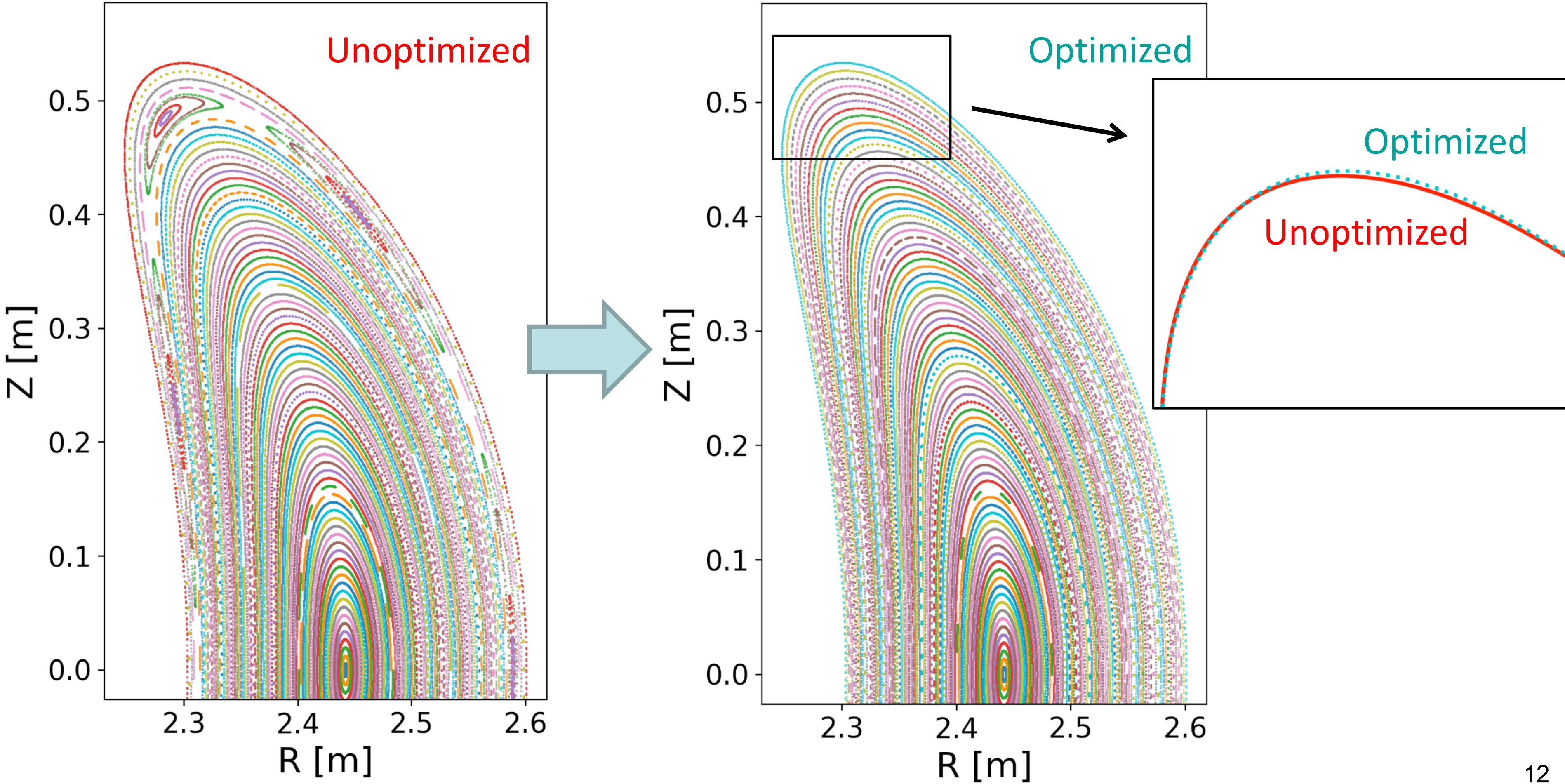
$$\begin{pmatrix} \delta R \\ \delta Z \end{pmatrix}_{\text{final}} = \overleftrightarrow{M} \begin{pmatrix} \delta R \\ \delta Z \end{pmatrix}_{\text{initial}}$$

Residue = 0 for a good surface.

Greene, *J Math Phys* (1979)

```
# Create an equilibrium object to optimize:
spec = Spec('QH-residues.sp')
spec.boundary.change_resolution(mpol=12, ntor=12)

# Define the parameter space for optimization:
spec.boundary.all_fixed()
spec.boundary.set_fixed('zs(6,1)', False)

# Main island chain has helicity iota = 8/7:
residue1 = Residue(spec, 8, 7)
residue2 = Residue(spec, 12, 11)

# Objective function is \sum_j residue_j ** 2
prob = LeastSquaresProblem([(residue1, 0, 1),
                            (residue2, 0, 1)])

least_squares_serial_solve(prob)
```

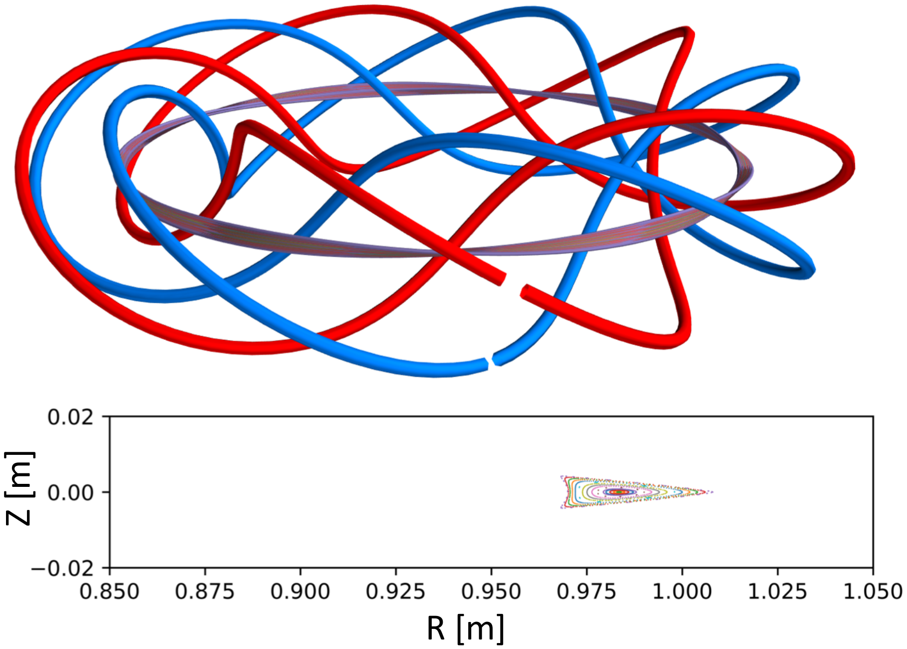
Optimization of boundary shape successfully results in good surfaces



