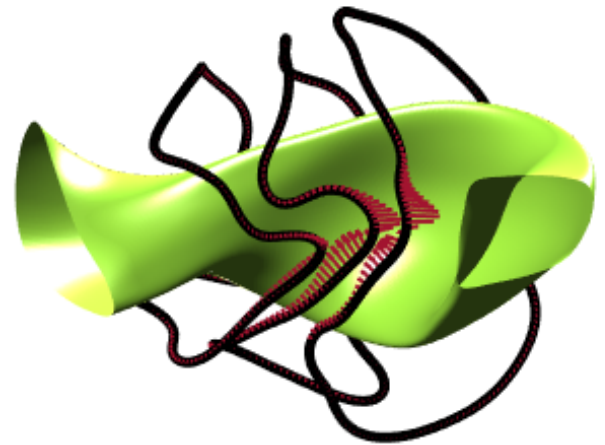


Adjoint methods for efficient stellarator optimization and sensitivity analysis

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University of Maryland, College Park

Sherwood Fusion Theory
Conference
April 15, 2019

Outline

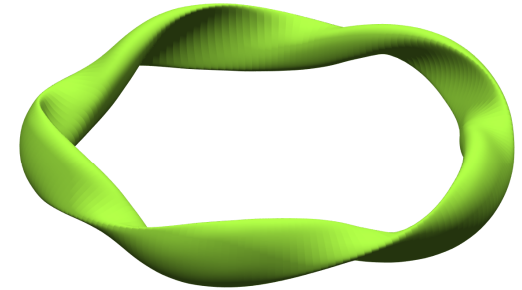
- **Introduction to shape optimization ideas**
- Adjoint stellarator coil design
- Adjoint drift kinetic equation for neoclassical optimization
- Shape gradients for MHD equilibria

Designing a stellarator requires shape optimization

MHD equilibria

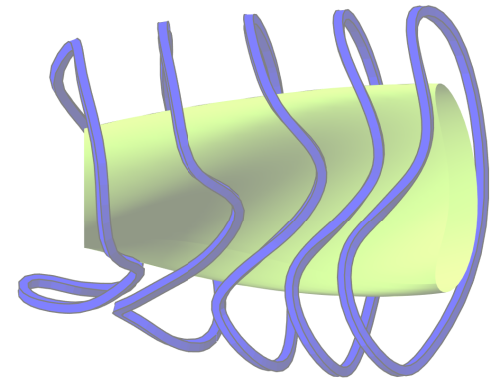
- Plasma boundary determines magnetic geometry
- Figures of merit depend on boundary shape (e.g. neoclassical confinement, stability)

How should one design boundary to obtain optimal configuration?



Coil design

How to design coils to obtain desired plasma boundary?
How sensitive is a figure of merit to coil displacements?

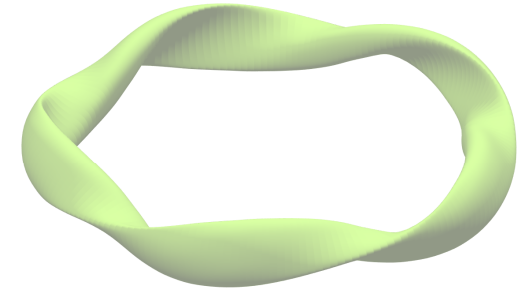


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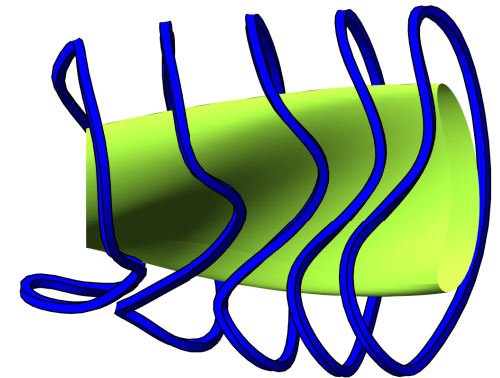
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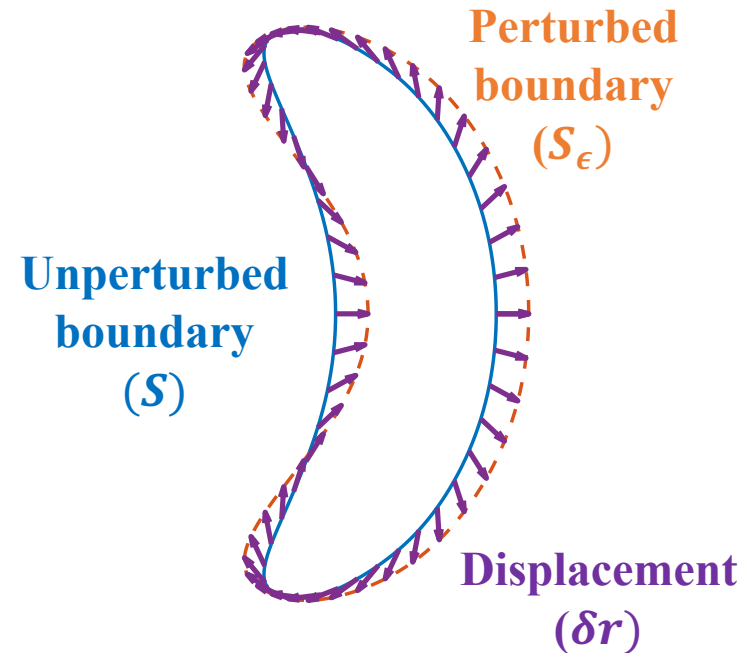
Describing derivatives with respect to shape

- Consider $f(S)$, a functional of surface, S
- Surface is displaced by vector field $\delta \mathbf{r}$

$$S_\epsilon = \{\mathbf{r}_0 + \epsilon \delta \mathbf{r} : \mathbf{r}_0 \in S\}$$

- Shape derivative of $f(S)$

$$\delta f(S; \delta \mathbf{r}) = \lim_{\epsilon \rightarrow 0} \frac{f(S_\epsilon) - f(S)}{\epsilon}$$



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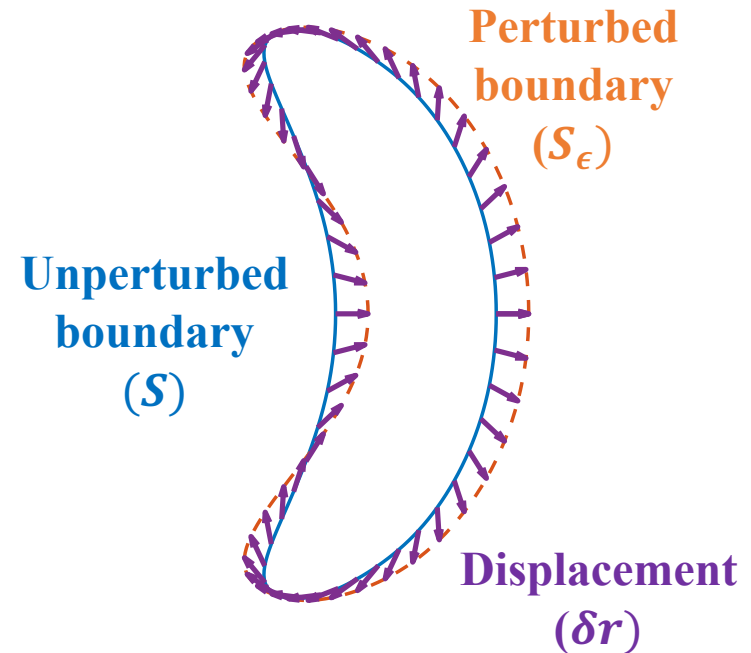
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$$\delta f(S; \delta \mathbf{r}) = \int_S d^2x \, \delta \mathbf{r} \cdot \mathbf{n} \, \mathcal{G}$$

- For *any* $\delta \mathbf{r}$, shape gradient, $\mathcal{G}$, provides change to figure of merit, δf



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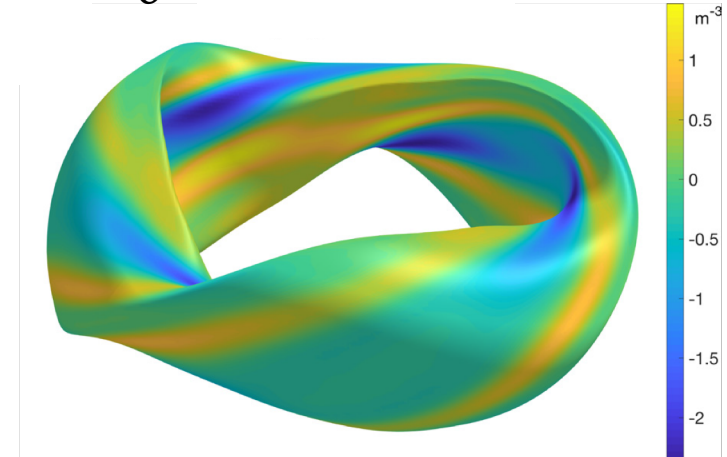
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$\mathcal{G}$ for rotational transform



M. Landreman & E.J. Paul, *Nuclear Fusion* 58 (2018).

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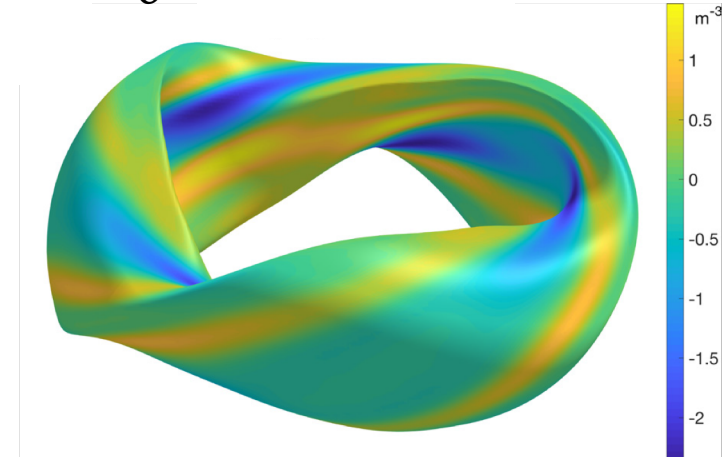
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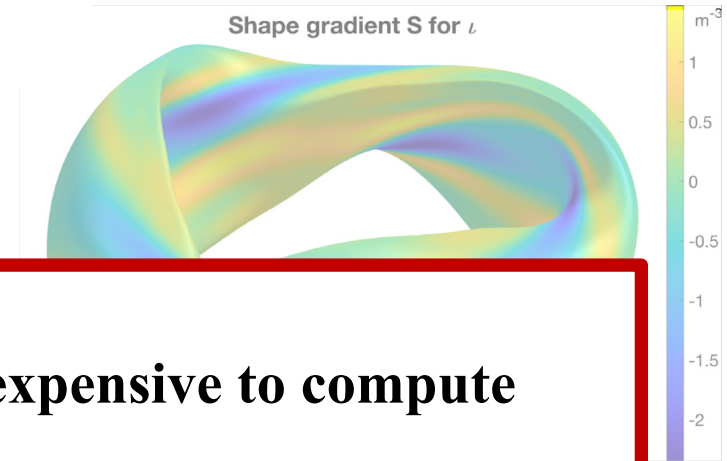
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Why is the shape gradient ($\mathcal{G}$) useful?

