Regcoil/Stellopt Fourier Winding Surfaces with BFGS Quasi-Newton Algorithm

John C. Schmitt

Thanks to **E. Paul** for QN/BFGS Analytic Fortran Starter Code

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- Overview of BFGS Q-N Algorithm
  - Description
  - Implementation
- Application: Winding Surface Fourier Coefficients to find ‘better’ surfaces
- Comparisons to L-M: Small test, Medium test
- QHS results
- Plans

- Backup slides

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QN BFGS

Algorithm 6.1 (BFGS Method).

Given starting point x_0, convergence tolerance $\epsilon > 0$,
    inverse Hessian approximation H_0;
$k \leftarrow 0$;
while $\|\nabla f_k\| > \epsilon$;
    Compute search direction

$$p_k = -H_k \nabla f_k; \tag{6.18}$$

    Set $x_{k+1} = x_k + \alpha_k p_k$ where α_k is computed from a line search
        procedure to satisfy the Wolfe conditions (3.6);
    Define $s_k = x_{k+1} - x_k$ and $y_k = \nabla f_{k+1} - \nabla f_k$;
    Compute H_{k+1} by means of (6.17);
    $k \leftarrow k + 1$;
end (while)

Numerical Optimization, Nocedal and Wright

The coupled STELLOPT/REGCOIL code

- Vary the winding surface via the Fourier series description
- Selection of results for BFGS and LM
- QHS (4 field period, $\langle R_0 \rangle$ = 6 m, Aspect ratio = 6.7)

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STELLOPT can now manipulate the set of Fourier coefficients that describe the coil winding surface

- Winding surface is specified by a set of Fourier coefficients in toroidal space $(\theta,\ \zeta)$
  - Coordinate system
    - Superimpose Cartesian (X, Y, Z) and spherical (R, ζ, Z)
    - $\theta = \text{atan}\left(\frac{Z}{R}\right)$ Poloidal angle (in the $\mathrm{R}-\mathrm{Z}$ plane)
    - $\zeta = \text{atan}\left(\frac{Y}{Z}\right)$ Toroidal angle (in the $\mathrm{X}-\mathrm{Y}$ plane)
  - The surface (2D manifold) is defined by the locus of point given by

$$R(\theta,\zeta) = \sum R_{m,n,c} \cos(m\theta + n\zeta) + \sum R_{m,n,s} \sin(m\theta + n\zeta)$$

$$\mathrm{Z}(\theta,\zeta) = \sum Z_{m,n,c} \cos(m\theta + n\zeta) + \sum Z_{m,n,s} \sin(m\theta + n\zeta)$$

- Stellarator symmetry is enforced for now
  - With stellarator symmetry, many modes must be 0: All: $R_{m,n,s}$ All: $Z_{m,n,c}$, and some (m,n) combinations
  - The ability to allow non-stellarator symmetry has been implemented, but not tested

- For the work here:
  - Only one 'target': Minimize the residual $|B_{norm}|$ on the target surface
  - Initial guess: A winding surface with a uniform separation (See previous presentations)

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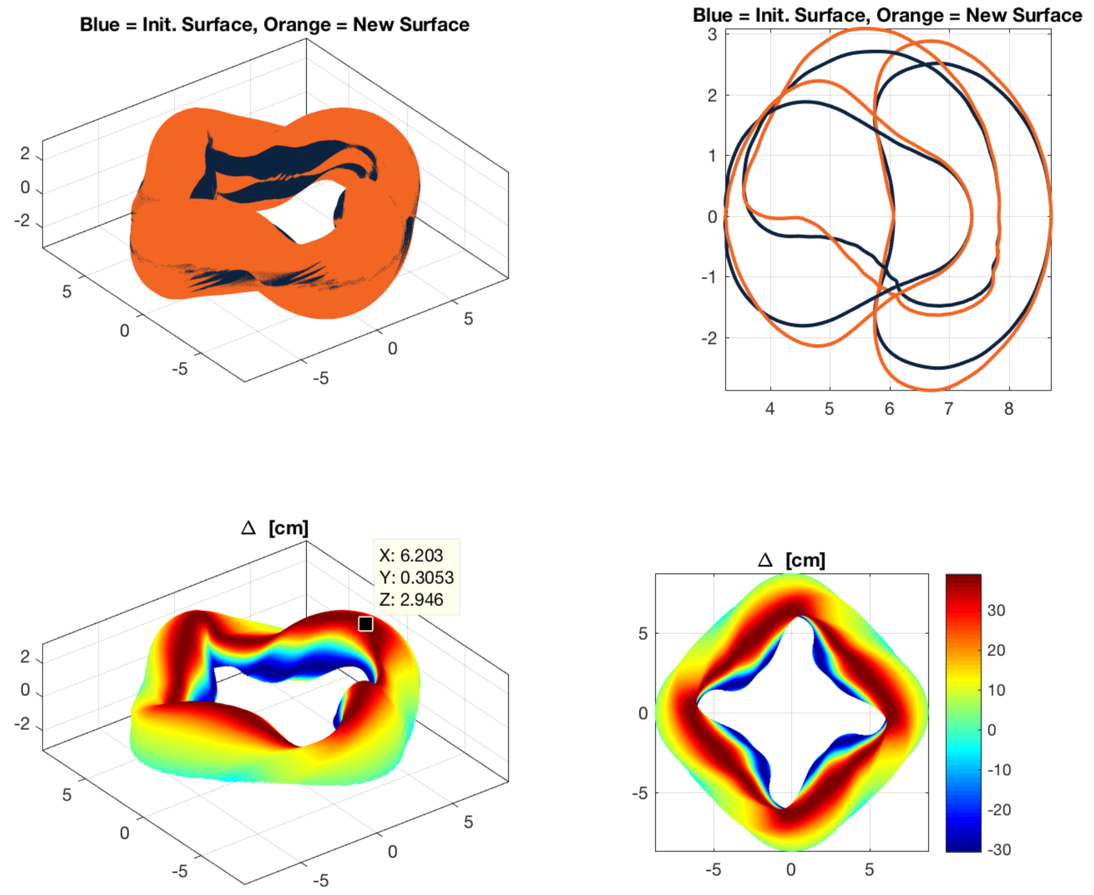
Additional 'recent updates'

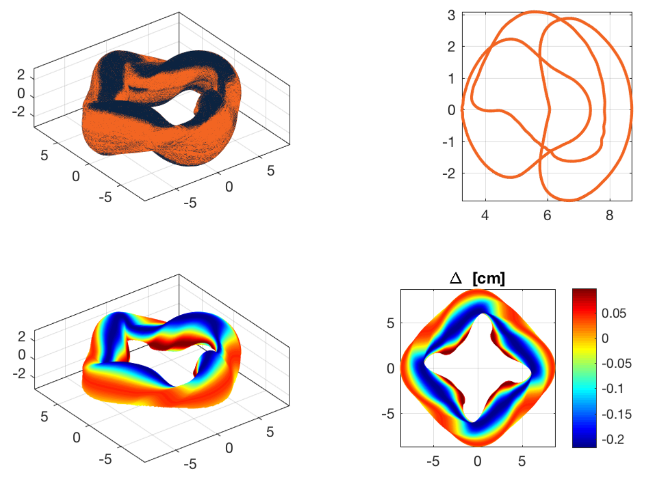
- Quasi-Newton search
  - Shares some aspects of L-M (trust-region finite-difference scheme)
  - The change in the Jacobian between iterations is used to build up an approximation of the (inverse) Hessian
- Version with analytic derivatives -> E. Paul
- Call to Finite Differencing schemes, parallelization -> J. Schmitt

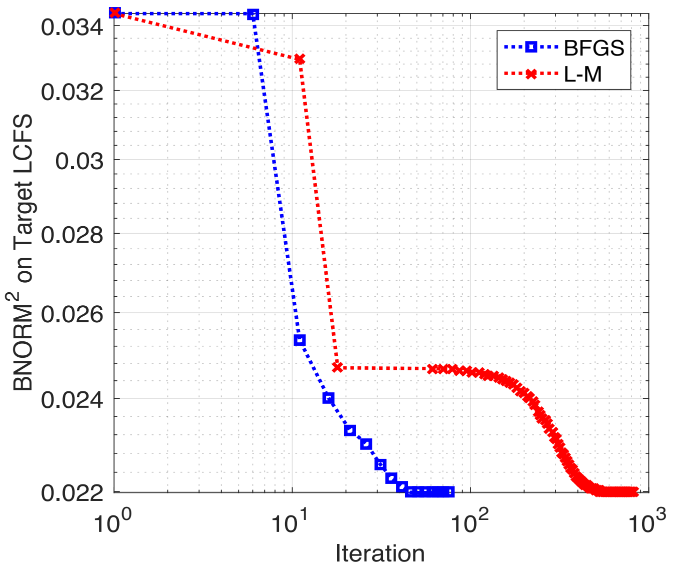
Preliminary comparison, limited spectrum BFGS vs. L-M

- Not quite an 'apples-to-apples' comparison
  - Internal function call count is does not include backtrack.
    - Backtrack calls tend to be in the range of (,)
    - When close to the solution, backtracking calls are in the range of (,)
  - This is fixed in the plots below

’Small’ Test (BFGS & L-M)