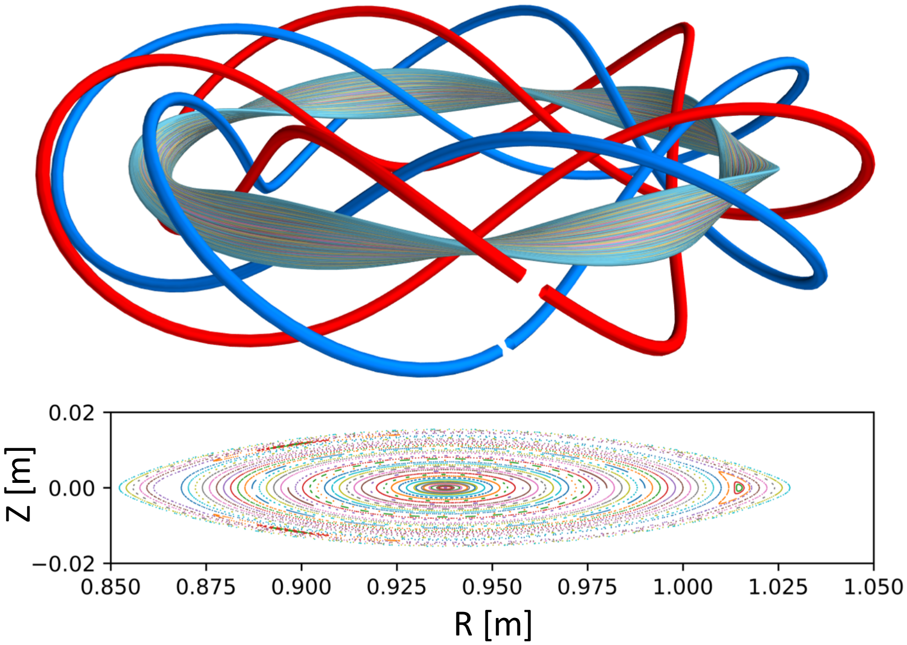
Optimization for good surfaces can also be done in the parameter space of coil shapes rather than the boundary shape

Reproduction of Cary & Hanson (1986) with simsopt by Rogerio Jorge

Unoptimized

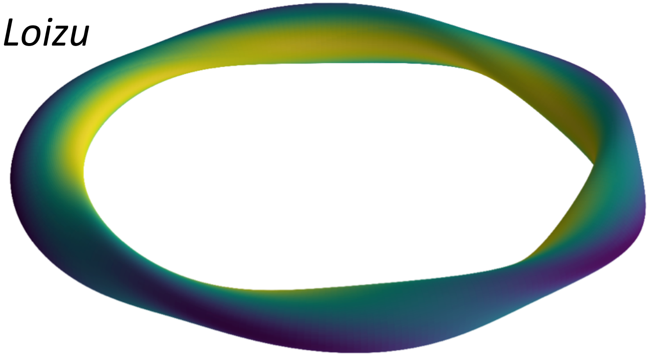


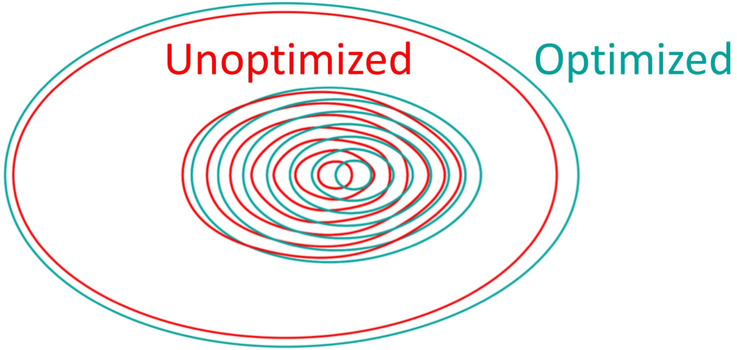
Optimized

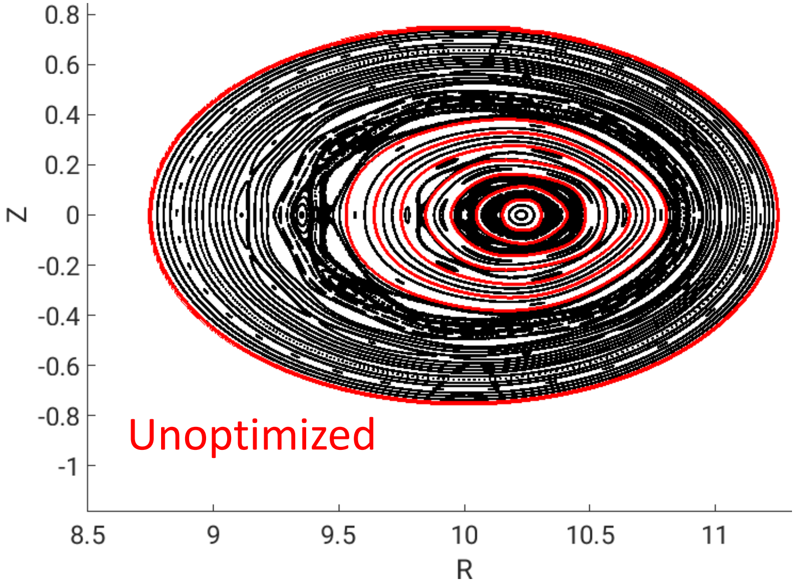


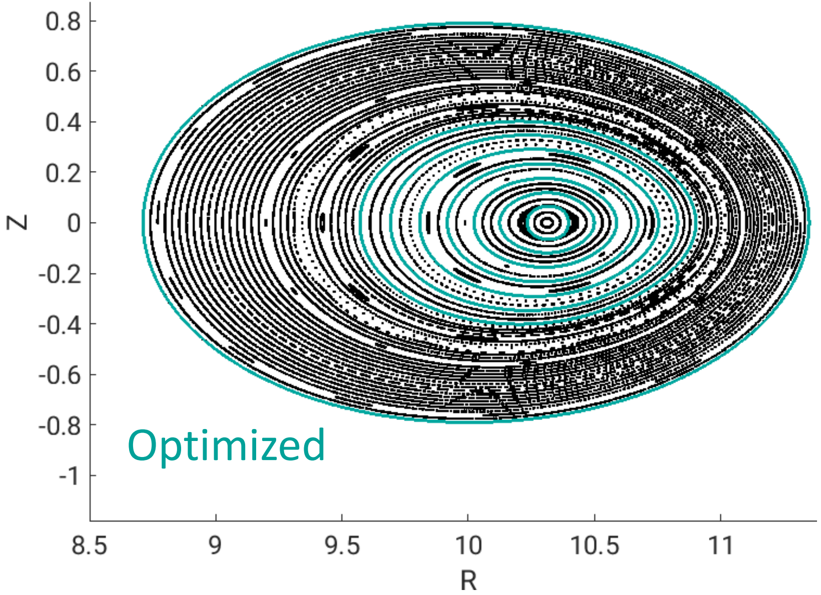
We are now optimizing for integrability with plasma current & pressure