- *Local* sensitivity information
- Quantifying engineering tolerances
- Gradient-based optimization

Describing derivatives with respect to shape

- Consider $f(S)$, a functional of surface, S
- Surface is displaced by vector field $\delta \mathbf{r}$



Problem: shape gradient generally expensive to compute

- Surface S described by parameters, Ω
- Computing shape gradient of $f(S)$ with finite difference parameter derivatives requires $\geq N_\Omega + 1$ evaluations of $f(S)$

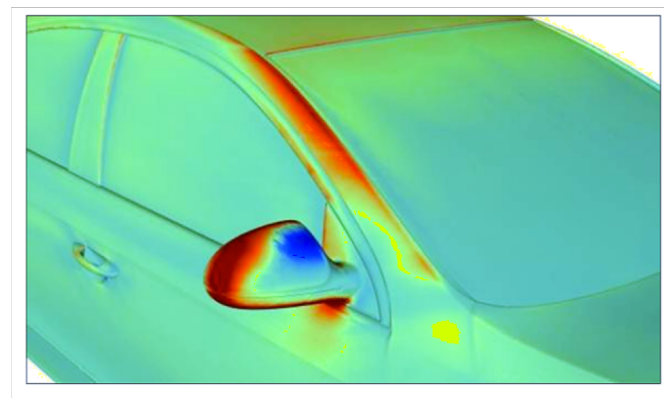
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Adjoint method provides efficient shape gradient computation

- Figure of merit $f(\mathbf{x})$ depends on solution to system of equations, $\mathbf{L}(\mathbf{x}) = 0$
- Goal: compute derivative of $f(\mathbf{x})$ with respect to parameters $\Omega = \{\Omega_i\}_{i=1}^{N_\Omega}$
- Adjoint method requires 1 additional solve (rather than $\geq N_\Omega$ from finite differences)
- No noise from finite difference step size

Adjoint methods widely used in computational fluid dynamics



Inward for smaller drag

Outward for smaller drag

C. Othmer, *J. Math. Industry* 4, (2014).

Adjoint method for a linear system

$$\overleftrightarrow{A}x = b$$

- Goal: compute $\partial f / \partial \Omega$ for parameters $\Omega = \{\Omega_i\}_{i=1}^{N_\Omega}$

$$f = x^T c$$

- Expensive to get $\partial f / \partial \Omega$ with finite differences ($\geq N_\Omega + 1$ solutions of system)

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- Compute derivative with chain rule

$$\frac{\partial f}{\partial \Omega_i} = c^T \frac{\partial x}{\partial \Omega_i} = c^T (\overleftrightarrow{A})^{-1} \left(\frac{\partial b}{\partial \Omega_i} - \frac{\partial \overleftrightarrow{A}}{\partial \Omega_i} x \right) \quad \longrightarrow \quad \frac{\partial f}{\partial \Omega_i} = ((\overleftrightarrow{A}^T)^{-1} c)^T \left(\frac{\partial b}{\partial \Omega_i} - \frac{\partial \overleftrightarrow{A}}{\partial \Omega_i} x \right)$$

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- Solve adjoint equation

$$\overleftrightarrow{A}^T q = c$$

- Get derivative with **2 solutions of linear system** (x, q)

$$\frac{\partial f}{\partial \Omega_i} = q^T \left(\frac{\partial b}{\partial \Omega_i} - \frac{\partial \overleftrightarrow{A}}{\partial \Omega_i} x \right)$$

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REGCOIL¹ method for coil optimization

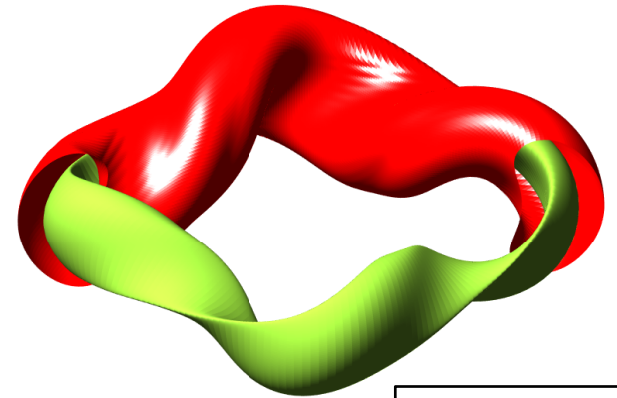
Given desired plasma and winding surface, obtain coil shapes with linear least-squares method

- Assume all coils lie on toroidal winding surface
- Approximate coils by current density $\mathbf{K}$ on winding surface

$$\mathbf{K} = \mathbf{n} \times \nabla \Phi$$

- Minimize $\chi^2 = (\text{field error}) + \lambda(\text{coil complexity})$
- Linear least-squares solution for Fourier-discretized Φ

$$\overleftrightarrow{\mathbf{A}}\Phi = \mathbf{b}$$



Winding
surface

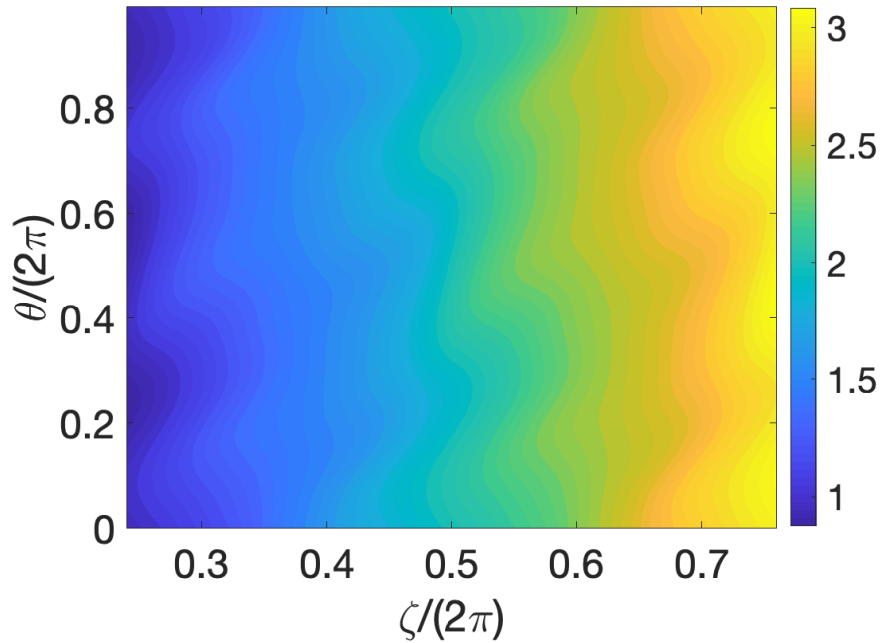
Plasma
surface

¹M. Landreman, *Nuclear Fusion* 57 (2017).

Current potential provides coil shapes

$$\mathbf{K} = n \times \nabla \Phi$$

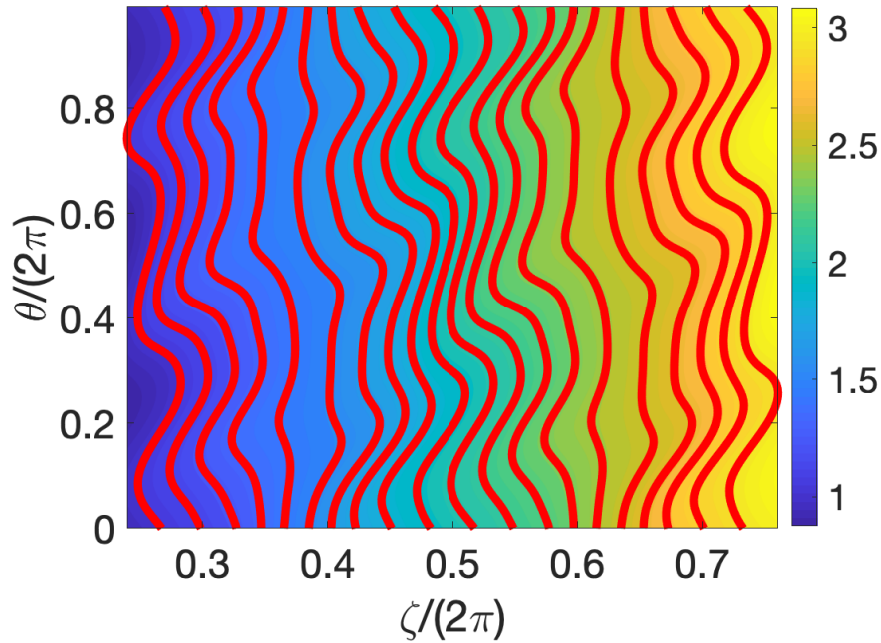
Current Potential (Φ) [A]



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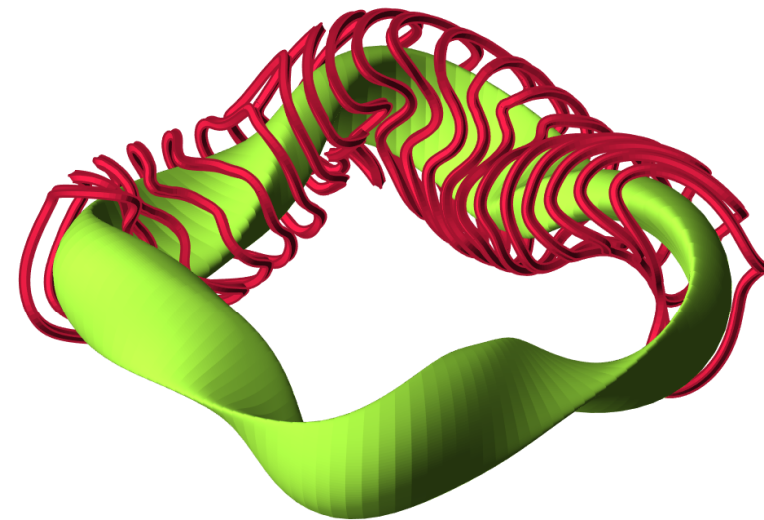
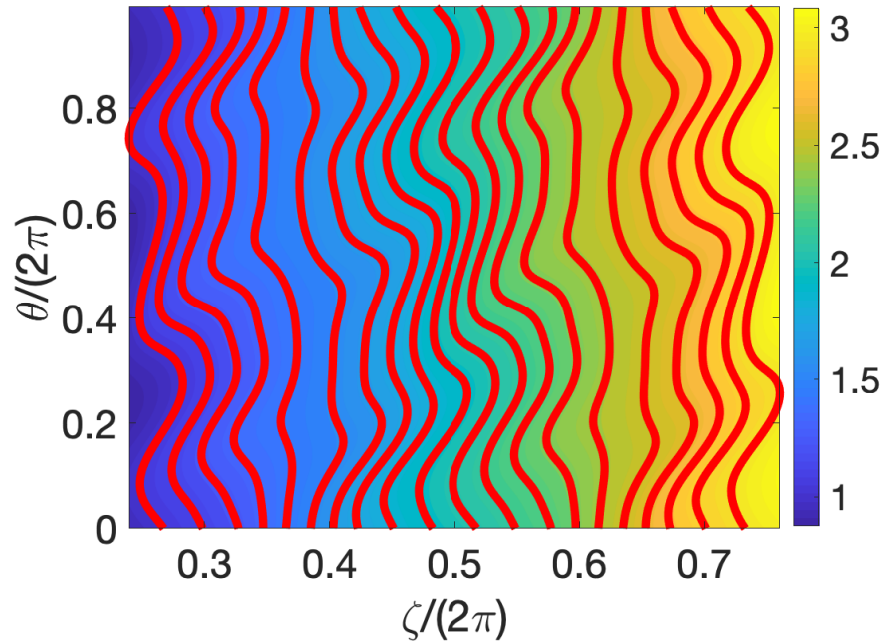
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Current Potential (Φ) [A]