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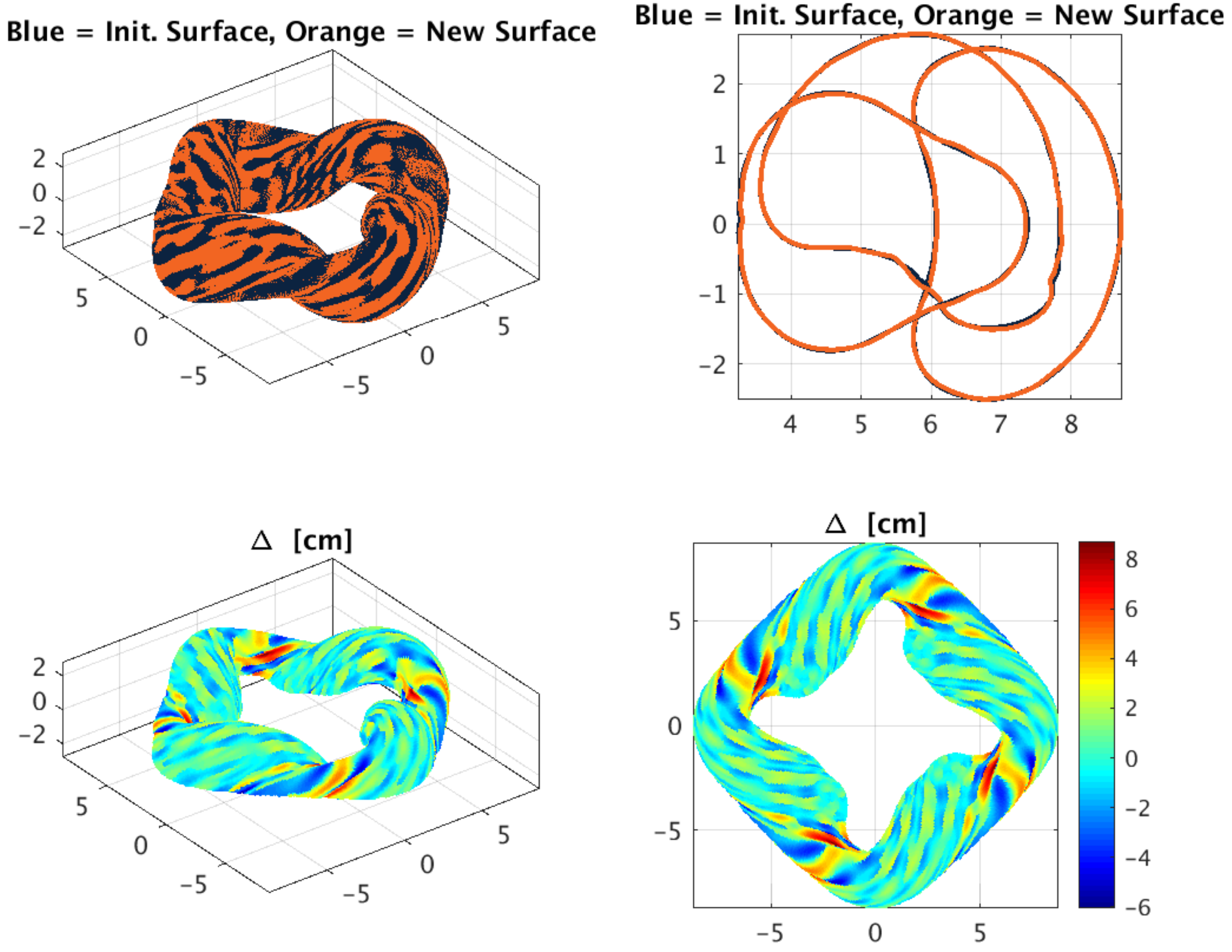
‘Medium’ Tests (BFGS)



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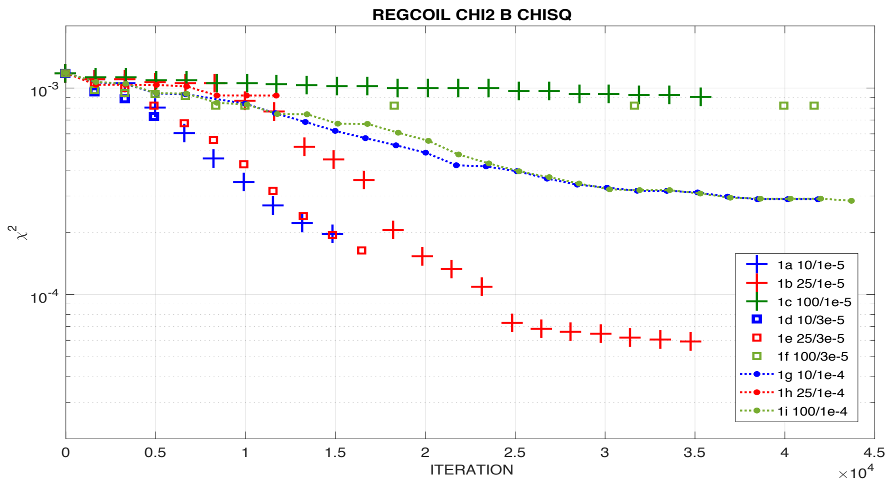
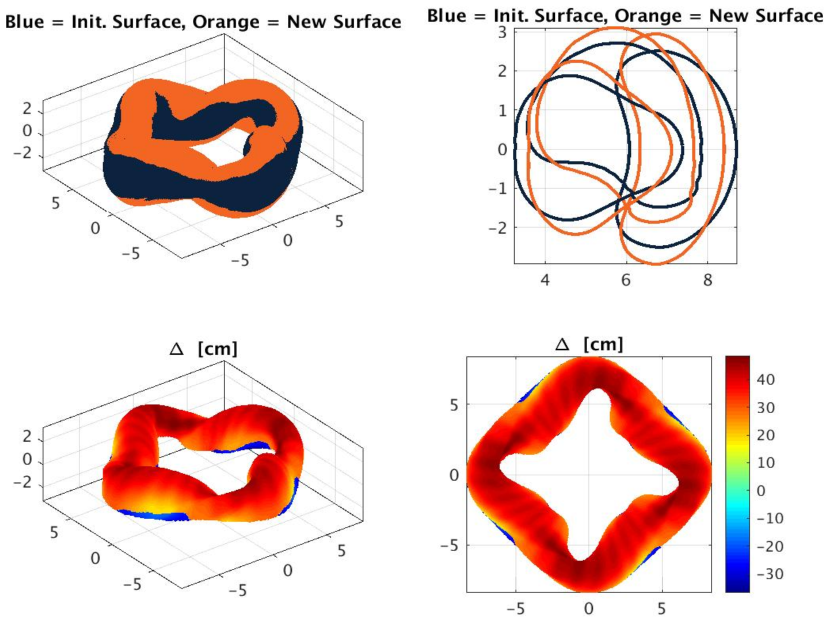
'Large' test (L-M) QHS





- n this test, 1617 harmonics of the winding surface were allowed to be varied ($M \in [0,24]$, $N \in [-16,16]$).
- χ^2 vs Iteration count for several STELLOPT runs with different L-M control parameters, EPSFCN and FACTOR
- Initial winding surface (blue) and Final winding surface (orange). Upper right: Initial and Final surfaces at three toroidal angles in a ½-field period. Lower plots: The distance, in cm, between equivalent grid points of the Initial and Final winding surfaces, color-coded according bar on the right

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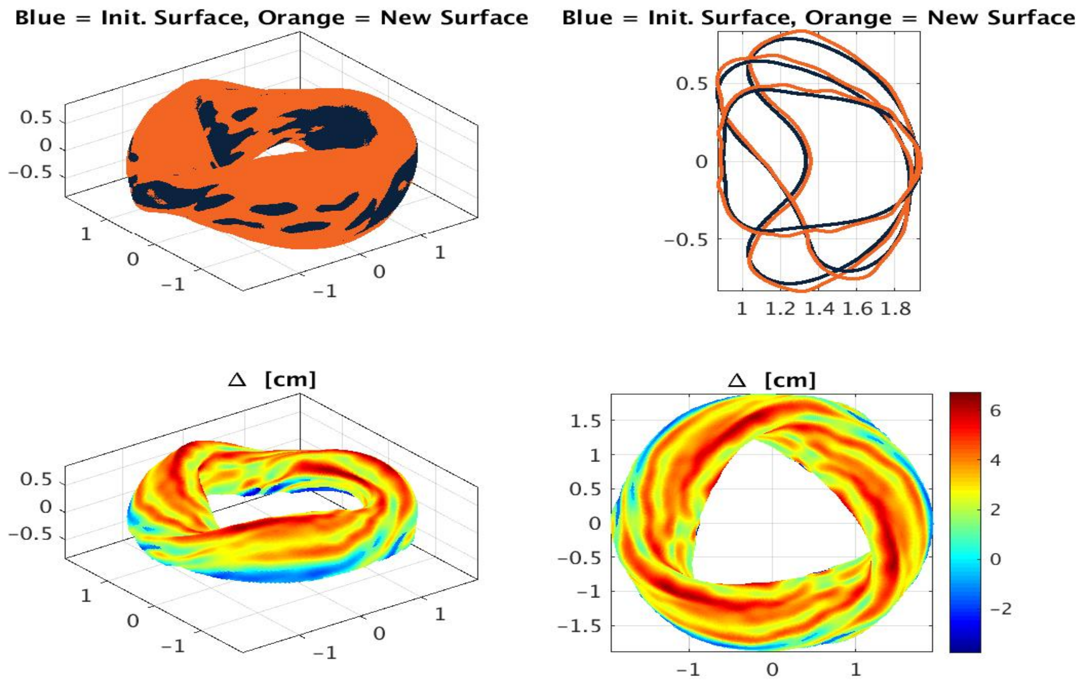
'Large' test (L-M) QHS