Baillod & Loizu



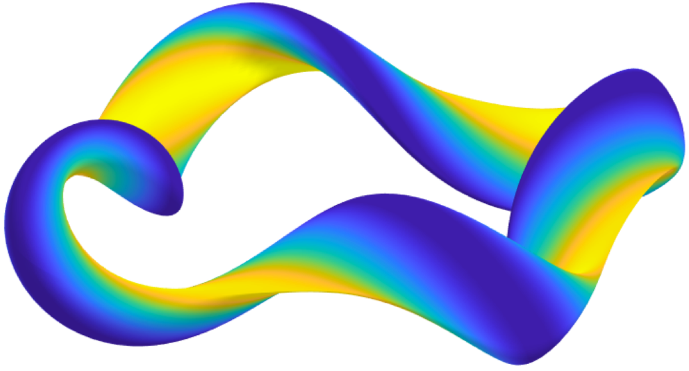


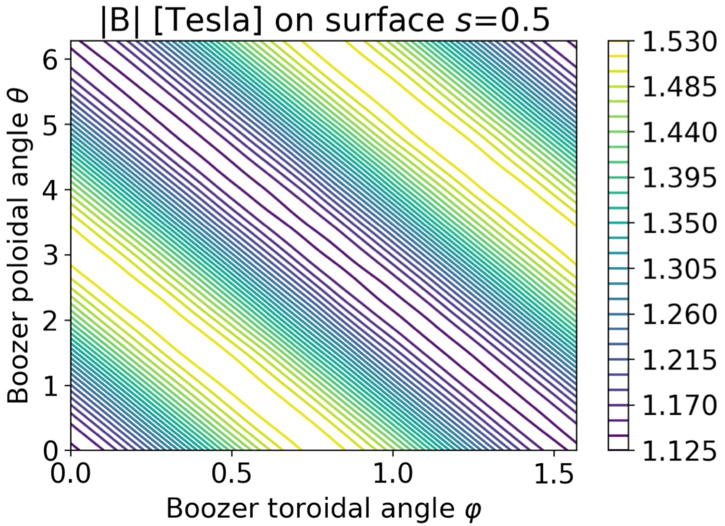




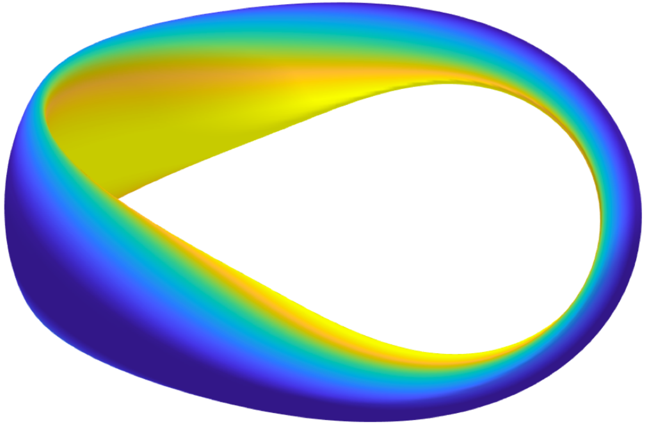
Like STELLOPT & ROSE, SIMSOPT can optimize VMEC configurations for quasisymmetry

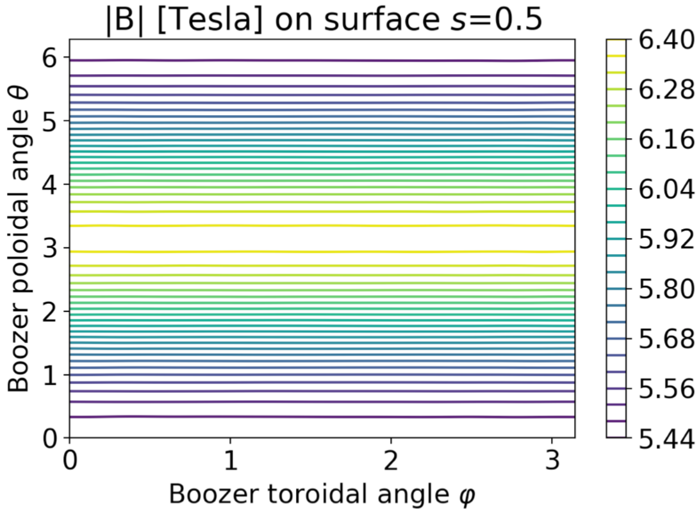
```
mpi = MpiPartition()
vmec = Vmec("input.nfp4_QH”, mpi)

# Define parameter space:
surf = vmec.boundary
surf.all_fixed()
surf.fixed_range(mmin=0, mmax=3,
                 nmin=-3, nmax=3, fixed=False)
surf.set_fixed("rc(0,0)") # Average major radius

# Set parameters for quasisymmetry objective:
qs = Quasisymmetry(Boozer(vmec),
                   0.5, # Radius to target.
                   1, 1) # (M, N) you want in |B|.

# Define objective function:
prob = LeastSquaresProblem([(qs, 0, 1),
                            (vmec.aspect, 7, 1)])

least_squares_mpi_solve(prob, mpi, grad=True)
```




|B| [Tesla] on surface s=0.5
Boozer poloidal angle θ
0
1
2
3
4
5
6
Boozer toroidal angle φ
0.0
0.5
1.0
1.5
1.530
1.485
1.440
1.395
1.350
1.305
1.260
1.215
1.170
1.125

Scripting allows dynamic increase in resolution during optimization

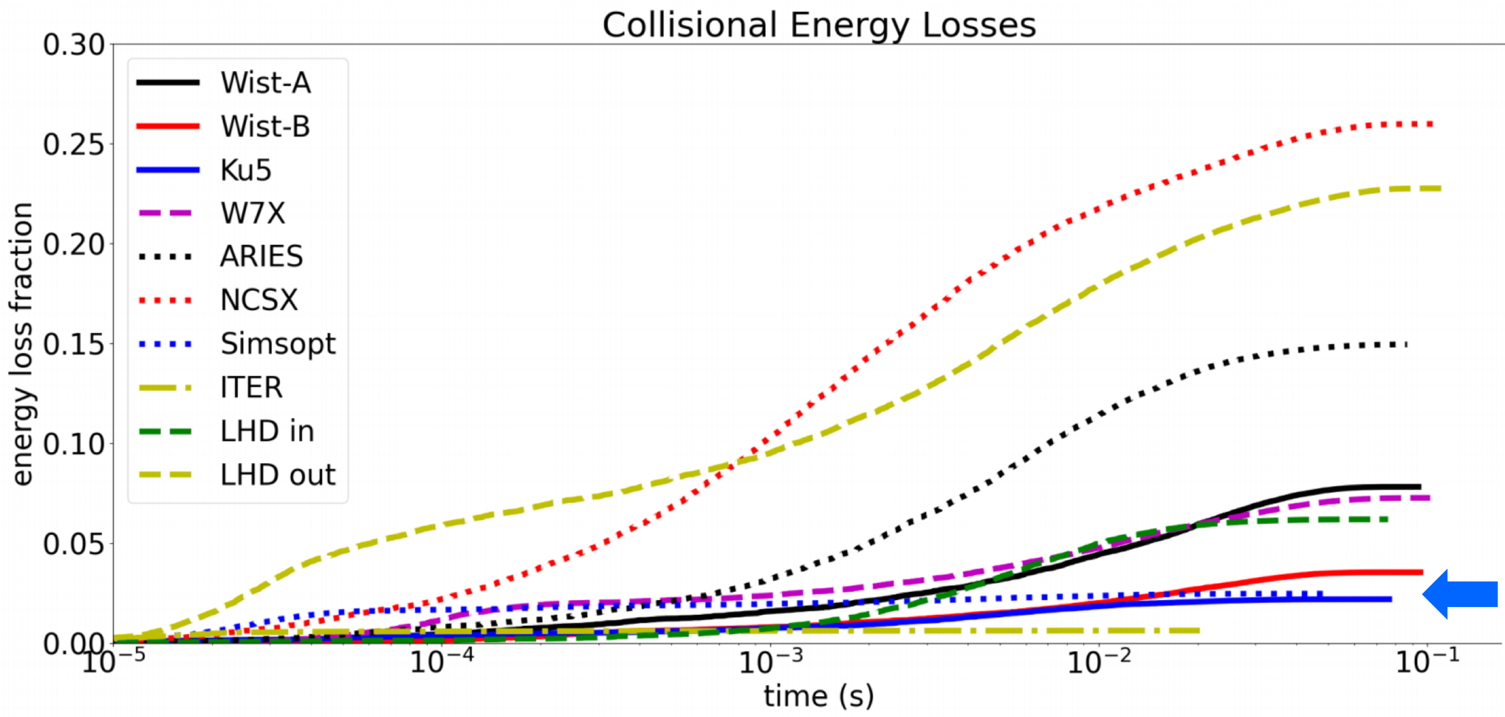


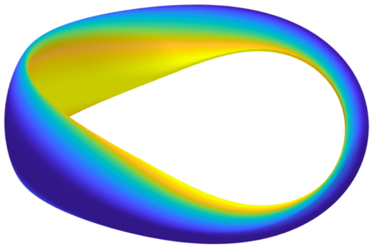


```
mpi = MpiPartition()
vmec = Vmec("input.nfp2_QA", mpi=mpi)
surf = vmec.boundary

# Configure quasisymmetry objective:
boozer = Boozer(vmec)
qs = Quasisymmetry(boozer, 0.5, # Radius to target
                   1, 0) # (M, N) you want in |B|

# Define objective function:
prob = LeastSquaresProblem([(vmec.aspect, 6, 1),
                            (vmec.iota_axis, 0.465, 1),
                            (vmec.iota_edge, 0.495, 1),
                            (qs, 0, 1)])

for step in range(4):
    vmec.indata.mpol = 3 + step # Increase resolution
    vmec.indata.ntor = vmec.indata.mpol
    boozer.mpol = 16 + step * 8 # Increase resolution
    boozer.ntor = boozer.mpol

    # Parameter space gets larger each step:
    surf.all_fixed()
    max_mode = step + 1
    surf.fixed_range(mmin=0, mmax=max_mode,
                     nmin=-max_mode, nmax=max_mode,
                     fixed=False)
    surf.set_fixed("rc(0,0)") # Major radius

    least_squares_mpi_solve(prob, mpi, grad=True)
```