**Coils on winding
surface**

**Plasma
surface**

Optimize winding surface with adjoint method¹ to improve coils

Objective function

$$f(S_{\text{coil}}, \Phi(S_{\text{coil}})) = f_{\text{plasma}} + \alpha_{\text{coil}} f_{\text{coil}} + \alpha_{\text{spacing}} f_{\text{spacing}}$$

- $f_{\text{plasma}} = \int_{S_{\text{plasma}}} d^2x (\mathbf{B} \cdot \mathbf{n})^2 \rightarrow$ reproduce desired plasma surface
- $f_{\text{coil}} = (\int_{S_{\text{coil}}} d^2x K^2 / A_{\text{coil}})^{1/2} \rightarrow$ improve engineering properties of coils
- $f_{\text{spacing}} = -V_{\text{coil}}^{1/3} \rightarrow$ minimize coil ripple, increase coil-plasma distance

¹E.J. Paul et al, *Nuclear Fusion* 58 (2018)

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Use adjoint method for analytic derivatives

- Optimization space: Ω = parameterization of S_{coil}
- Solve linear adjoint equation

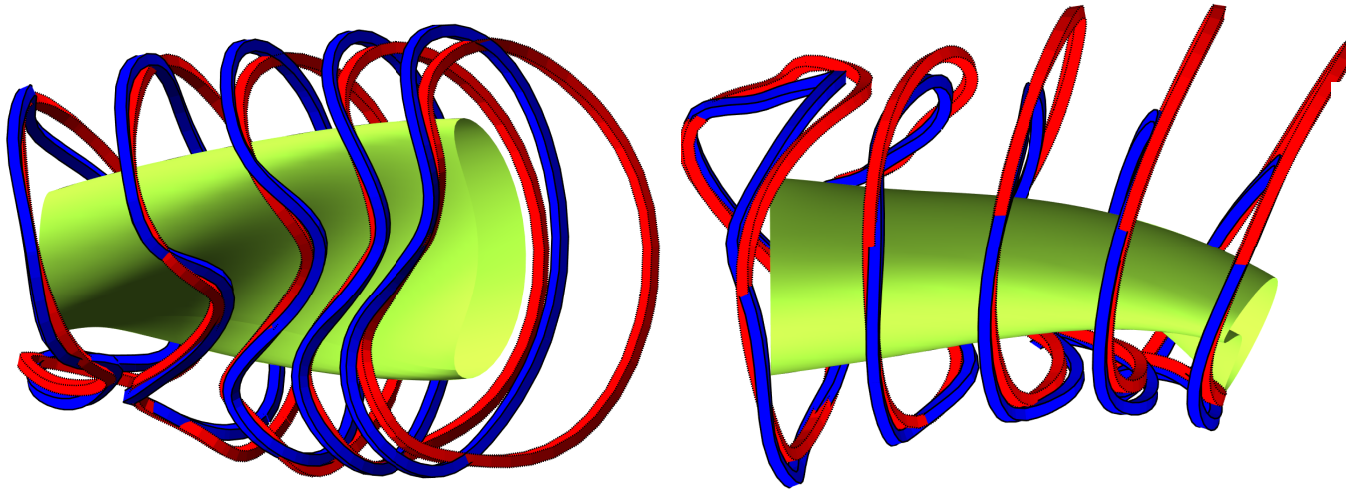
$$\vec{A}^T \mathbf{q} = \frac{\partial f}{\partial \Phi}$$

- Compute $\partial f / \partial \Omega$ from Φ and adjoint solution $\mathbf{q}$

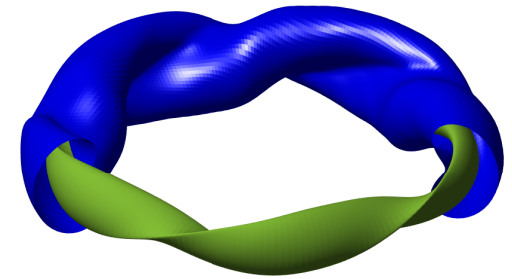
$$\frac{\partial f}{\partial \Omega_i} = \left(\frac{\partial f}{\partial \Omega_i} \right)_{\Phi} + \mathbf{q}^T \left(\frac{\partial \mathbf{b}}{\partial \Omega_i} - \frac{\partial \vec{A}}{\partial \Omega_i} \Phi \right)$$

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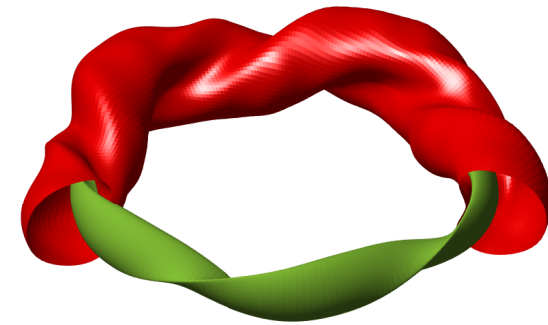
Example - optimizing W7-X winding surface



Actual W7-X winding
surface (initial)

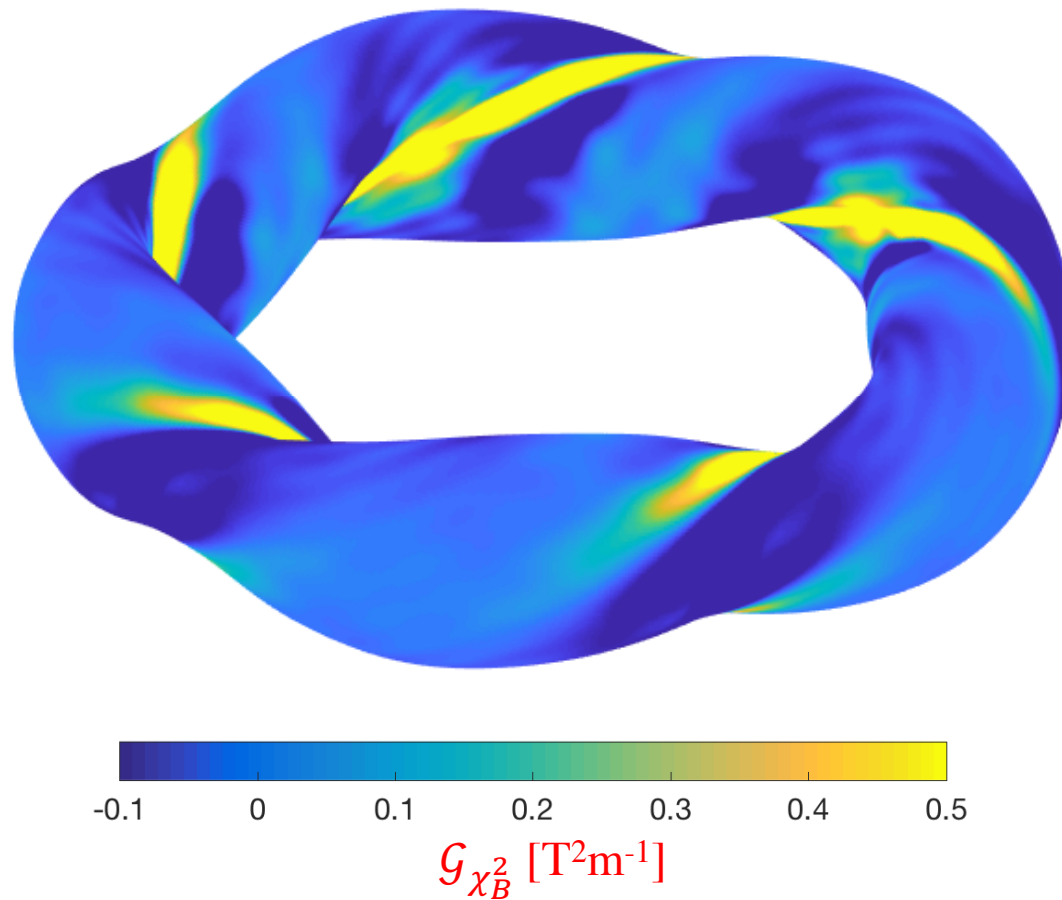


Optimized



	Initial	Optimized
Min. coil-coil distance [m]	0.22	0.27
Max curvature [m^{-1}]	9.01	4.84
Max toroidal extent [rad.]	0.22	0.20
Mean normal field error	0.034	0.023

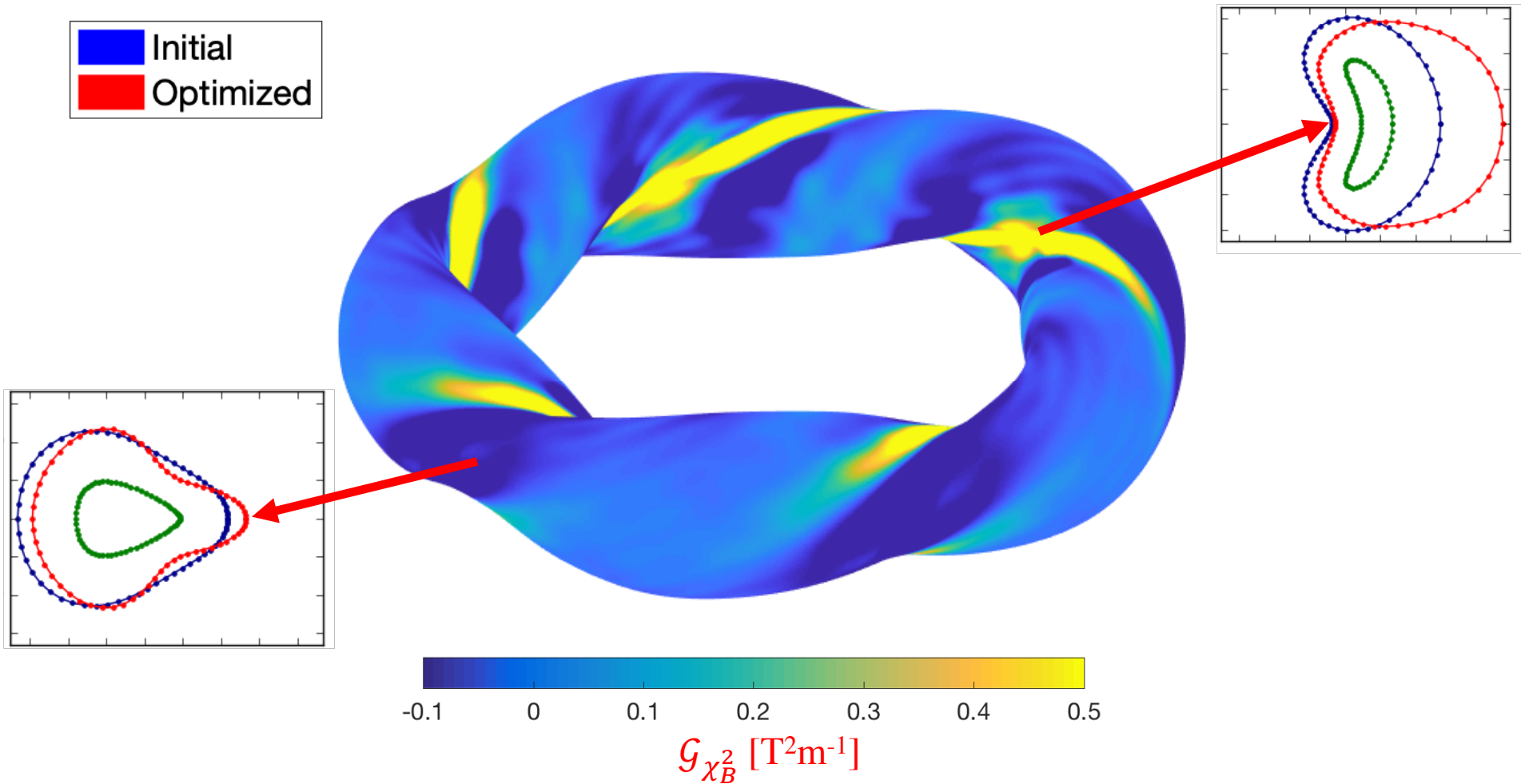
Shape gradient indicates regions of large field error sensitivity