- *Initial winding surface (blue) and Final winding surface (orange). Upper right: Initial and Final surfaces at three toroidal angles in a ½-field period. Lower plots: The distance, in cm, between equivalent grid points of the Initial and Final winding surfaces, color-coded according to the bar on the right.*

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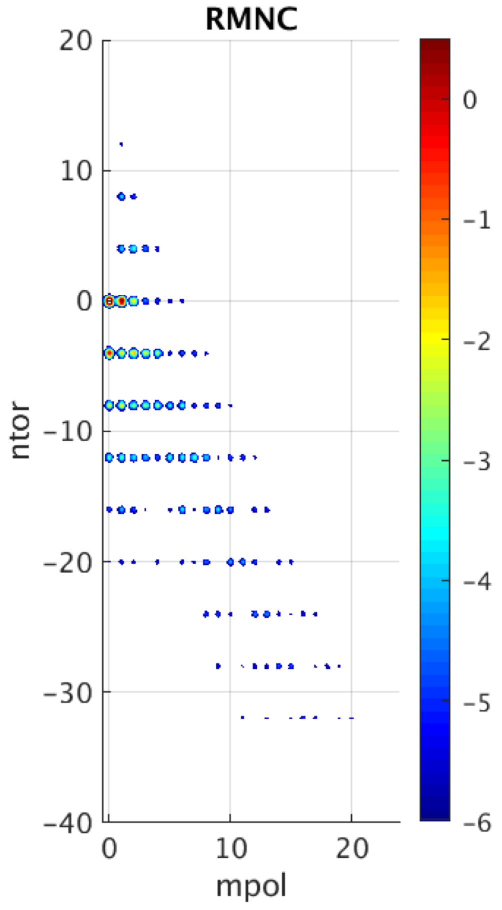
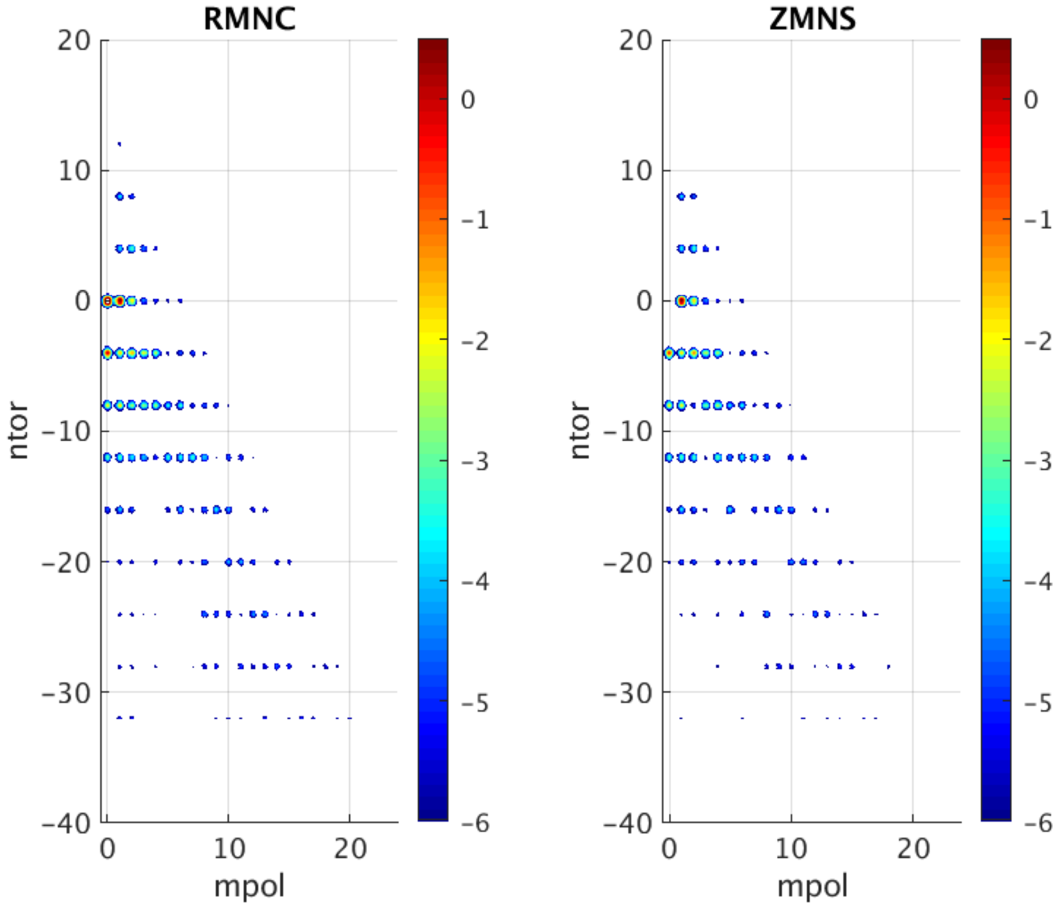
Spectrum Observations





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Next steps

- Fix fcnt implementation
- Fix nprocs ‘bug/feature?’
- Test with non-regcoil constraints
  - Multiple issues w/ other components of stellopt/single vmec equilibrium logic

Backup slides

Preliminary results

- The good
  - Many ‘better’ solutions are found
- The bad
  - L-M routine is extremely finicky
- The ugly
  - Repeated runs with identical starting points, input files and batch submission requests arrive at different solutions

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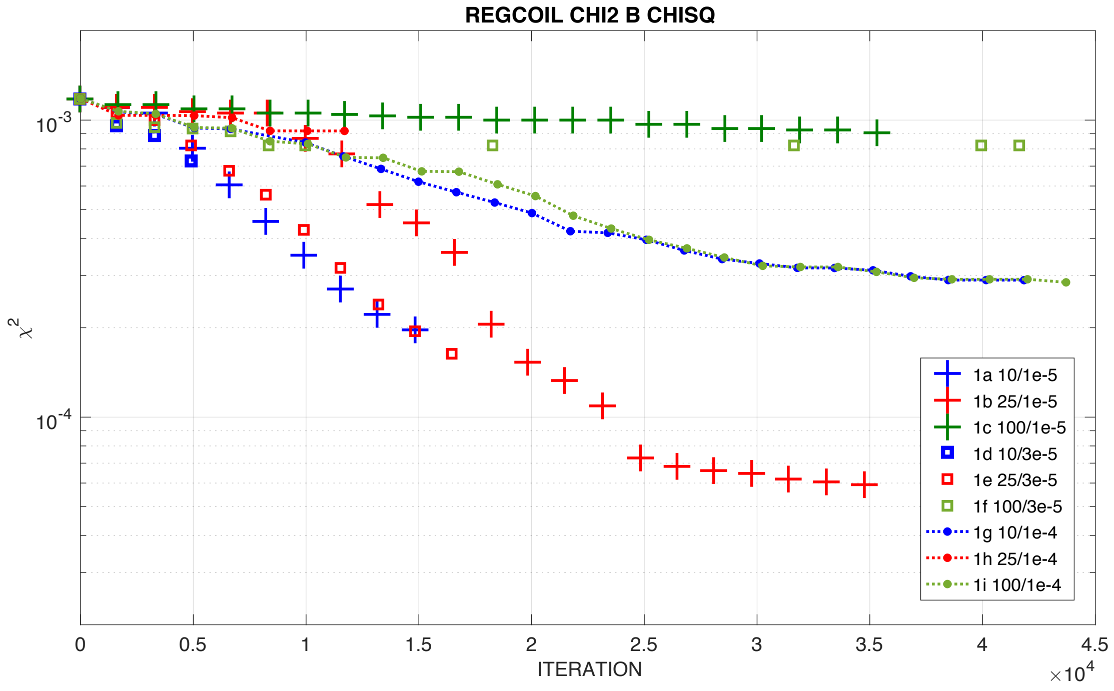
Additional ‘recent updates’

- Equil_type = ‘vmec2000_oneeq’
  - Static MHD VMEC equilibrium: Solve only on the 0^{th} iteration and reuse for all further iterations
  - Useful for coil-optimization loop where equilibrium is not changing
- Quasi-Newton search
  - Shares some aspects of L-M (trust-region finite-difference scheme)
  - The change in the Jacobian between iterations is used to build up an approximation of the Hessian
- Include existing coil sets in calculation – discussed with Matt; Should be straight-forward to implement; Add to list of goals?

STELLOPT finds a better solutions (smaller residual $|B_{norm}|$ on the target surface) when manipulating the Fourier coefficients. A reduction by one order of magnitude compared to the uniform winding surface.