Simsopt can generate configurations with decent alpha particle confinement

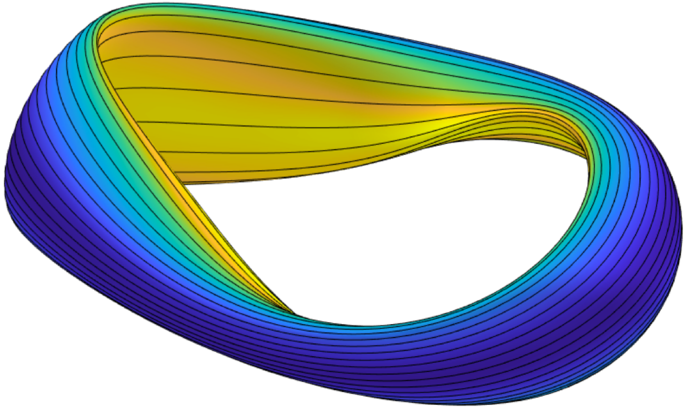
Bader et al, arXiv:2106.00716





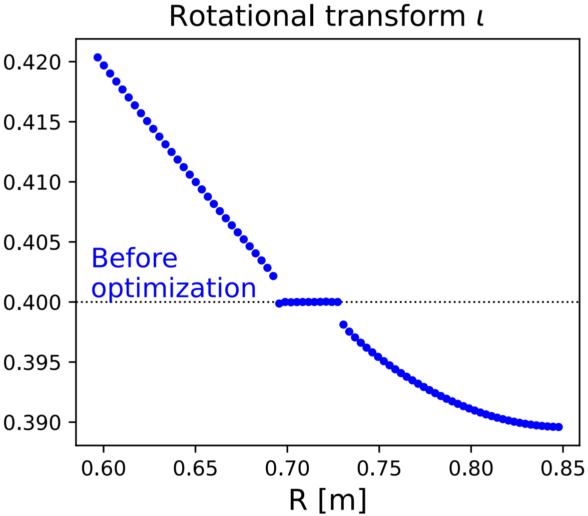
Configurations scaled to the ARIES-CS volume and average |B|.

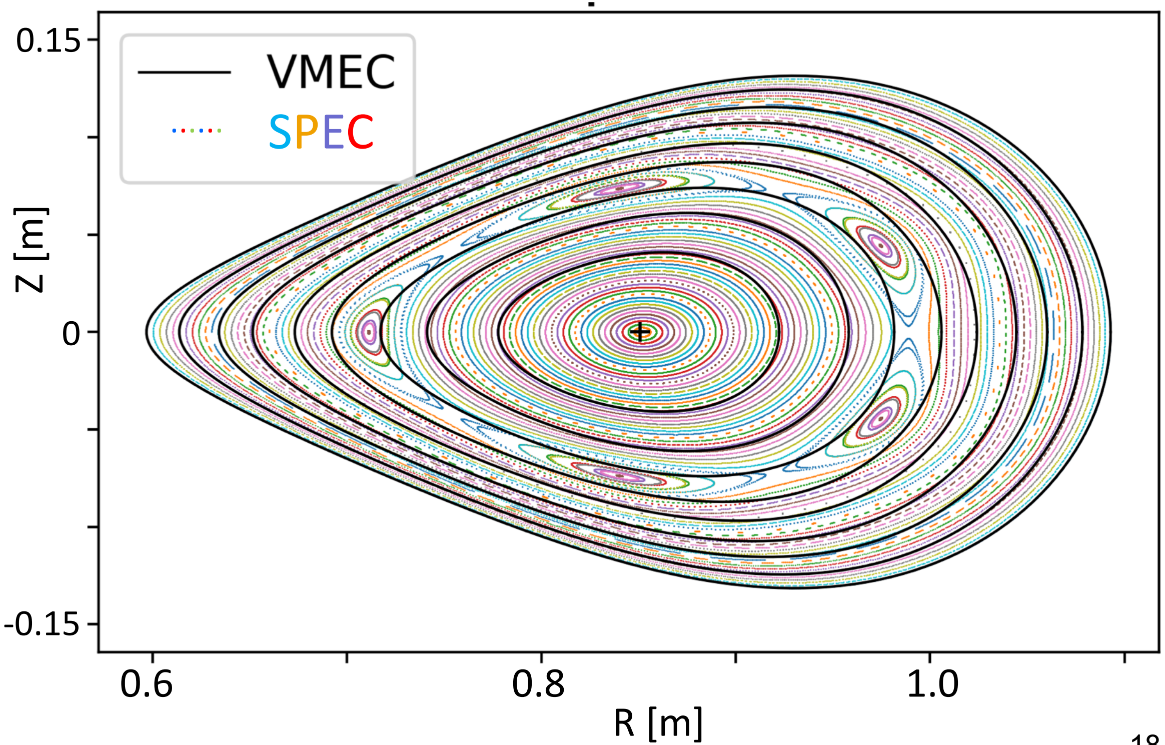
Simsopt can also optimize for quasisymmetry & good surfaces simultaneously, with both VMEC and SPEC in the loop.