$$\delta\chi_B^2(S_{\text{coil}}; \delta\mathbf{r}) = \int_{S_{\text{coil}}} d^2x \, \delta\mathbf{r} \cdot \mathbf{n} \, \mathcal{G}_{\chi_B^2}$$

$$\chi_B^2 = \int_{S_{\text{plasma}}} d^2x \, (\mathbf{B} \cdot \mathbf{n})^2$$

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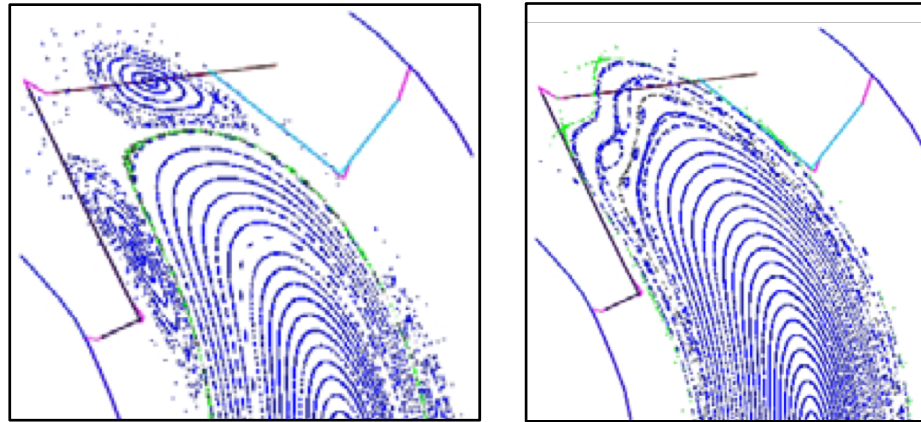
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- Adjoint stellarator coil design
- **Adjoint drift kinetic equation for neoclassical optimization**
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Stellarators must be optimized with neoclassical physics

- Semi-analytic reduced models historically used
 - Effective ripple in $1/\nu$ regime ($\epsilon_{\text{eff}}^{3/2}$) [V. Nemov et al., *Phys. of Plasmas* 12, 4622 (1999)]
 - Low collisionality bootstrap model [K.-C. Shaing et al., *Phys. of Fluids B* 1, 148 (1989)]

Minimal J_b needed for proper island divertor operation

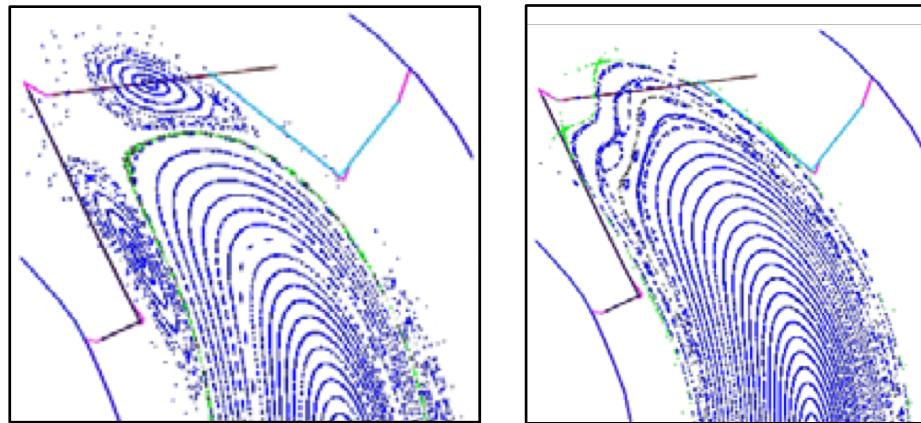


Geiger et al, *Contributions to Plasma Physics* 50, 770 (2010).

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Our approach – no assumption on E_r or collisionality

Optimizing for neoclassical parameters

- Solve local drift kinetic equation (DKE) for f_1 with SFINCS¹

$$(\nu_{\parallel} \mathbf{b} + \mathbf{v}_E) \cdot \nabla f_1 - C(f_1) = -\mathbf{v}_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}$$

- Moments (particle flux, bootstrap current) computed from inner product with f_1

$$\Gamma_{\psi} = \langle \widetilde{\Gamma_{\psi}}, f_1 \rangle = \left\langle \int d^3v \frac{\widetilde{\Gamma_{\psi}} f_1}{f_M} \right\rangle_{\psi}$$

- Geometric parameters enter DKE through B (and several flux functions)

$$B = \sum_{mn} B_{mn} \cos(m\theta - n\zeta)$$

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Requires $\geq N_{modes}+1$ solutions of DKE with finite differences

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Adjoint approach allows efficient neoclassical optimization

- Solve DKE

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- Derivative computed with (f_1 and $q^{\Gamma\psi}$)

$$\begin{aligned} & \frac{\partial \Gamma_\psi}{\partial B_{mn}} \\ &= \left(\frac{\partial \Gamma_\psi}{\partial B_{mn}} \right)_{f_1} + \left\langle q^{\Gamma\psi}, \left(\frac{\partial S}{\partial B_{mn}} - \frac{\partial \mathbb{L}}{\partial B_{mn}} f_1 \right) \right\rangle \end{aligned}$$

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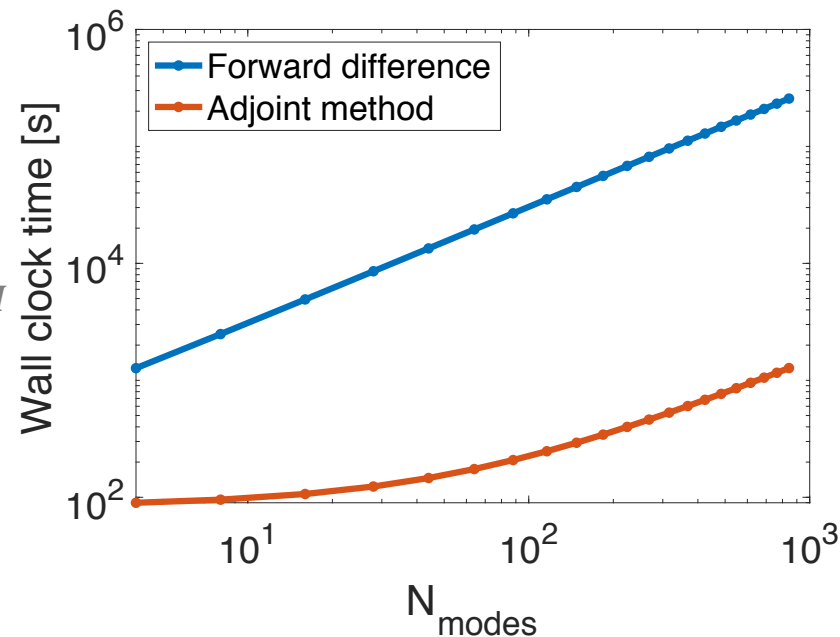
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Adjoint approach requires 2 DKE solutions with SFINCS¹
($N_{\text{modes}} + 1$ for forward difference)



¹E.J. Paul, et al, *Submitted to J. Plasma Phys.* (2019).

Local magnetic sensitivity computed with adjoint approach

Define magnetic sensitivity

$$\delta\mathcal{R}(B; \delta B) = \langle S_{\mathcal{R}} \delta B \rangle_{\psi}$$

Solve linear system for $S_{\mathcal{R}}$

$$\frac{\partial \mathcal{R}}{\partial B_{mn}} = \langle S_{\mathcal{R}} \cos(m\theta - n\zeta) \rangle_{\psi}$$

Local magnetic sensitivity computed with adjoint approach

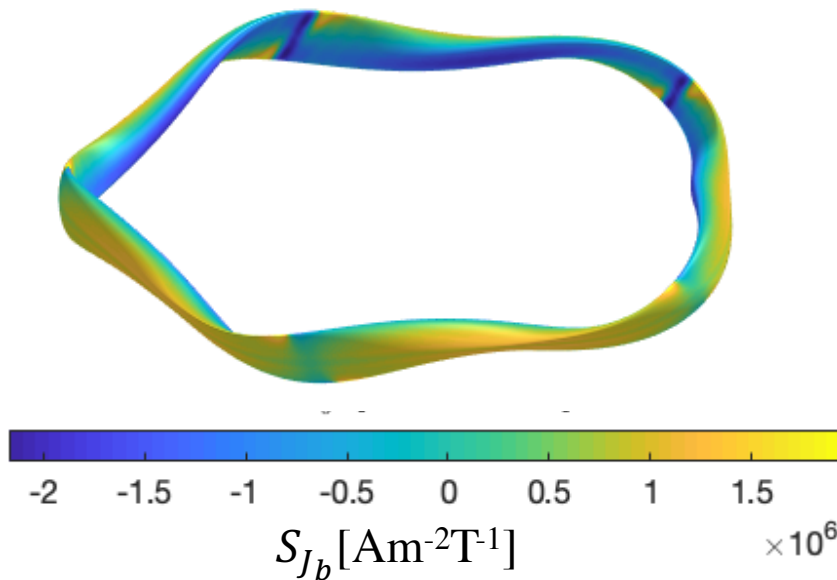
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Solve linear system for $S_{\mathcal{R}}$

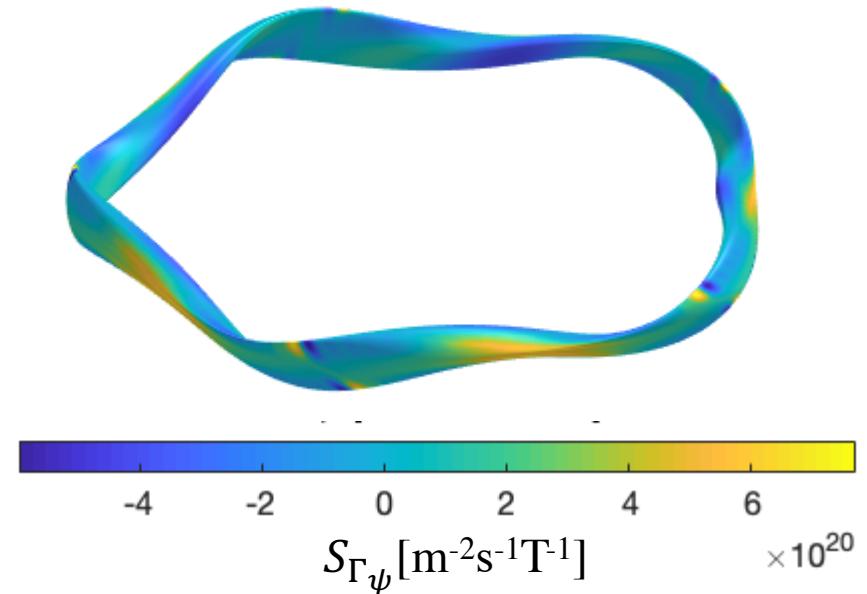
$$\frac{\partial \mathcal{R}}{\partial B_{mn}} = \langle S_{\mathcal{R}} \cos(m\theta - n\zeta) \rangle_{\psi}$$