- Initial guess was a winding surface with uniform separation, K_{RMS}= 2.82e6 A/m
- 1618 total harmonics were allowed to be varied
- 1618 identical targets of $\chi^2_{B_{norm}}$
- Behavior exhibits a dependence on L-M optimizer run parameters of FACTOR / EPSFCN
- Time limit reached
  - Cases b, c, f, g, i
- “algorithm estimates that the relative error between x and the solution is at most xtol”
  - Cases a, d, e, h



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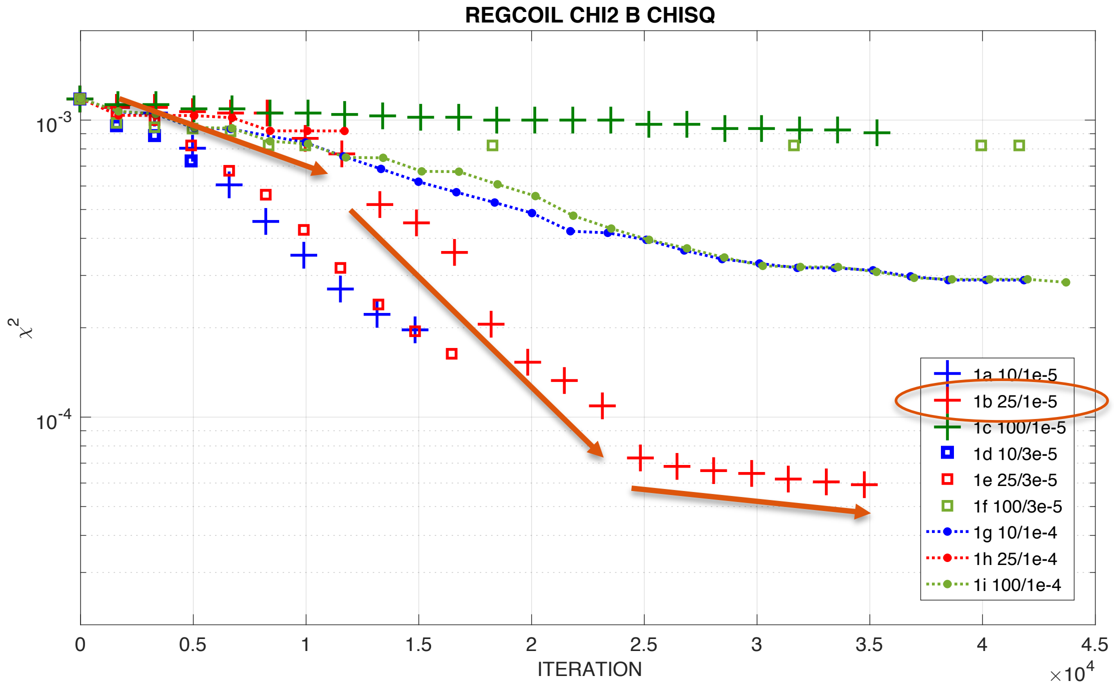
The largest reduction is for L-M options: FACTOR=25; EPSFCN = 1e-5

- This is the case shown in red ‘+’ symbols, see arrows



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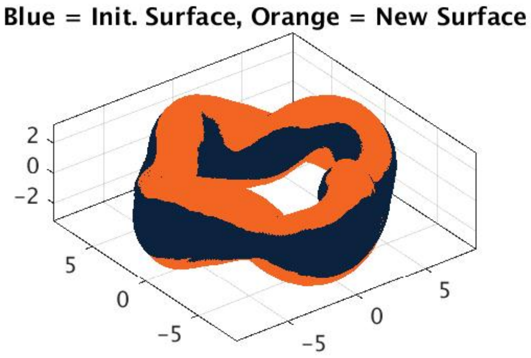
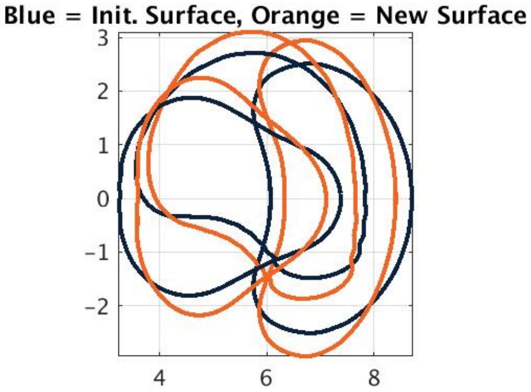
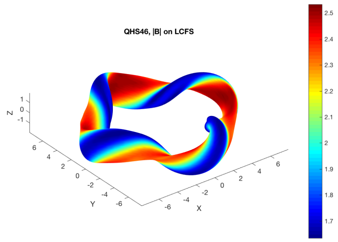
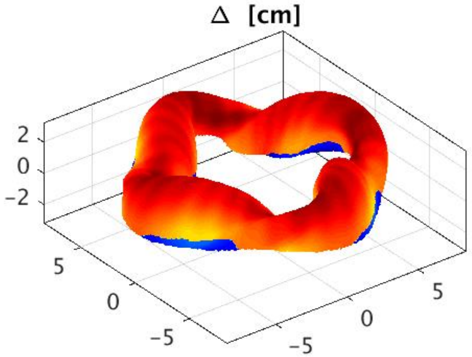
Final iteration of highlighted case

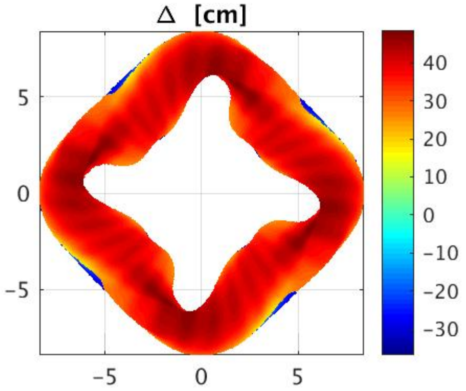
- The solution after the last iteration is teller and narrower than the starting position
- Recall: The starting position was a ‘uniform distance’ away from the plasma boundary











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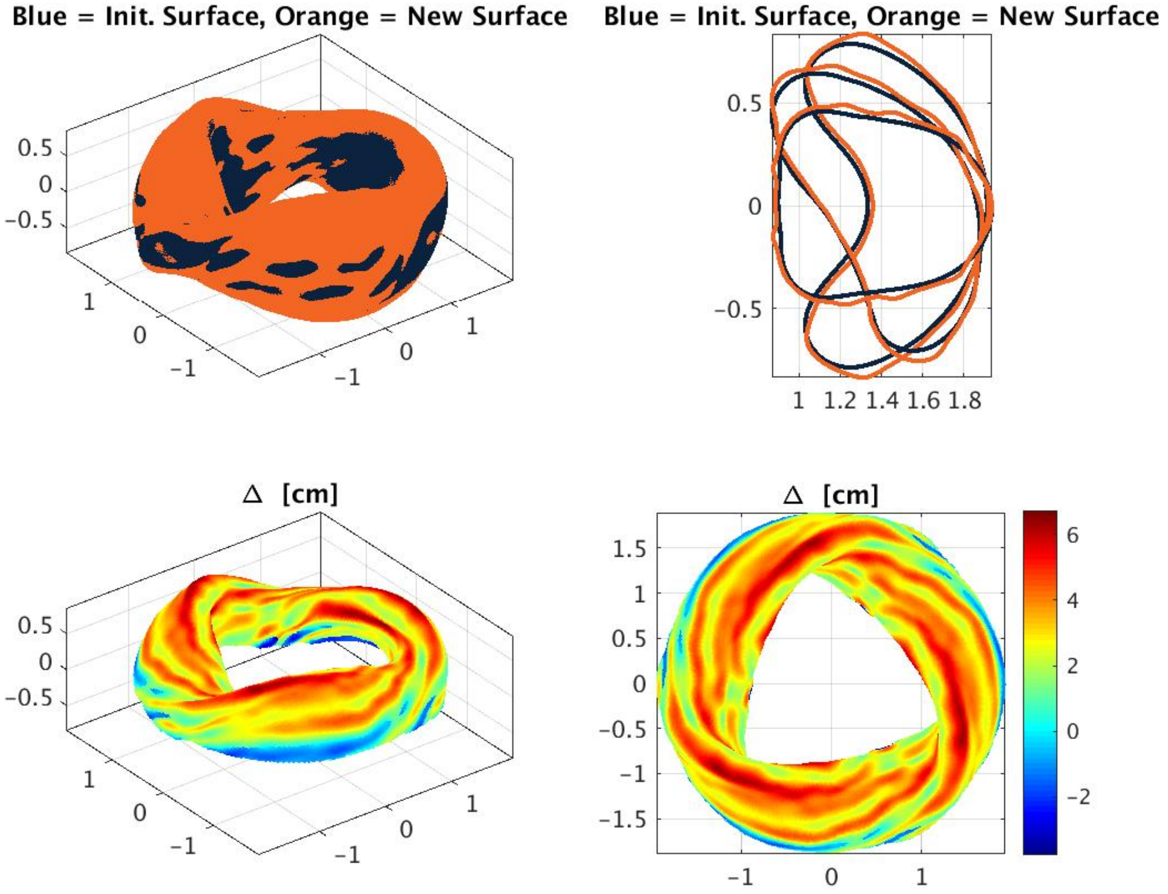
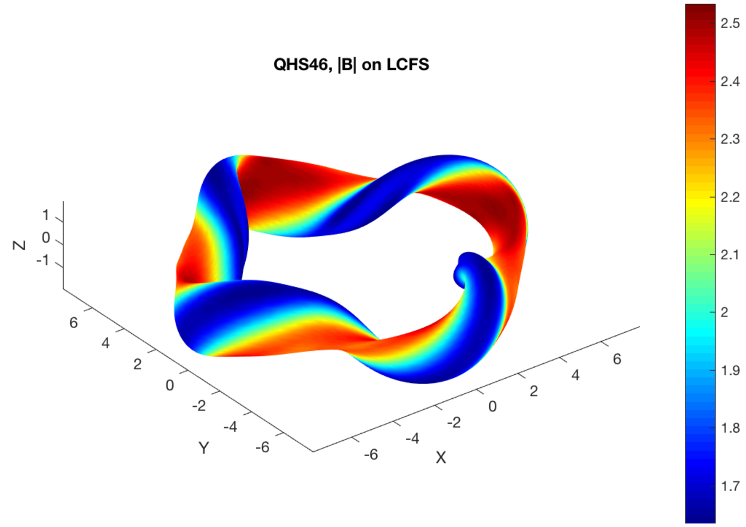
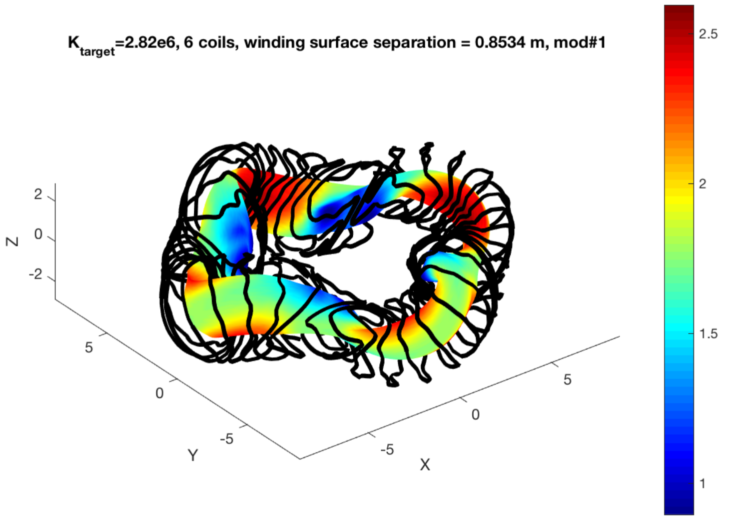
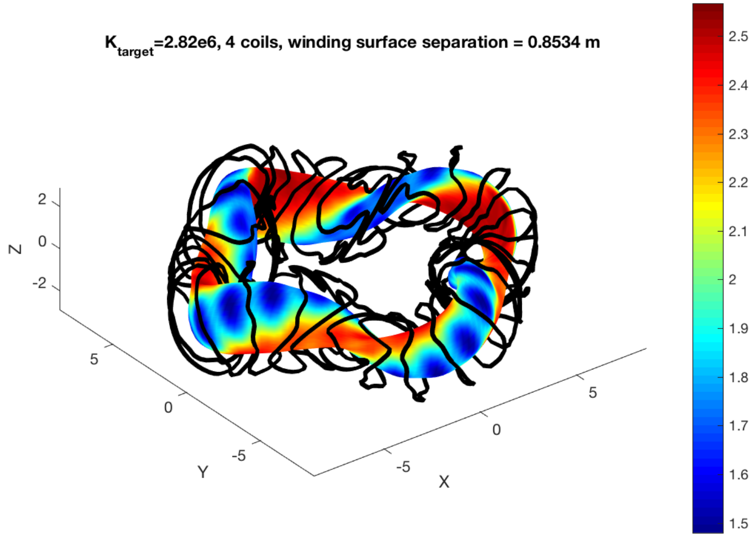
Results for QAS share some characteristics