Starting point: nfp=2, QA, aspect = 6,

Island chain at iota = 2/5 = 0.4





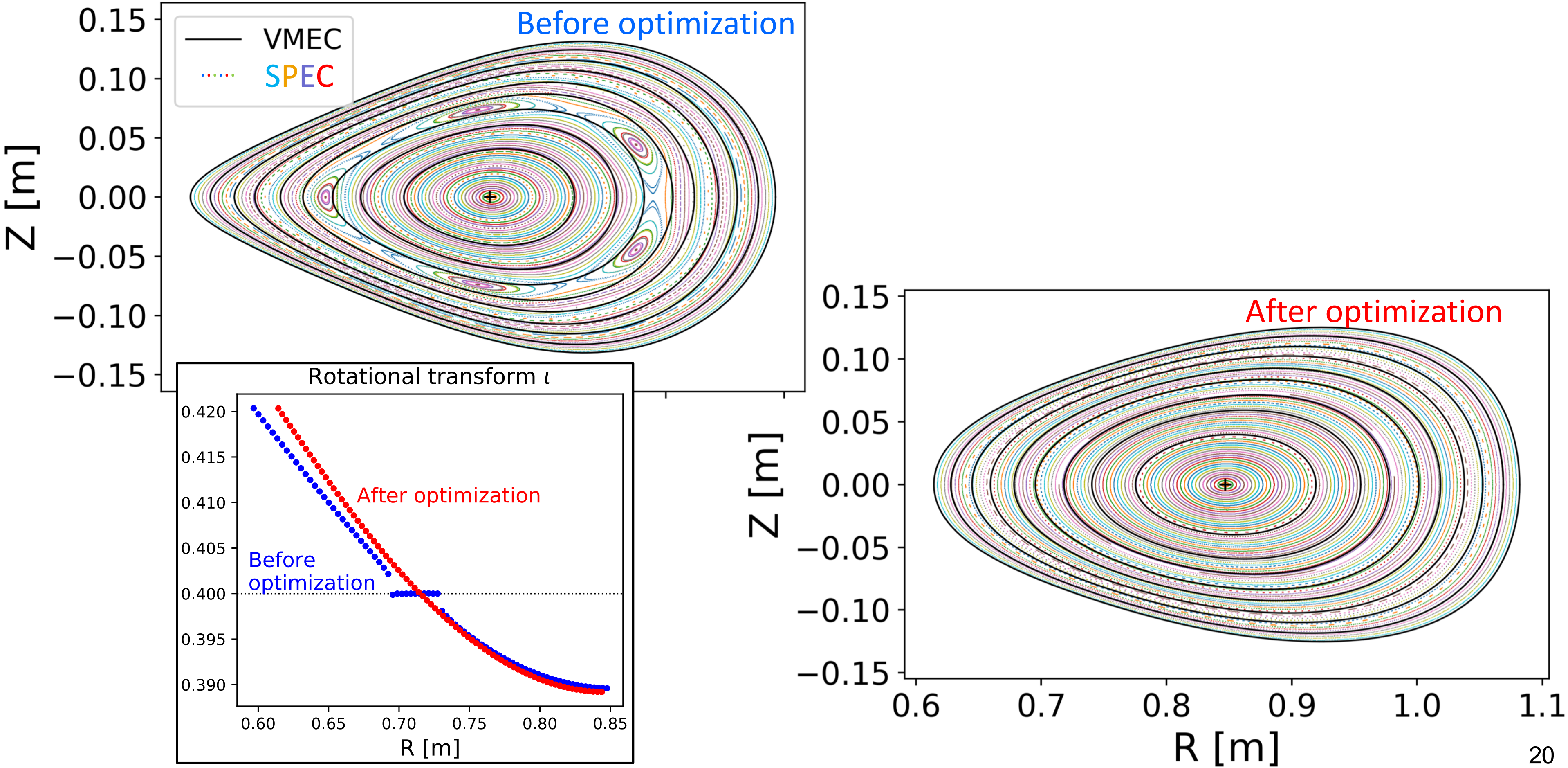
Simsopt driver script applied:

SPEC told to use the same boundary surface object as VMEC.

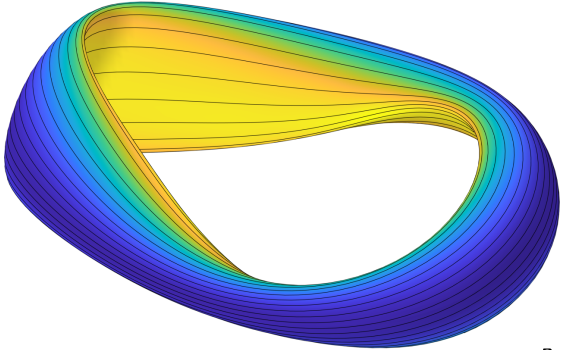
```
mpi = MpiPartition()
vmec = Vmec("input.nfp2_QA”, mpi)
surf = vmec.boundary

spec = Spec("nfp2_QA.sp", mpi)
spec.boundary = surf

# Define parameter space:
surf.all_fixed()
surf.fixed_range(mmin=0, mmax=3,
                 nmin=-3, nmax=3, fixed=False)
surf.set_fixed("rc(0,0)") # Major radius

# Configure quasisymmetry objective:
qs = Quasisymmetry(Boozer(vmec),
                   0.5, # Radius s to target
                   1, 0) # (M, N) you want in |B|

# Specify resonant iota = p / q
p = -2; q = 5
residue1 = Residue(spec, p, q)
residue2 = Residue(spec, p, q, theta=np.pi)

# Define objective function
prob = LeastSquaresProblem([(vmec.aspect, 6, 1),
                            (vmec.iota_axis, 0.39, 1),
                            (vmec.iota_edge, 0.42, 1),
                            (qs, 0, 2),
                            (residue1, 0, 2),
                            (residue2, 0, 2)])

least_squares_mpi_solve(prob, mpi, grad=True)
```

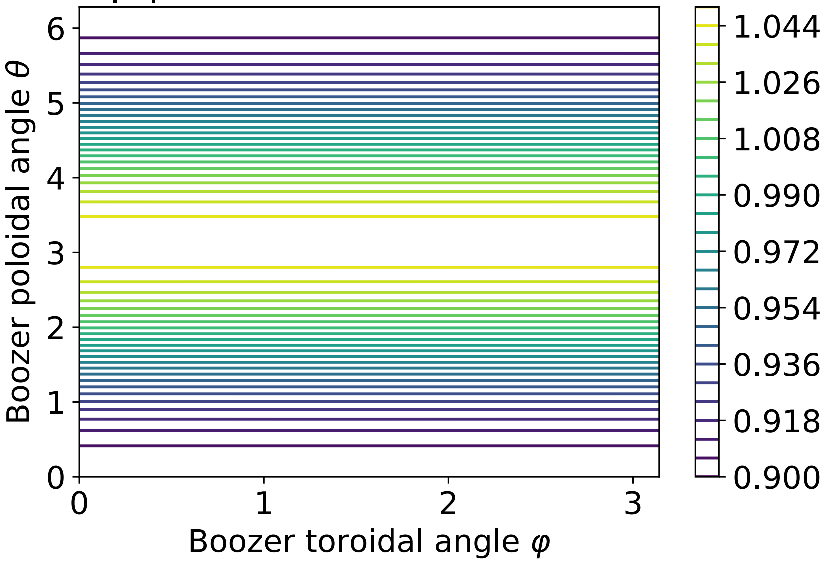
Objective function includes both quasisymmetry from VMEC + booz_xform and residues from SPEC + pyoculus.

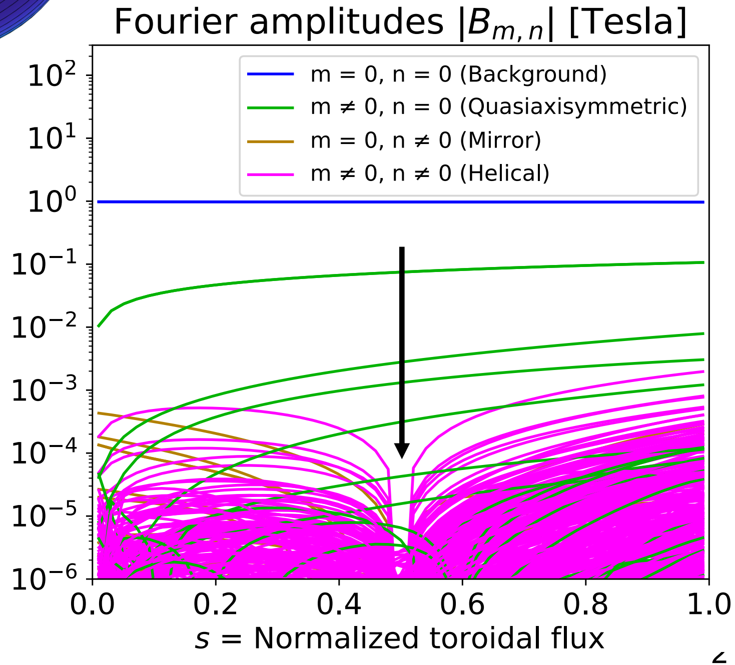
The optimization eliminates the islands



Quasisymmetry is simultaneously improved during the optimization

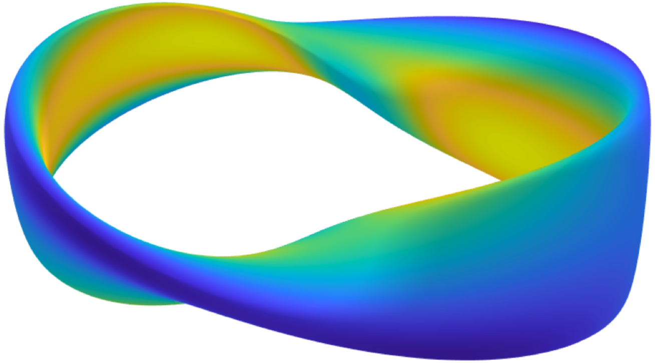



|B| [Tesla] on surface s=0.5
Boozer poloidal angle θ
0
1
2
3
4
5
6
Boozer toroidal angle φ
0
1
2
3
1.044
1.026
1.008
0.990
0.972
0.954
0.936
0.918
0.900