Bootstrap current sensitivity



$$\delta J_b(B; \delta B) = \left\langle S_{J_b} \delta B \right\rangle_{\psi}$$

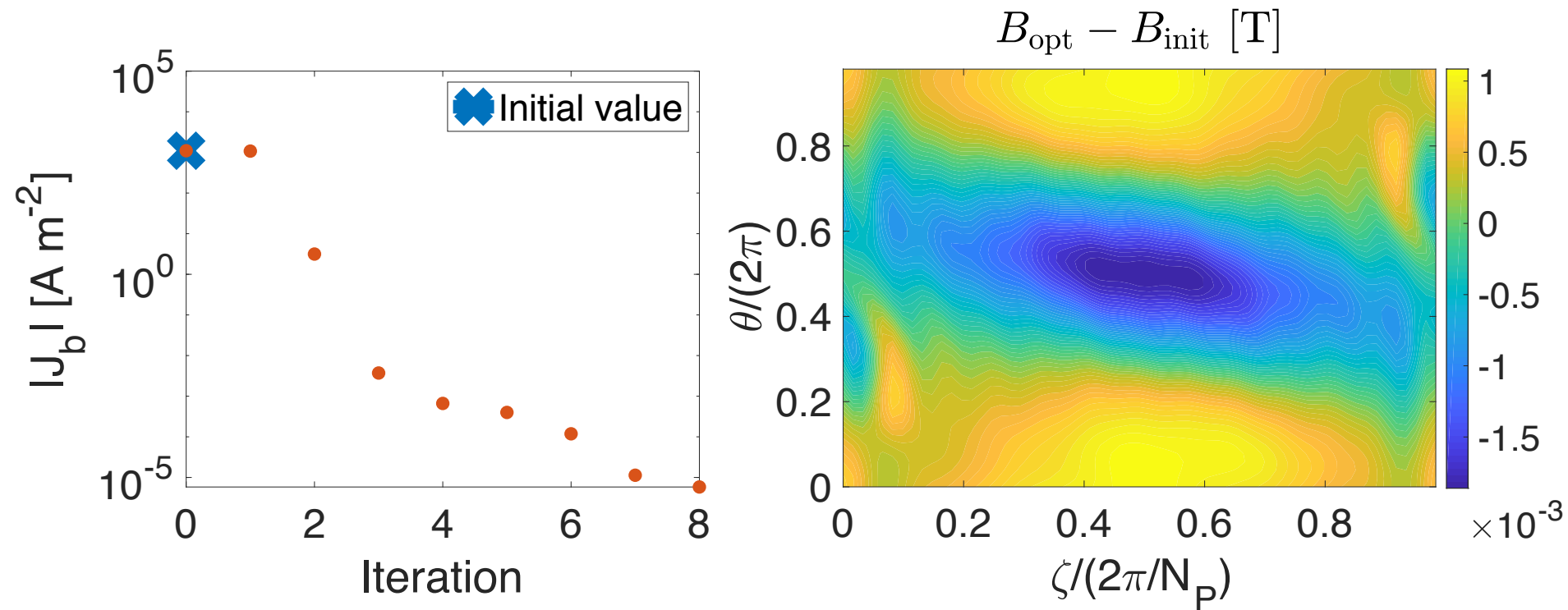
Particle flux sensitivity



$$\delta \Gamma_{\psi}(B; \delta B) = \left\langle S_{\Gamma_{\psi}} \delta B \right\rangle_{\psi}$$

Adjoint-based bootstrap current optimization

- W7-X standard configuration ($\rho = \sqrt{\psi/\psi_0} = 0.7$)
- BFGS (quasi-Newton) method with backtracking line search



Outline

- Introduction to shape optimization ideas
- Adjoint stellarator coil design
- Adjoint drift kinetic equation for neoclassical optimization
- **Shape gradients for MHD equilibria**

Computing MHD shape derivatives directly is expensive

- MHD equilibrium with specified $p(\psi)$ and $\iota(\psi)$ and boundary S_{plasma}

$$0 = \frac{(\nabla \times \mathbf{B}) \times \mathbf{B}}{4\pi} - \nabla p$$

- Goal: compute $\delta f(S_{\text{plasma}}; \delta \mathbf{r})$, for any displacement $\delta \mathbf{r}$

Computing MHD shape derivatives directly is expensive

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$$0 = \frac{(\nabla \times \mathbf{B}) \times \mathbf{B}}{4\pi} - \nabla p$$

- Goal: compute $\delta f(S_{\text{plasma}}; \delta \mathbf{r})$, for any displacement $\delta \mathbf{r}$
- Perturbation with fixed $\iota(\psi)$ and $p(\psi)$ determined from ξ_1

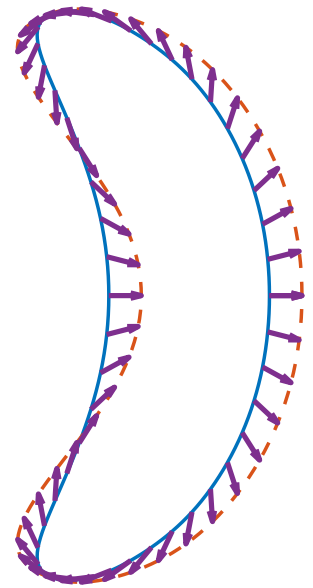
$$\delta \mathbf{B}_1 = \nabla \times (\xi_1 \times \mathbf{B})$$

$$\delta p(\xi_1) = -\xi_1 \cdot \nabla p$$

- Perturbed equilibrium with specified $\delta \mathbf{r} \cdot \mathbf{n}|_{S_{\text{plasma}}}$ satisfies

$$\mathbf{F}(\xi_1) = \frac{(\nabla \times \mathbf{B}) \times \delta \mathbf{B}_1 + \nabla \times (\delta \mathbf{B}_1) \times \mathbf{B}}{4\pi} - \nabla \delta p(\xi_1) = 0 \quad (V_{\text{plasma}})$$

$$\xi_1 \cdot \mathbf{n} = \delta \mathbf{r} \cdot \mathbf{n} \quad (S_{\text{plasma}})$$



Unperturbed
boundary

Perturbed
boundary

Displacement
(ξ_1)

Computing MHD shape derivatives directly is expensive

- MHD equilibrium with specified $p(\psi)$ and $\iota(\psi)$ and boundary S_{plasma}

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- Goal: compute $\delta f(S_{\text{plasma}}; \delta \mathbf{r})$, for any displacement $\delta \mathbf{r}$

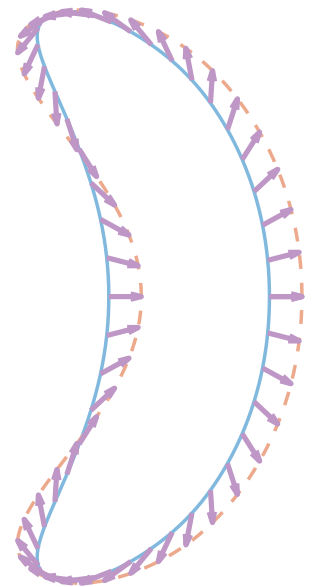
- Perturbation with

Requires computing force balance for many ($\sim 10^2$) possible boundary perturbations

- Perturbed equilibrium with specified $\delta \mathbf{r} \cdot \mathbf{n}|_{S_{\text{plasma}}}$ satisfies

$$\mathbf{F}(\xi_1) = \frac{(\nabla \times \mathbf{B}) \times \delta \mathbf{B}_1 + \nabla \times (\delta \mathbf{B}_1) \times \mathbf{B}}{4\pi} - \nabla \delta p(\xi_1) = 0 \quad (V_{\text{plasma}})$$

$$\xi_1 \cdot \mathbf{n} = \delta \mathbf{r} \cdot \mathbf{n} \quad (S_{\text{plasma}})$$



**Unperturbed
boundary**
**Perturbed
boundary**
**Displacement
(ξ_1)**

Computing MHD shape gradient with adjoint approach¹

Take advantage of self-adjointness of MHD force operator

$$\int_{V_{\text{plasma}}} d^3x (-\mathbf{F}(\xi_1) \cdot \xi_2 + \mathbf{F}(\xi_2) \cdot \xi_1) + \frac{1}{4\pi} \int_{S_{\text{plasma}}} d^2x \mathbf{n} \cdot (\xi_1 \delta \mathbf{B}_2 \cdot \mathbf{B} - \xi_2 \delta \mathbf{B}_1 \cdot \mathbf{B}) = 0$$

- Compute shape derivative (in terms of ξ_1) for figure of merit, $f(S_{\text{plasma}})$

$$\delta f(S_{\text{plasma}}; \xi_1) = \int_{V_{\text{plasma}}} d^3x \xi_1 \cdot \mathbf{A}_1 + \int_{S_{\text{plasma}}} d^2x \mathbf{n} \cdot \xi_1 \mathbf{A}_2$$

¹T. Antonsen Jr., E.J. Paul et al, *J. Plasma Phys.* 85 (2019)

Computing MHD shape gradient with adjoint approach¹

Take advantage of self-adjointness of MHD force operator

$$\int_{V_{\text{plasma}}} d^3x (-\mathbf{F}(\xi_1) \cdot \xi_2 + \mathbf{F}(\xi_2) \cdot \xi_1) + \frac{1}{4\pi} \int_{S_{\text{plasma}}} d^2x \mathbf{n} \cdot (\xi_1 \delta \mathbf{B}_2 \cdot \mathbf{B} - \xi_2 \delta \mathbf{B}_1 \cdot \mathbf{B}) = 0$$

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- Adjoint displacement ξ_2 satisfies

$$\mathbf{F}(\xi_2) = -\mathbf{A}_1(V_{\text{plasma}})$$

$$\xi_2 \cdot \mathbf{n} = 0 \text{ (} S_{\text{plasma}} \text{)}$$

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Computing MHD shape gradient with adjoint approach¹

Take advantage of self-adjointness of MHD force operator

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$$\mathbf{F}(\xi_2) = -\mathbf{A}_1(V_{\text{plasma}})$$

$$\xi_2 \cdot \mathbf{n} = 0 \quad (S_{\text{plasma}})$$

- Apply self-adjointness relation

$$\mathcal{G} = \left(\frac{\delta \mathbf{B}_2 \cdot \mathbf{B}}{4\pi} + A_2 \right)$$

¹T. Antonsen Jr., E.J. Paul et al, *J. Plasma Phys.* 85 (2019)