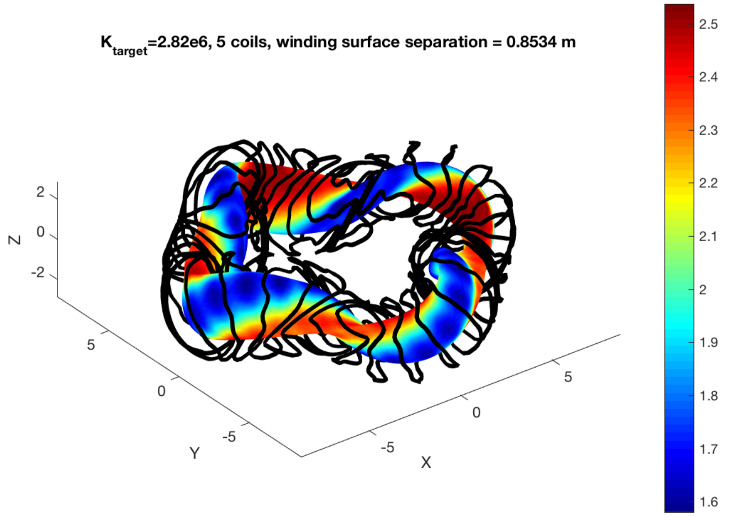


Previous results:
4, 5, or 6 Coils / field period
Uniform winding surface, 2.82e6 A/m









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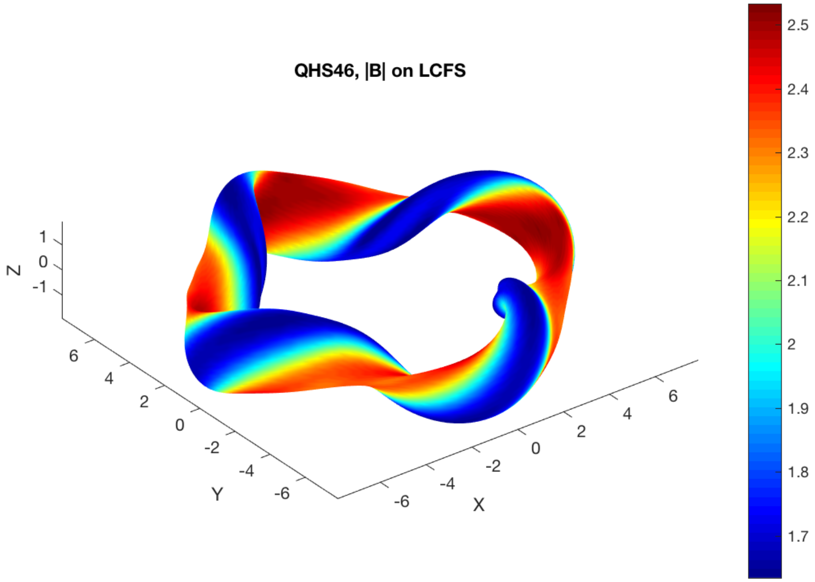
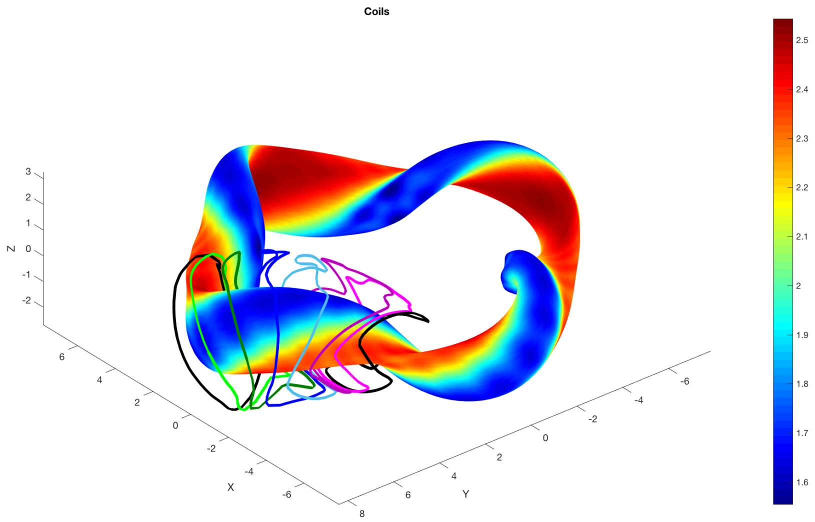
6 Coils / field period
Fourier/Optimized winding surface
2.82e6 A/m on winding surface; 1.5 MA in each coil





Also see the interactive matlab figure:

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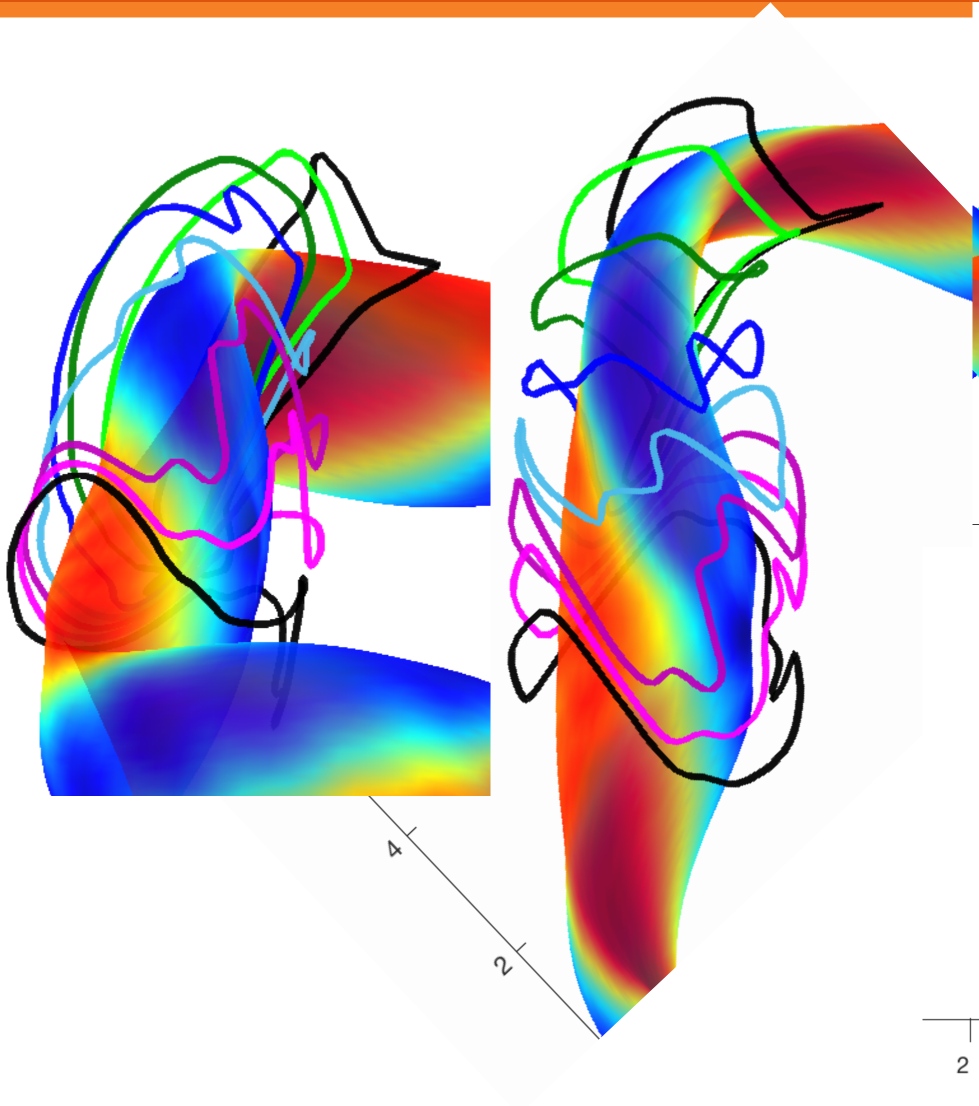
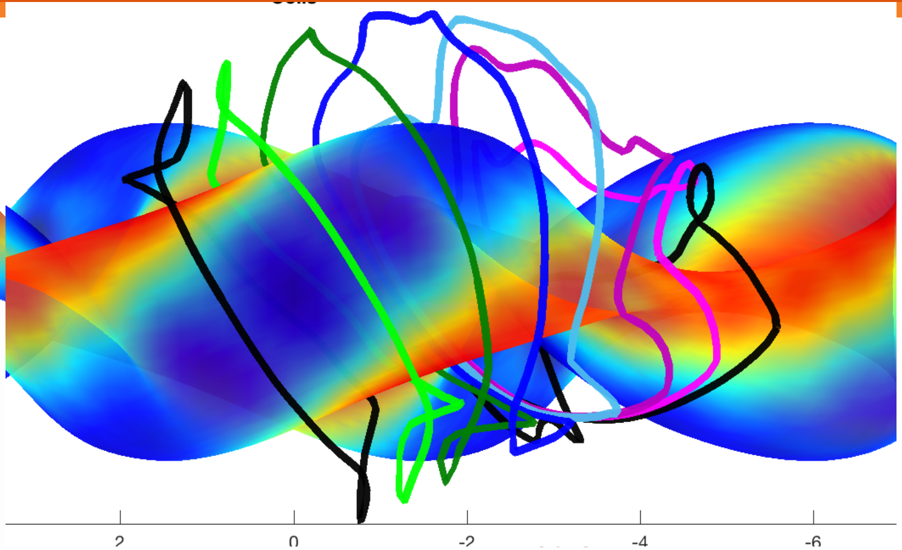
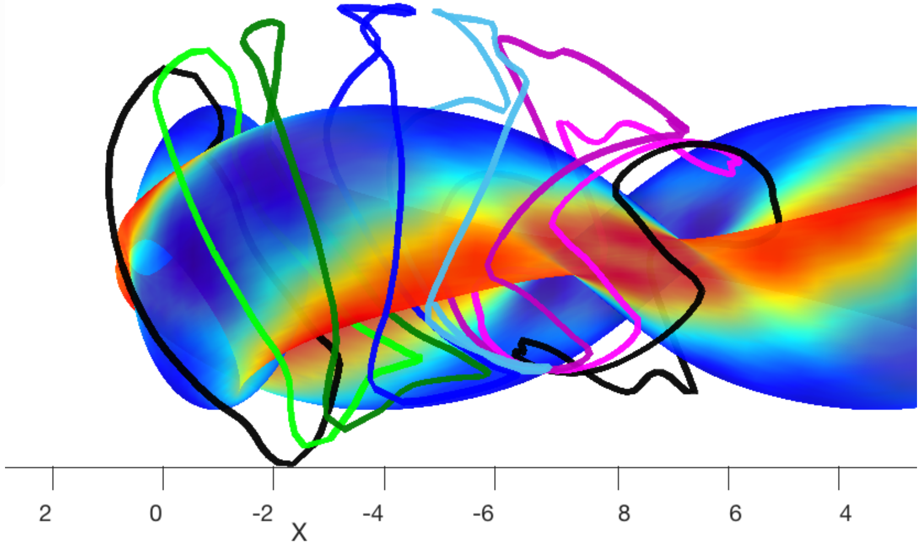
6 Coils / field period
Fourier/Optimized winding surface







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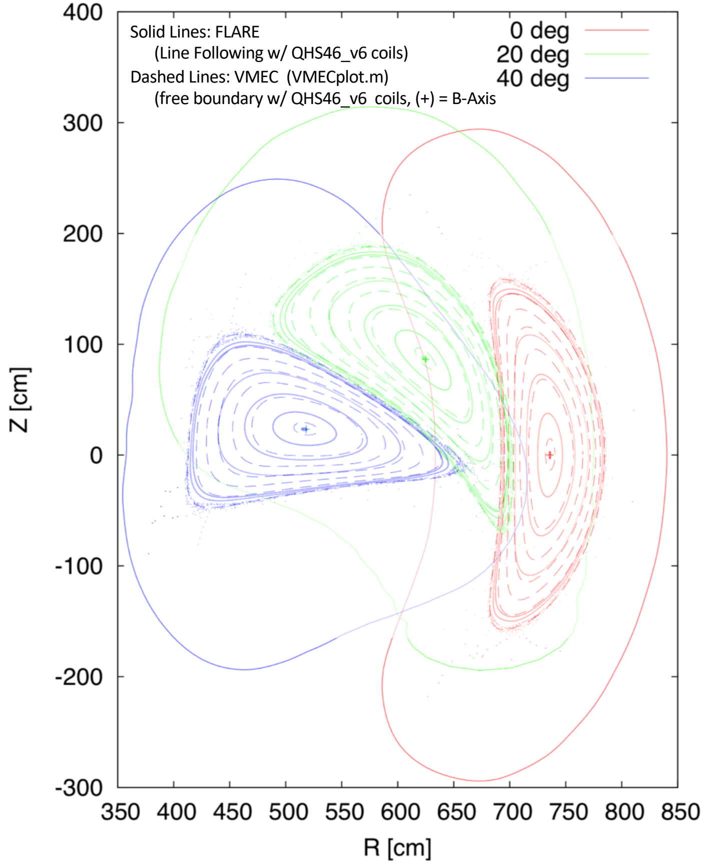
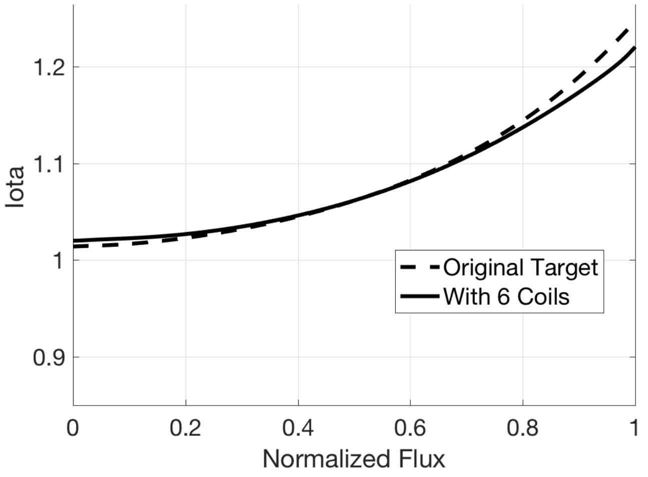
Poincaré plot with field line following compared to VMEC surfaces show agreement up to rational surface at edge

- VMEC vacuum surfaces agree well with field line following* (by eye)
  - Axis is close
  - Shapes are qualitatively similar
  - VMEC's 'last closed flux surface' encloses a small stochastic region
    - Not unexpected





* H. Frerichs, UW

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Preliminary conclusions

- With the freedom to vary the coil winding surface, the stellopt/regcoil search finds many solutions that produce a reduction in Bnorm
  - Lots of ‘local’ solutions
  - Global solution not obvious
  - Adding additional constraints will change this behavior
- For at least one case (QHS), a set of 6 finite (filamentary) coils produce satisfactory results (VMEC and Field-line following)

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Next steps

- Optimization
  - Make sure target, variable and L-M options are correct/consistent; Loose ends?
  - How do the coils change from their ‘optimal locations’ with Small, Medium, and Large changes in target K_{RMS}
    - On static winding surface (for small changes) and on varying one (via Fourier coeffs)
  - Add more constraints

- Code development
  - Target (penalize) plasmas with cusps
  - Target (RMS) current density
  - Coil-cutting (2D manifold contour map of a scalar gradient in 3D space)
  - Include existing coil sets in calculation
  - Q-N (*Partially complete)