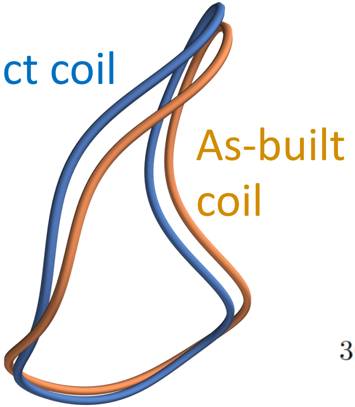


Simsopt objective functions can be plugged into outside libraries

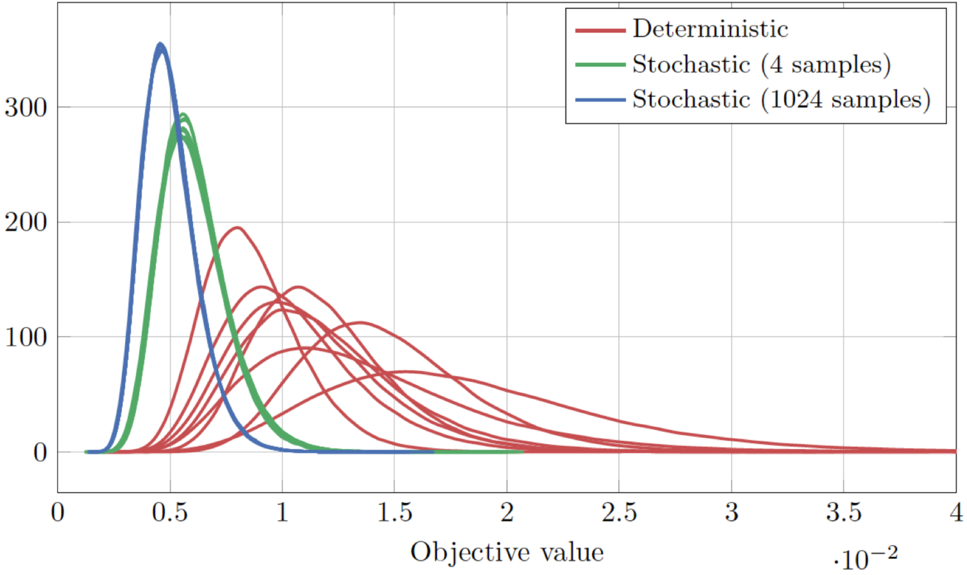
```
# E.g., Bayesian global optimization library TuRBO
from turbo import TurboM
from simsopt import LeastSquaresProblem, ...

# Define objective function as in previous slides:
...
prob = LeastSquaresProblem([(vmec.aspect, 6, 1),
                            (vmec.iota_axis, 0.465, 1),
                            (vmec.iota_edge, 0.495, 1),
                            (qs, 0, 1)])

turbo = TurboM(prob.objective, ...)
turbo.optimize()
```



Simsopt is used for NYU derivative-based stochastic coil optimization



Distribution of objective function given coil shape errors



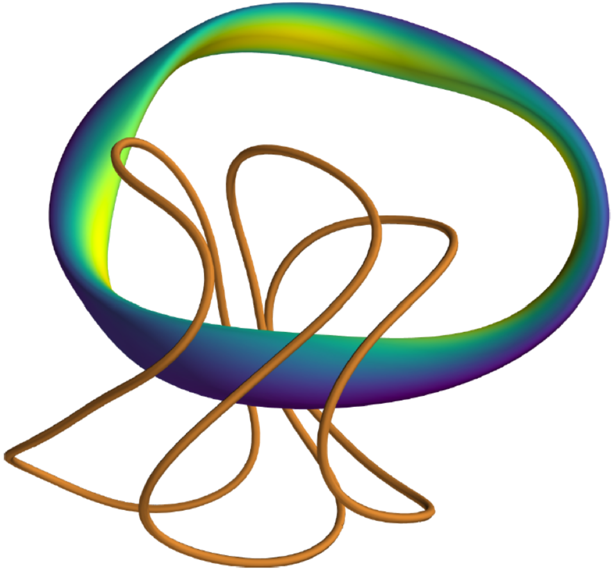
Wechsung, Giuliani, Stadler, et al

- Vision
- Examples
- Design
- Next steps

Design aspects

- Driver and infrastructure is in python.
- New compiled code is in C++, via pybind11.
- Fortran codes (e.g. VMEC, SPEC) interfaced via f90wrap.

A variety of geometric objects and **B** field types have been implemented



Curve subclasses:

CurveXYZFourier, CurveRZFourier, CurveHelical, JaxCurveXYZFourier, RotatedCurve

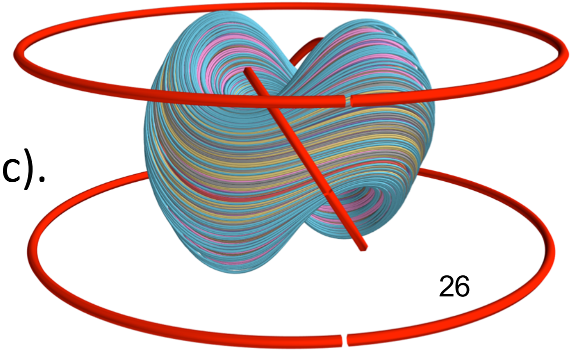
Surface subclasses:

SurfaceRZFourier, SurfaceGarabedian, SurfaceXYZFourier, SurfaceXYZTensorFourier

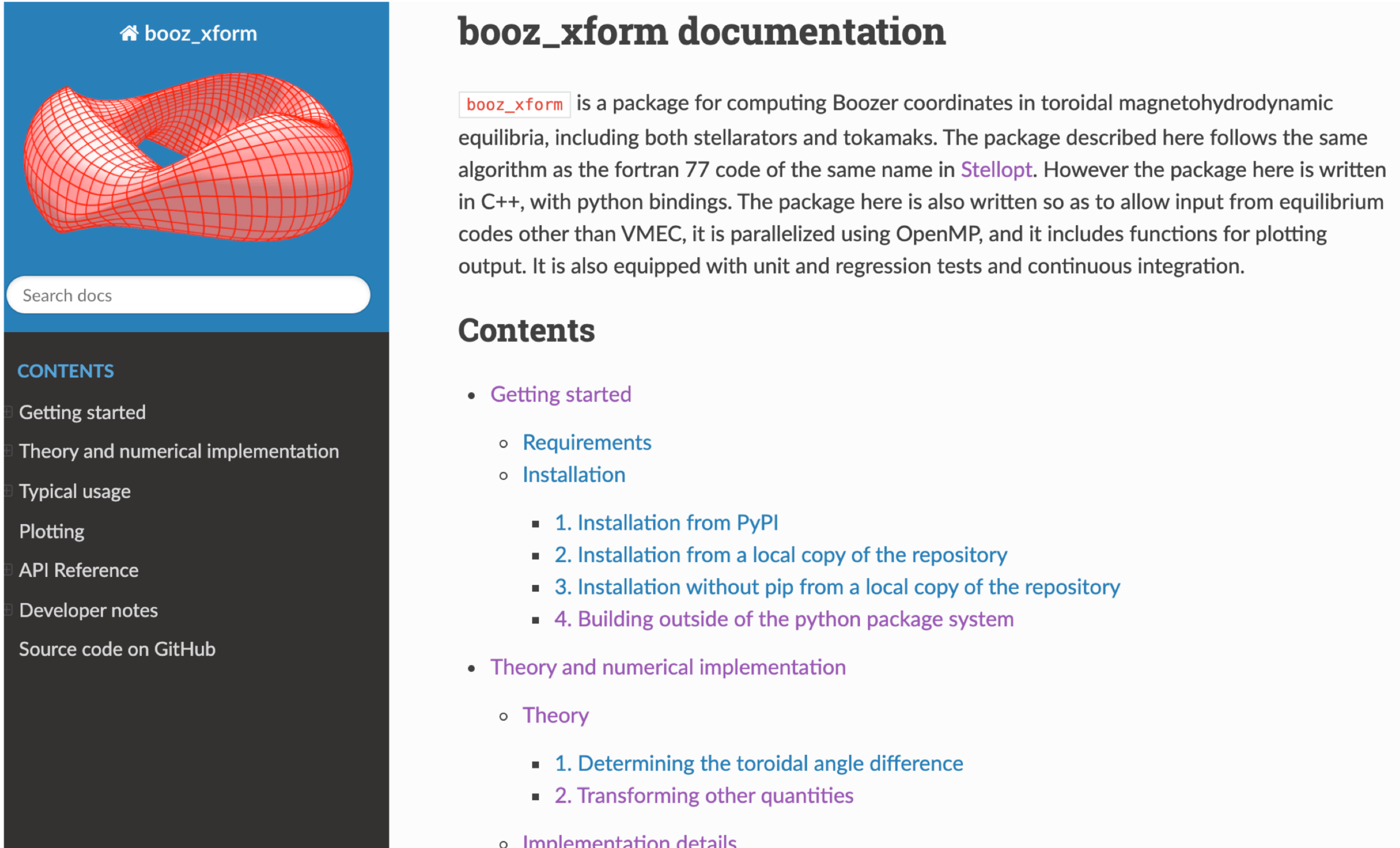
MagneticField subclasses:

BiotSavart, ToroidalField, CircularCoil, Dommaschk, ScalarPotentialRZMagneticField, MagneticFieldSum

- All include 1 or 2 derivatives.
- All can include code in C++ (for speed) & python (for plotting etc).
- All have caching to avoid repeated calculations.
- Example with automatic differentiation is included.



As an example of a new standalone physics module, booz_xform has been re-written



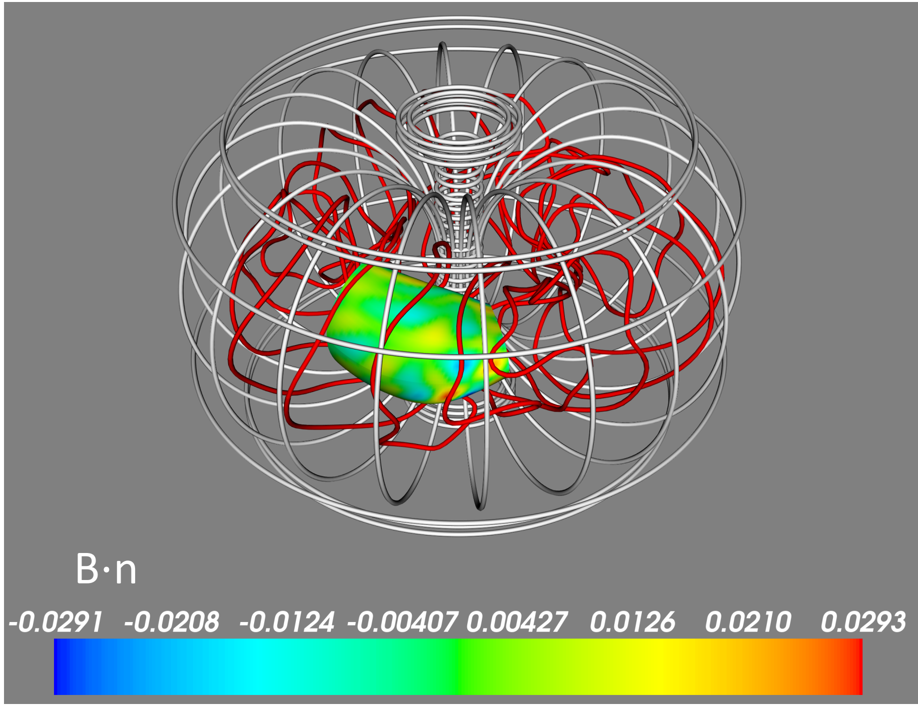
booz_xform documentation

`booz_xform` is a package for computing Boozer coordinates in toroidal magnetohydrodynamic equilibria, including both stellarators and tokamaks. The package described here follows the same algorithm as the fortran 77 code of the same name in Stellopt. However the package here is written in C++, with python bindings. The package here is also written so as to allow input from equilibrium codes other than VMEC, it is parallelized using OpenMP, and it includes functions for plotting output. It is also equipped with unit and regression tests and continuous integration.