Computing MHD shape gradient with adjoint approach¹

Take advantage of self-adjointness of MHD force operator

$$\int_{V_{\text{plasma}}} d^3x (-\mathbf{F}(\xi_1) \cdot \xi_2 + \mathbf{F}(\xi_2) \cdot \xi_1) + \frac{1}{4\pi} \int_{S_{\text{plasma}}} d^2x \mathbf{n} \cdot (\xi_1 \delta \mathbf{B}_2 \cdot \mathbf{B} - \xi_2 \delta \mathbf{B}_1 \cdot \mathbf{B}) = 0$$

Shape derivative with respect to *any* perturbation computed with *one* additional force balance solve

- Compute shape

$$\delta f(S_{\text{plasma}};$$

$$f(S_{\text{plasma}})$$

$$\xi_1 A_2$$

- Adjoint displacement ξ_2 satisfies

$$\mathbf{F}(\xi_2) = -\mathbf{A}_1(V_{\text{plasma}})$$

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- Apply self-adjointness relation

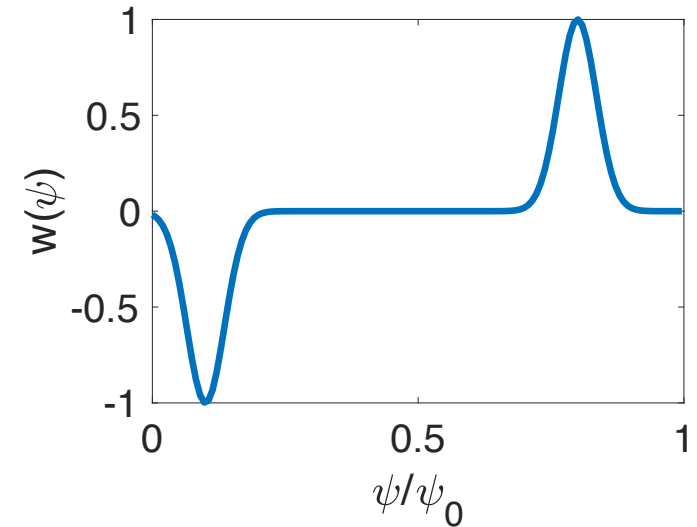
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¹T. Antonsen Jr., E.J. Paul et al, *J. Plasma Phys.* 85 (2019)

Magnetic well shape gradient computed with 2 VMEC¹ calls

$$f_W = \int_{V_{\text{plasma}}} d\psi V'(\psi) w(\psi)$$

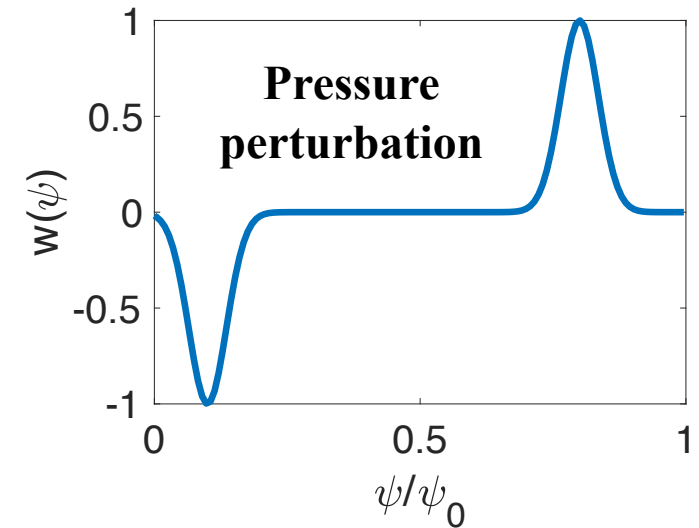
$f_W < 0$ favorable for stability



¹S. Hirshman & J.C. Whitson, *Physics of Fluids* 26, 3553 (1983).

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$$f_W < 0 \text{ favorable for stability}$$



Adjoint perturbation satisfies

$$\mathbf{F}(\xi_2) = \nabla(w(\psi)) (V_{\text{plasma}})$$

$$\xi_2 \cdot \mathbf{n} = 0 (S_{\text{plasma}})$$

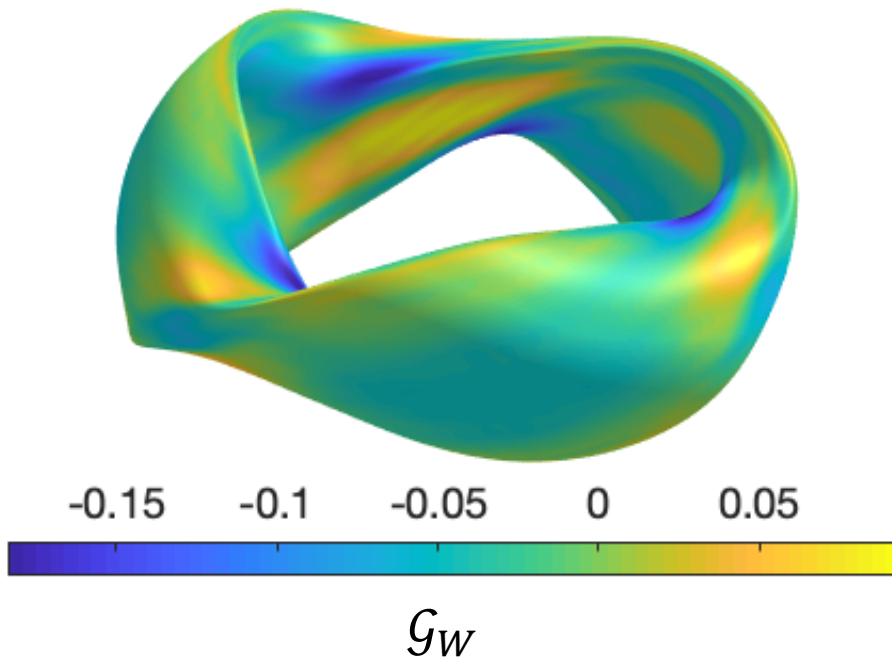
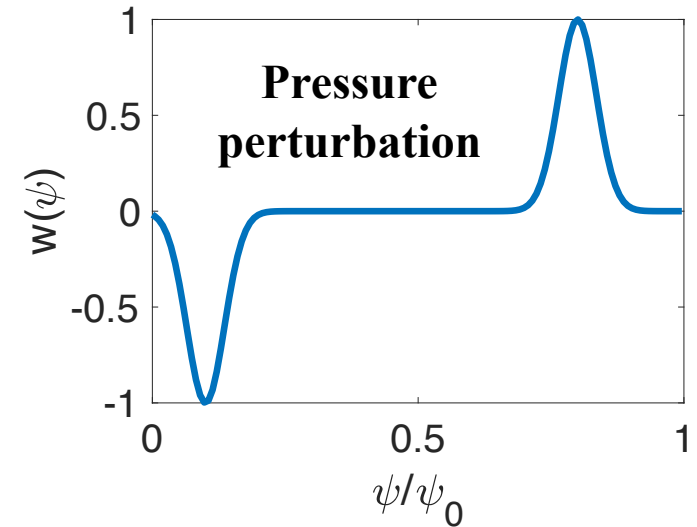
$$\mathcal{G}_W = \frac{\delta \mathbf{B}_2 \cdot \mathbf{B}}{4\pi} + w(\psi)$$

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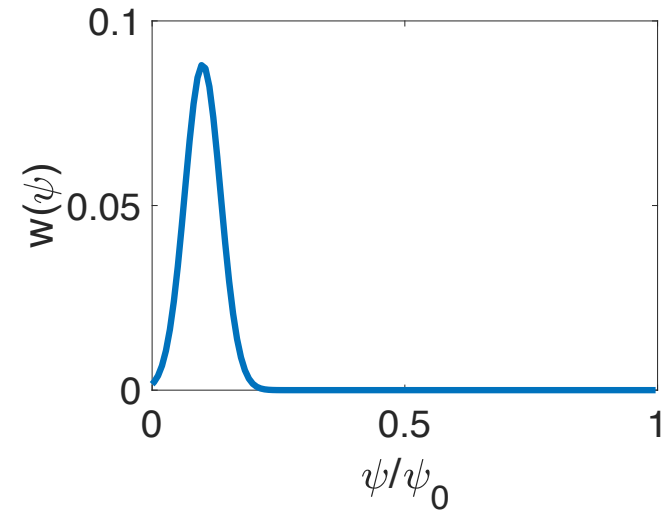
Coil shape gradient for ι computed with 2 VMEC calls

$$\delta f(C; \delta \mathbf{r}_C) = \sum_k \int_{C_k} dl \, \mathbf{s}_k \cdot \delta \mathbf{r}_{C_k}$$

$\mathbf{s}_k$, shape gradient for coil k , gives
perturbation δf for *any* $\delta \mathbf{r}_{C_k}$

Coil shape gradient for ι computed with 2 VMEC calls

$$f_{\iota} = \int_{V_{\text{plasma}}} d\psi w(\psi) \iota(\psi)$$

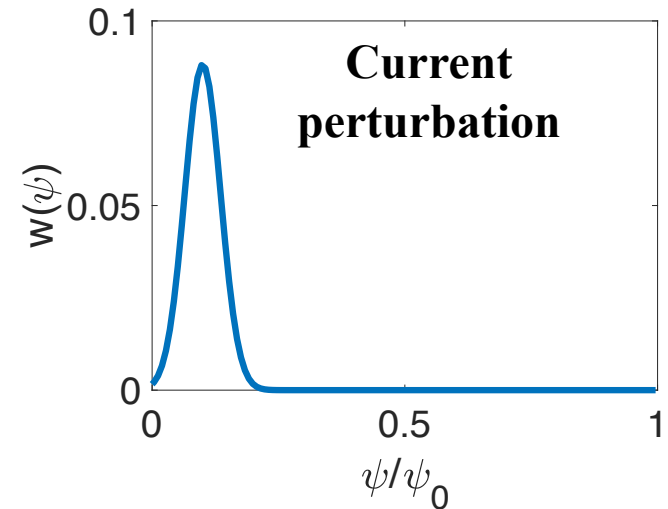


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$\mathbf{s}_k$, shape gradient for coil k , gives perturbation δf for any $\delta \mathbf{r}_{C_k}$

Coil shape gradient for ι computed with 2 VMEC calls

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$\mathbf{s}_k$, shape gradient for coil k , gives perturbation δf for any $\delta \mathbf{r}_{C_k}$