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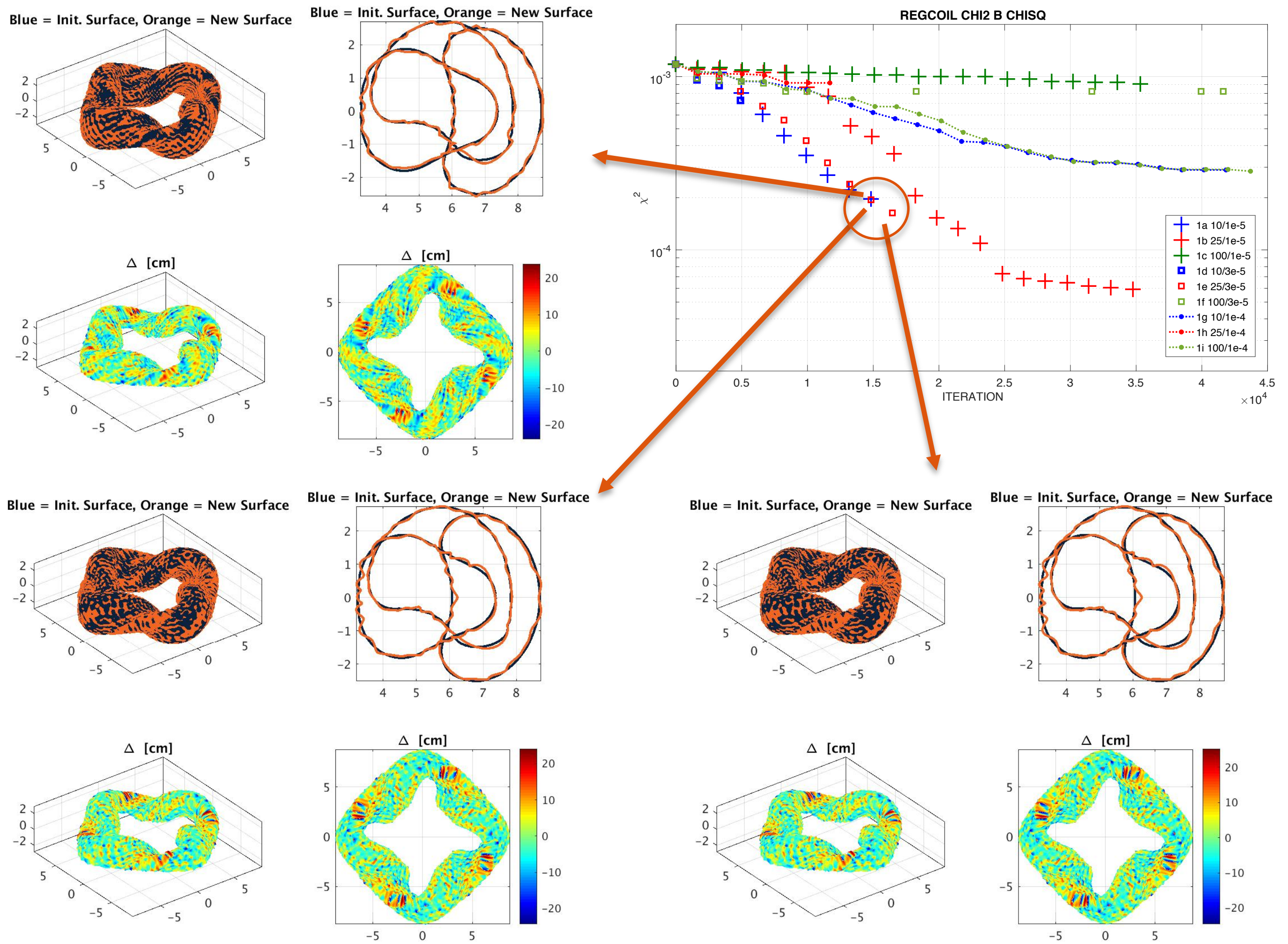
Extra slides

The optimizer runs that demonstrated the most rapid descent A) look a little different, B) are still evolving, and C) terminated because the solver was in a local minimum (I think)

- The surfaces of the two branches that descend more rapidly, but are truncated, look a little different
- blue +'s (upper left)
- red squares (lower left)

- The red square descent path has one extra step – see lower right plots

➢ **The solver got stuck in a local minimum?**
  ➢ "algorithm estimates that the relative error between x and the solution is at most xtol"



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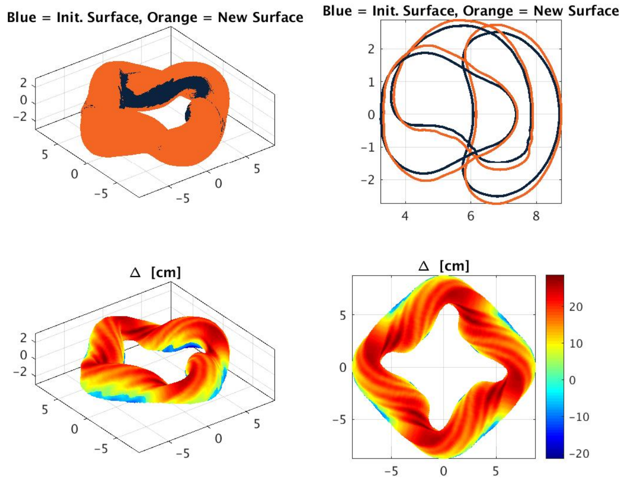
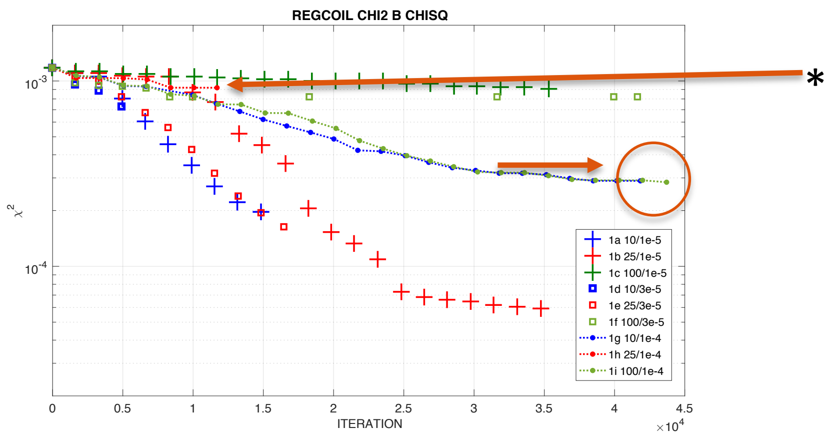
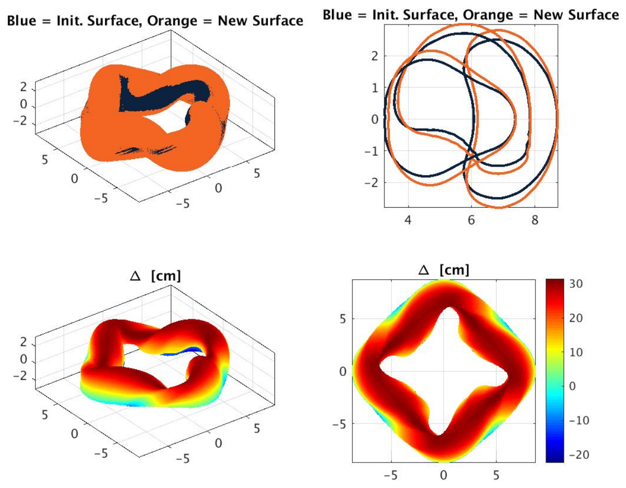
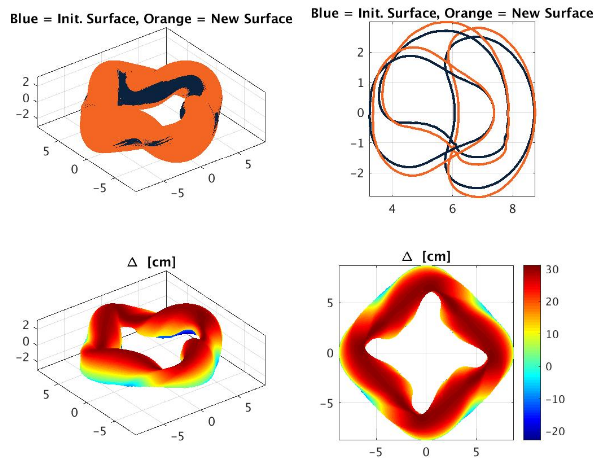
The optimizer branch that descends more slowly looks vaguely like the ‘best’ case: Taller, **but less narrow**!