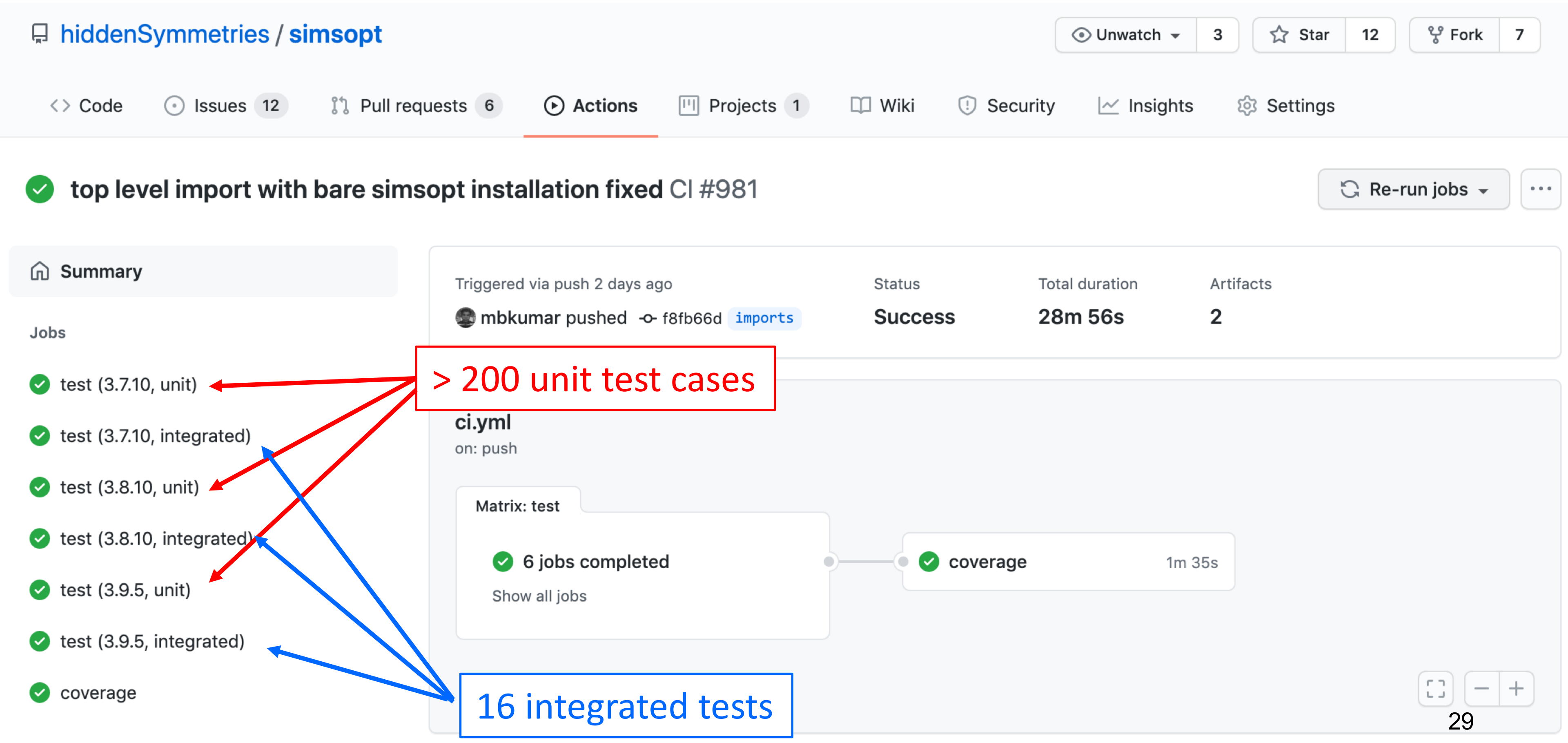
Contents

Simsopt is being designed to handle both derivative-free and derivative-based problems

- Curves, surfaces, and magnetic fields all have 1-2 derivatives implemented.
- Curve types with automatic differentiation are implemented.
- Stage-2 coil optimization with derivatives (FOCUS) with simsopt classes works.
- Presently, simsopt handles naïve multiplication of Jacobians for the chain rule.
- In process of updating the system for defining problems with derivatives, to allow user-controlled forward vs reverse-mode chain rule.



Comprehensive tests are automatically run after every push to GitHub



hiddenSymmetries / simsopt

✓ top level import with bare simsopt installation fixed CI #981

Jobs

- ✓ test (3.7.10, unit)
- ✓ test (3.7.10, integrated)
- ✓ test (3.8.10, unit)
- ✓ test (3.8.10, integrated)
- ✓ test (3.9.5, unit)
- ✓ test (3.9.5, integrated)
- ✓ coverage

Triggered via push 2 days ago	Status	Total duration	Artifacts
mbkumar pushed f8fb66d imports	Success	28m 56s	2

ci.yml
on: push

Matrix: test
✓ 6 jobs completed
Show all jobs

✓ coverage 1m 35s

> 200 unit test cases

16 integrated tests

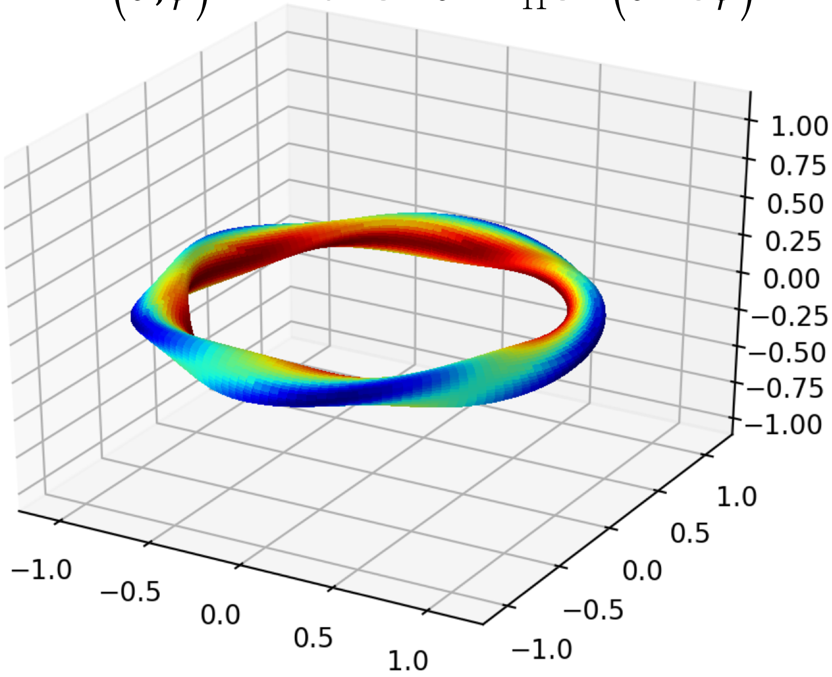
Several benchmark problems have been characterized. Simsopt+spec, simsopt+vmec, and stellopt give the same answer.

`github.com/landreman/stellopt_scenarios`

Boundary:

$$R(\theta,\varphi) = 1 + 0.1\cos\theta + R_{11}\cos(\theta - 5\varphi),$$

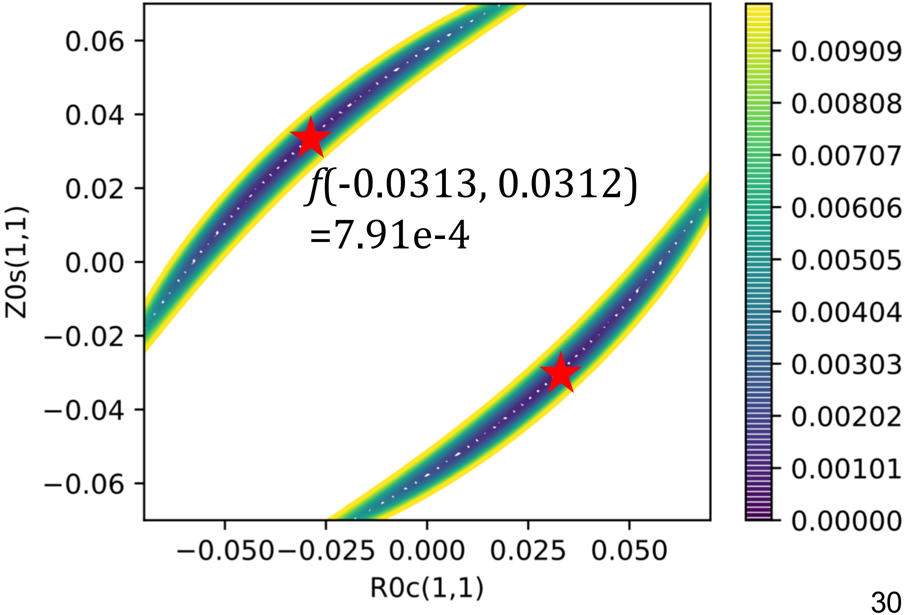
$$Z(\theta,\varphi) = \quad 0.1\sin\theta + Z_{11}\sin(\theta - 5\varphi)$$



Independent variables: $\{R_{11},\ Z_{11}\}$

Objective function:

$$f = (\iota_0 - 0.41)^2 + (\text{volume} - 0.15)^2$$



f(-0.0313, 0.0312) =7.91e-4

- Vision
- Examples
- Design
- Next steps

There are many ways you could contribute

- Parallel global optimization algorithms
- Multi objective algorithms
- Make sure the infrastructure can handle likely use cases
- Adjoint problems by E Paul & A Geraldini
- Set up container for HPC
- Write mgrid files, free boundary VMEC & SPEC
- Implement more measures of integrability
- Interface more physics objectives & codes
- Connect more equilibrium codes: GVEC, DESC, BIEST
- Guiding center trajectory integration
- Add more graphing tools
- …

Closing questions

Any suggested modifications to the structure?

What to prioritize next?

Global optimization, multi-objective optimization, …

What other use cases would you like to be able to handle?

Join the project!

- *Development meetings: Mondays @ 9am NY, 3pm Europe*
- *simsopt slack workspace, #developers channel*
- *mattland@umd.edu*