Adjoint perturbation satisfies

$$\mathbf{F}(\xi_2) = 0 \quad (V_{\text{plasma}})$$

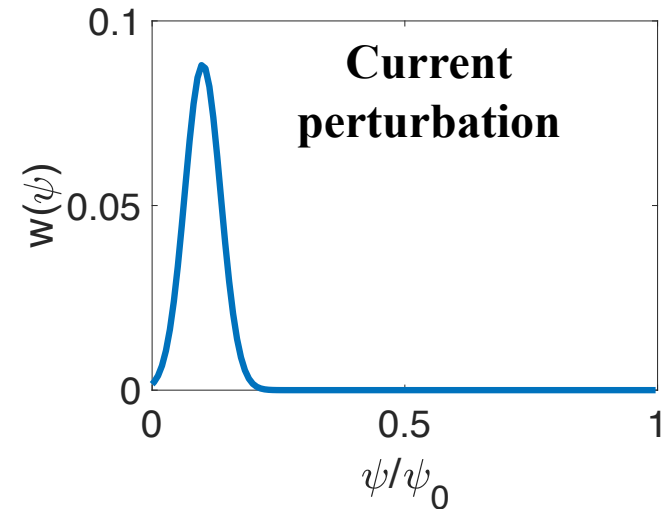
$$\delta \mathbf{r}_{C_k} = 0 \quad (C_k)$$

$$\delta I_2(\psi) = w(\psi)$$

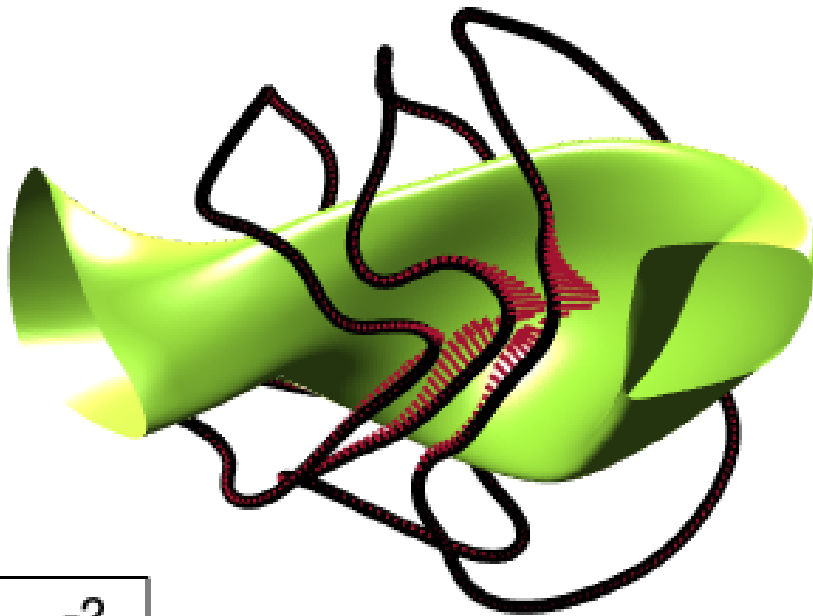
$$\mathbf{s}_k = \left. \frac{I_{C_k} \mathbf{t} \times \delta \mathbf{B}_2}{2\pi} \right|_{C_k}$$

Coil shape gradient for ι computed with 2 VMEC calls

$$f_{\iota} = \int_{V_{\text{plasma}}} d\psi w(\psi) \iota(\psi)$$



NCSX coil shape gradient for f_{ι}



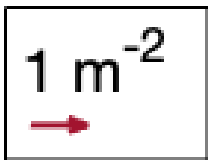
Adjoint perturbation satisfies

$$\mathbf{F}(\xi_2) = 0 \quad (V_{\text{plasma}})$$

$$\delta \mathbf{r}_{C_k} = 0 \quad (C_k)$$

$$\delta I_2(\psi) = w(\psi)$$

$$\mathbf{s}_k = \left. \frac{I_{C_k} \mathbf{t} \times \delta \mathbf{B}_2}{2\pi} \right|_{C_k}$$



Conclusions

- Adjoint methods allow efficient computation of geometric derivatives
 - Gradient-based optimization
 - Sensitivity and tolerance analysis
- Several applications demonstrated for stellarator design
 - Optimization of coil shapes [E.J. Paul et al, *Nuclear Fusion* 58 (2018)]
 - Optimization of neoclassical quantities with adjoint drift kinetic equation [E.J. Paul et al, *Submitted to J. Plasma Phys.* (2019)]
 - Shape gradients for fixed and free-boundary MHD equilibria [T. Antonsen Jr., E.J. Paul et al, *J. Plasma Phys.* 85 (2019)]
- Ongoing work
 - Adjoint MHD shape gradient for other figures of merit

Extra Slides

Optimization of current potential in REGCOIL

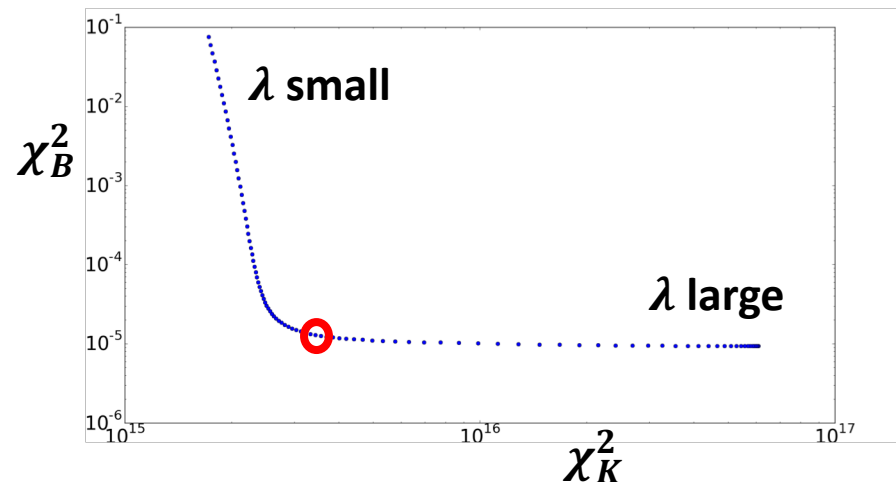
- Secular terms of Φ fixed by total poloidal and toroidal current

$$\Phi = \Phi_{SV} + \frac{G\zeta}{2\pi} + \frac{I\theta}{2\pi}$$

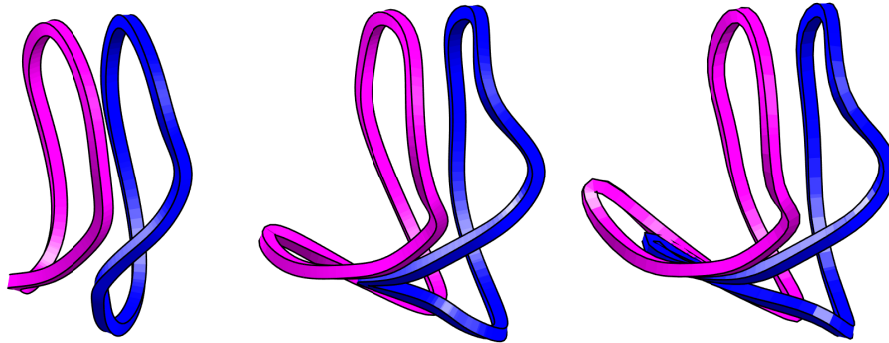
- Single-valued current potential is Fourier decomposed

$$\Phi_{SV} = \sum_{mn} \Phi_{mn} \sin(m\theta - n\zeta)$$

- Our task: $\min_{\Phi} \chi^2 = \chi_B^2 + \lambda \chi_K^2$
 - $\chi_K^2 = \int_{S_{\text{coil}}} d^2x K^2 \rightarrow$ Increase coil-coil spacing
 - $\chi_B^2 = \int_{S_{\text{plasma}}} d^2x (\mathbf{B} \cdot \mathbf{n})^2 \rightarrow$ Fidelity in reproducing plasma surface
- Regularization parameter (λ) chosen to meet engineering tolerance (e.g. max K)

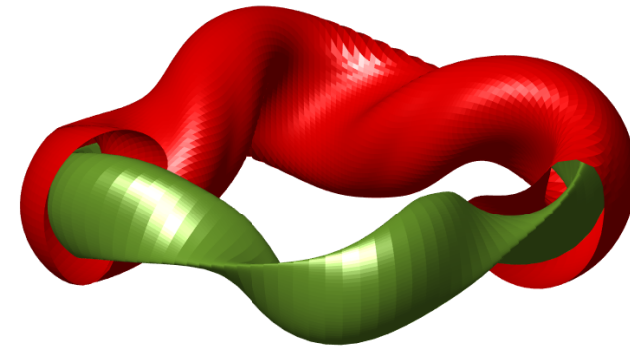


Adjoint method for winding surface optimization



Increasing $||\mathbf{K}||_2 \rightarrow$

Winding surface
(varying)



Plasma surface
(fixed)

Optimization parameters $\Omega = \{R_{mn}^c, Z_{mn}^s\}$

$$f(\Omega, \Phi(\Omega)) = \chi_B^2 + \alpha_K ||\mathbf{K}||_2 - \alpha_V V_{\text{coil}}^{1/3}$$

- $\chi_B^2 \rightarrow$ reproduce plasma surface
- $||\mathbf{K}||_2 \rightarrow$ improve engineering properties of coils
- $V_{\text{coil}}^{1/3} \rightarrow$ minimize coil ripple, increase coil-plasma distance

Our goal:

$$\min_{\Omega} f \quad \text{s.t.} \quad K_{\max} = K_{\max}^{\text{target}} \quad \text{and} \quad \min(d^{\text{coil-plasma}}) \geq d_{\text{target}}^{\text{coil-plasma}}$$

W7-X coil optimization metrics

	Initial	Optimized	Actual coil set
χ_B^2	0.115	0.0711	
$V_{\text{coil}} [\text{m}^3]$	156	190	
$ \mathbf{K} _2 [\text{MA/m}]$	2.21	2.16	
$\max K [\text{MA/m}]$	7.70	7.70	
Mean l [m]	8.51	8.95	8.69
Max l [m]	8.84	9.14	8.74
Mean $\Delta\zeta$ [rad.]	0.190	0.179	0.198
Max $\Delta\zeta$ [rad.]	0.222	0.197	0.208
Mean κ [m^{-1}]	1.21	1.10	1.20
Max κ [m^{-1}]	9.01	4.84	2.59
$d_{\text{coil-coil}}^{\min}$ [m]	0.223	0.271	0.261

Adjoint method for neoclassical optimization

- Define adjoint equation with respect to the inner product between set of distribution functions ($F = \{f_{1s}\}_{s=1}^{N_{\text{species}}}$)

$$\langle F, G \rangle = \sum_s \left\langle \int d^3v \frac{f_{1s} g_{1s}}{f_{Ms}} \right\rangle_\psi$$

- Moments of f_{1s} can be written as inner products (e.g. $\tilde{\Gamma}_s = f_{Ms} \mathbf{v}_{ms} \cdot \nabla \psi$)
 $\Gamma_s = \langle F, \tilde{\Gamma}_s \rangle \quad Q_s = \langle F, \tilde{Q}_s \rangle \quad V_{||,s} = \langle F, \tilde{V}_{||,s} \rangle$

- Compute derivatives of FOM

$$\left(\frac{\partial \Gamma_s}{\partial \Omega_i} \right)_{\mathbb{L}F=\mathbb{S}} = \left(\frac{\partial \Gamma_s}{\partial \Omega_i} \right)_F + \left\langle \frac{\partial F}{\partial \Omega_i}, \tilde{\Gamma}_s \right\rangle$$

- F satisfies linear system, where $\mathbb{L}(\Omega)$ and $\mathbb{S}(\Omega)$

$$\mathbb{L}F = \mathbb{S}$$

- $\partial F / \partial \Omega$ can be computed from finite differences

- Requires **N linear solves** of $M \times M$ system

$$\mathbb{L} \frac{\partial F}{\partial \Omega_i} = \left(\frac{\partial \mathbb{S}}{\partial \Omega_i} - \frac{\partial \mathbb{L}}{\partial \Omega_i} F \right)$$