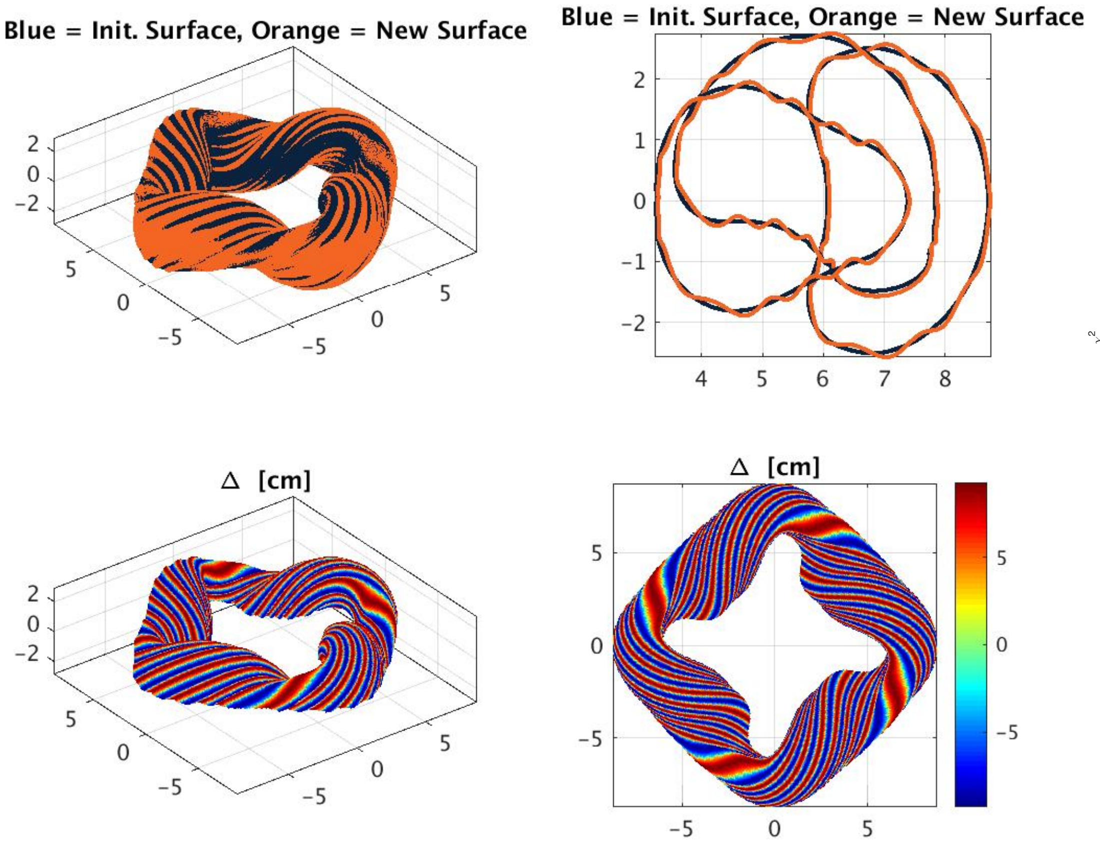


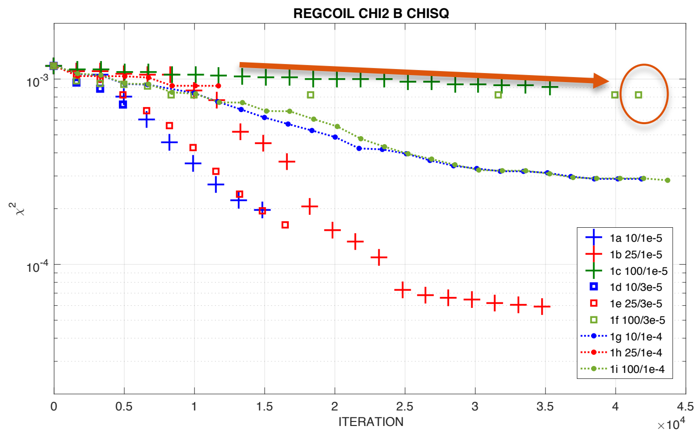




Helical Stripes: The runs that descend very slowly has very corrugated surfaces.

Helica has
very c





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Comparison of QHS46 Fourier Optimized coils to HSX coils which have been scaled to the same effective major radius as QHS46

- The (HSX) QHS configuration and coilset are scaled to match the same effective major radius as the QHS46 configuration that I have been using for the STELLOPT/REGCOIL studies
  - Scale factor: 6.025006 / 1.211364 (~ 5)
- The scaled QHS configuration was run through VMEC (fixed boundary)
  - Started with input.QHS_Rstart_1_513_32polmodes_18x24_axis_v2
  - Scaled the boundary. New filename: input.hsx_scaled_to_QHS46
    - I forgot to scale the axis; VMEC detected this, found a new axis and proceeded to converge
  - Started with coils.hsx_1fil
  - Scaled the coils (with read_coils_scaled.m, a modified version of read_coils.m)
  - Coil data structure is stored in matlab data file: HSX_coils_scaled_to_QHS.mat

- Slide 29: Short list of geometric quantities for the two configurations
- Slides 30-31: |B| on the LCFS and a subset of the coils for this scaled configuration are compared to the |B| and coils of QSH46 with the Fourier Optimized Winding Surface (FOWS)
- See additional slides: The individual coils are plotted on the same axes

Slide 32 – Final comments

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A comparison of a few geometric quantities (from the threed1 output files)

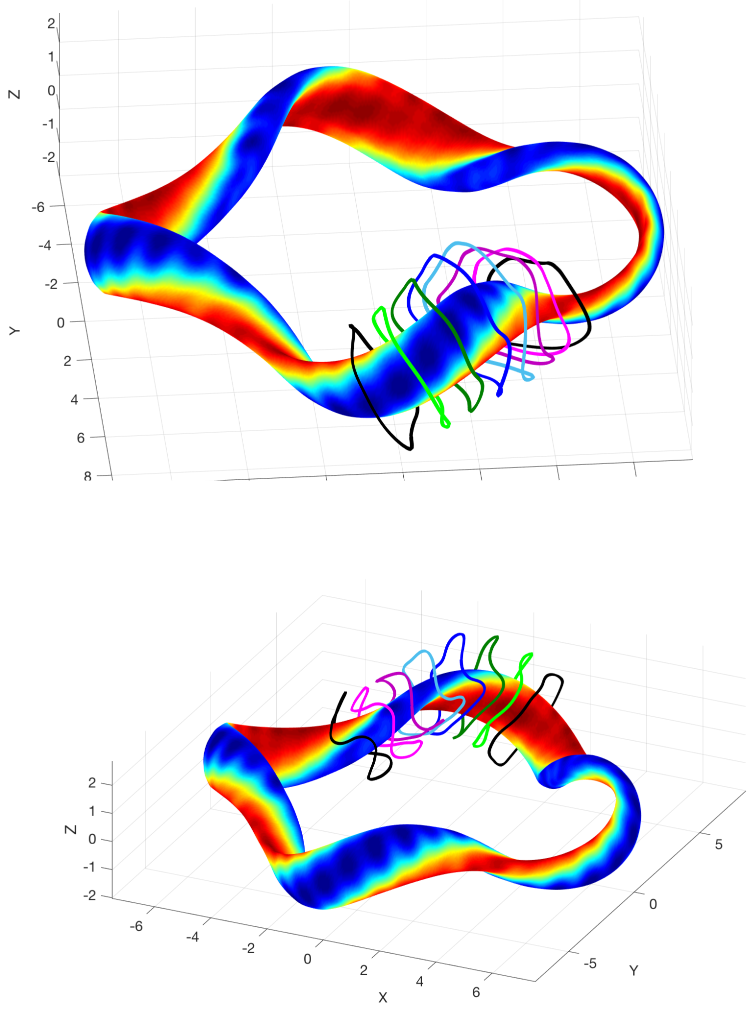
HSX, scaled

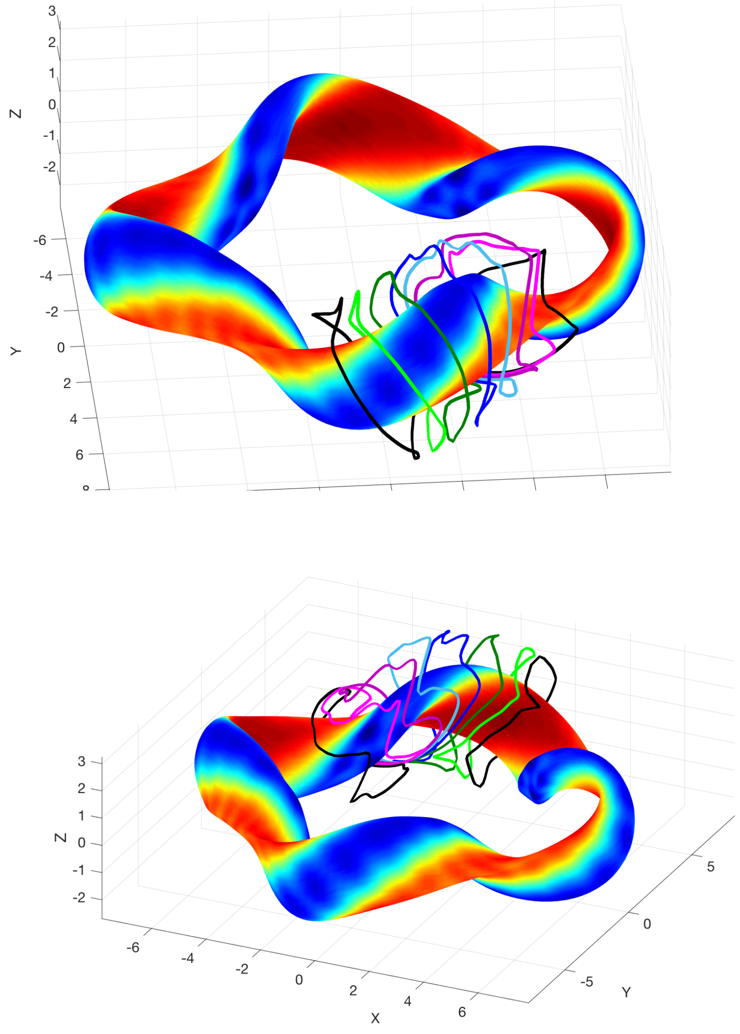
- **Aspect Ratio = 9.970152**
- Mean Elongation = 3.851684
- **Plasma Volume = 43.430845 [M**3]**
- **Cross Sectional Area = 1.147258 [M**2]**
- Normal Surface Area = 193.205616 [M**2]
- Poloidal Circumference= 4.693414 [M]
- **Major Radius = 6.025005 [M] (from Volume and Cross Section)**
- **Minor Radius = 0.604304 [M] (from Cross Section)**
- Minimum (inboard) R = 4.438649 [M]
- Maximum (outboard) R = 7.525447 [M]
- Maximum height Z = 1.562752 [M]

QHS46, 6 Coils on FOWS

- **Aspect Ratio = 6.699959**
- Mean Elongation = 4.064947
- **Plasma Volume = 96.174025 [M**3]**
- **Cross Sectional Area = 2.540507 [M**2]**
- Normal Surface Area = 293.721616 [M**2]
- Poloidal Circumference= 7.033194 [M]
- **Major Radius = 6.025006 [M] (from Volume and Cross Section)**
- **Minor Radius = 0.899260 [M] (from Cross Section)**
- Minimum (inboard) R = 4.108455 [M]
- Maximum (outboard) R = 7.840492 [M]
- Maximum height Z = 1.951591 [M]

Left: HSX (scaled)   Right: QHS46





Left: HSX (scaled)   Right: QHS46