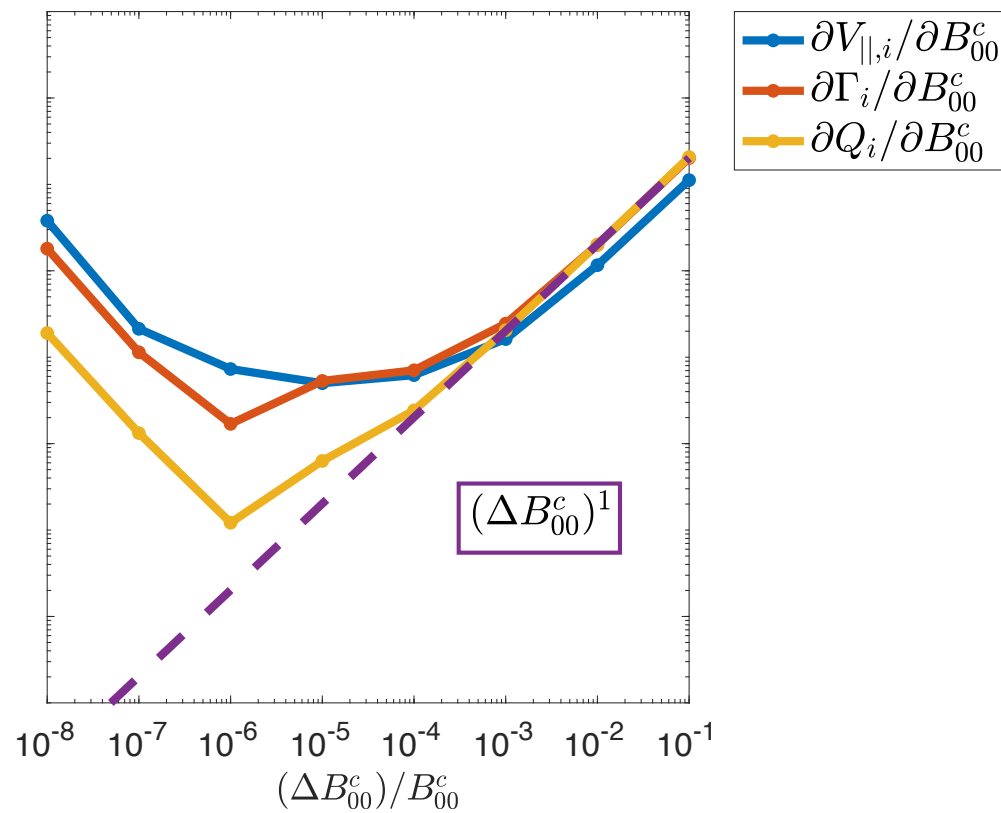
Adjoint method for neoclassical optimization

- Alternatively, solve adjoint equation once
 - Adjoint property: $\langle \mathbb{L}F, G \rangle = \langle F, \mathbb{L}^\dagger G \rangle$
 $\mathbb{L}^\dagger q^{\Gamma_s} = \tilde{\Gamma}_s$
- Use adjoint solution (q^{Γ_s}) and forward solution (F) to compute gradient with **2 linear solves** of $M \times M$ system

$$\begin{aligned}
 \left(\frac{\partial \Gamma_s}{\partial \Omega_i} \right)_{\mathbb{L}F=\mathbb{S}} &= \left(\frac{\partial \Gamma_s}{\partial \Omega_i} \right)_F + \left\langle \tilde{\Gamma}_s, \frac{\partial F}{\partial \Omega_i} \right\rangle \\
 &= \left(\frac{\partial \Gamma_s}{\partial \Omega_i} \right)_F + \left\langle \mathbb{L}^\dagger q^{\Gamma_s}, \mathbb{L}^{-1} \left(\frac{\partial \mathbb{S}}{\partial \Omega_i} - \frac{\partial \mathbb{L}}{\partial \Omega_i} F \right) \right\rangle \\
 &= \left(\frac{\partial \Gamma_s}{\partial \Omega_i} \right)_F + \left\langle q^{\Gamma_s}, \left(\frac{\partial \mathbb{S}}{\partial \Omega_i} - \frac{\partial \mathbb{L}}{\partial \Omega_i} F \right) \right\rangle
 \end{aligned}$$

- Compute solution to adjoint equation in addition to forward equation.
 $-(v_{||}\mathbf{b} + \mathbf{v}_E) \cdot \nabla q^{\Gamma_s} - C(q^{\Gamma_s}) = \tilde{\Gamma}_s$

Benchmark with forward difference derivatives



Generalization of self-adjointness relation

- Often toroidal current, $I_T(\psi)$, specified rather than $\iota(\psi)$ for equilibrium calculations
- Allow perturbations for which $\iota(\psi)$ can vary

$$\delta \mathbf{B}_1 = \nabla \times (\boldsymbol{\xi}_1 \times \mathbf{B} - \delta \Phi_1 \nabla \zeta)$$
- $\delta \iota(\psi)$ and $\delta I_T(\psi)$ coupled via generalized adjoint relation

$$\int_{V_P} d^3x [-\mathbf{F}(\boldsymbol{\xi}_1) \cdot \boldsymbol{\xi}_2 + \mathbf{F}(\boldsymbol{\xi}_2) \cdot \boldsymbol{\xi}_1] + \frac{1}{4\pi} \int_{S_P} d^2x \mathbf{n} \cdot [\boldsymbol{\xi}_1 \delta \mathbf{B}_2 \cdot \mathbf{B} - \boldsymbol{\xi}_2 \delta \mathbf{B}_1 \cdot \mathbf{B}] - \frac{2\pi}{c} \int_{V_P} d\psi \left(\delta I_{T,2} \frac{d\delta \Phi_1}{d\psi} - \delta I_{T,1} \frac{d\delta \Phi_2}{d\psi} \right) = 0$$

Direct perturbation

$$\begin{aligned} \boldsymbol{\xi}_1 \cdot \mathbf{n} &\neq 0 \\ \mathbf{F}(\boldsymbol{\xi}_1) &= 0 \\ \delta I_{T,1} &= 0 \end{aligned}$$

Adjoint perturbation

$$\begin{aligned} \boldsymbol{\xi}_2 \cdot \mathbf{n} &= 0 \\ \mathbf{F}(\boldsymbol{\xi}_2) &\neq 0 \\ \delta I_{T,2} &\neq 0 \end{aligned}$$

MHD free boundary shape gradients

Shape gradient for coils

$\mathbf{S}_k$, shape gradient for coil k , quantifies change in figure of merit δf resulting from perturbation to coil shape, $\delta \mathbf{r}_{C_k}$

$$\delta f(\delta \mathbf{r}_C; C) = \sum_k \int_{C_k} dl \mathbf{S}_k \cdot \delta \mathbf{r}_{C_k}$$

Free boundary adjoint relation

$$\int_{V_P} d^3x [-\mathbf{F}(\xi_1) \cdot \xi_2 + \mathbf{F}(\xi_2) \cdot \xi_1] + \frac{1}{c} \int_{V_V} d^3x (\delta J_{C_1} \cdot \delta \mathbf{A}_{V_2} - \delta J_{C_2} \cdot \delta \mathbf{A}_{V_1}) + \frac{2\pi}{c} \int_{V_P} d\psi \left(\delta \Phi_1 \frac{d\delta I_{T,2}}{d\psi} - \delta \Phi_2 \frac{d\delta I_{T,1}}{d\psi} \right) = 0$$

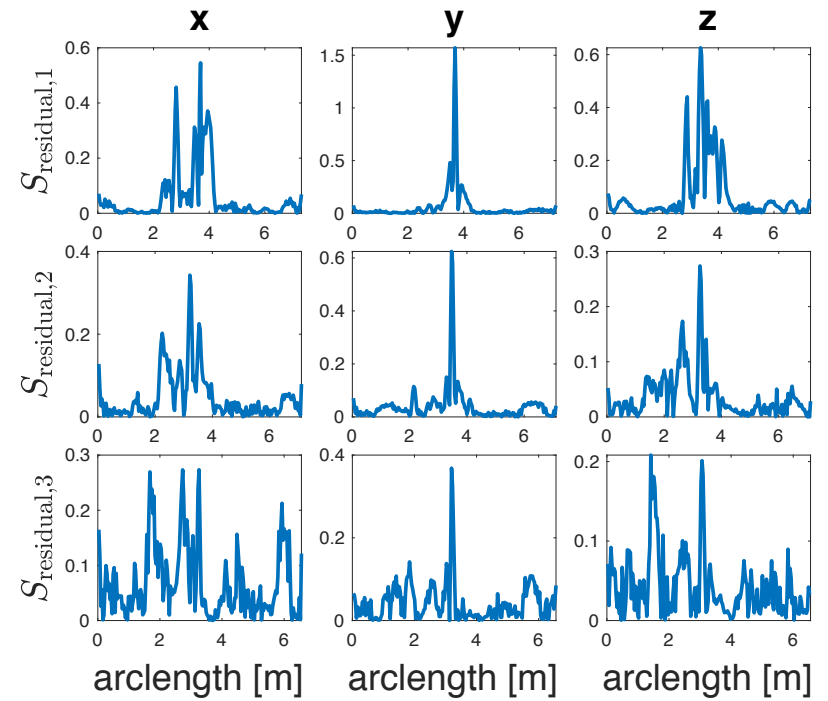
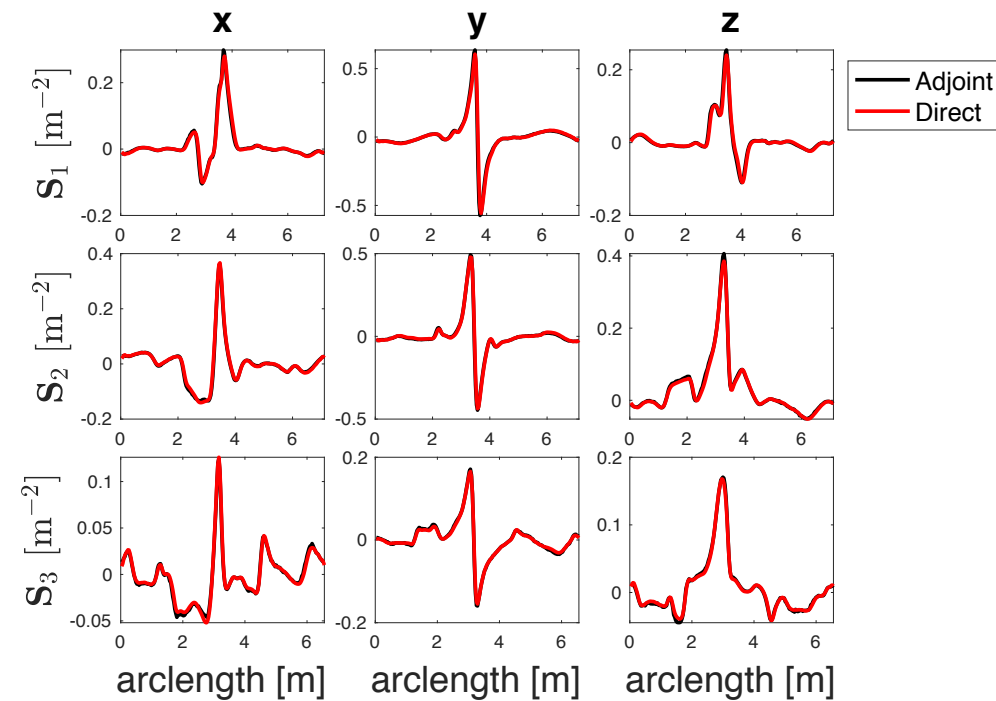
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Adjoint perturbation

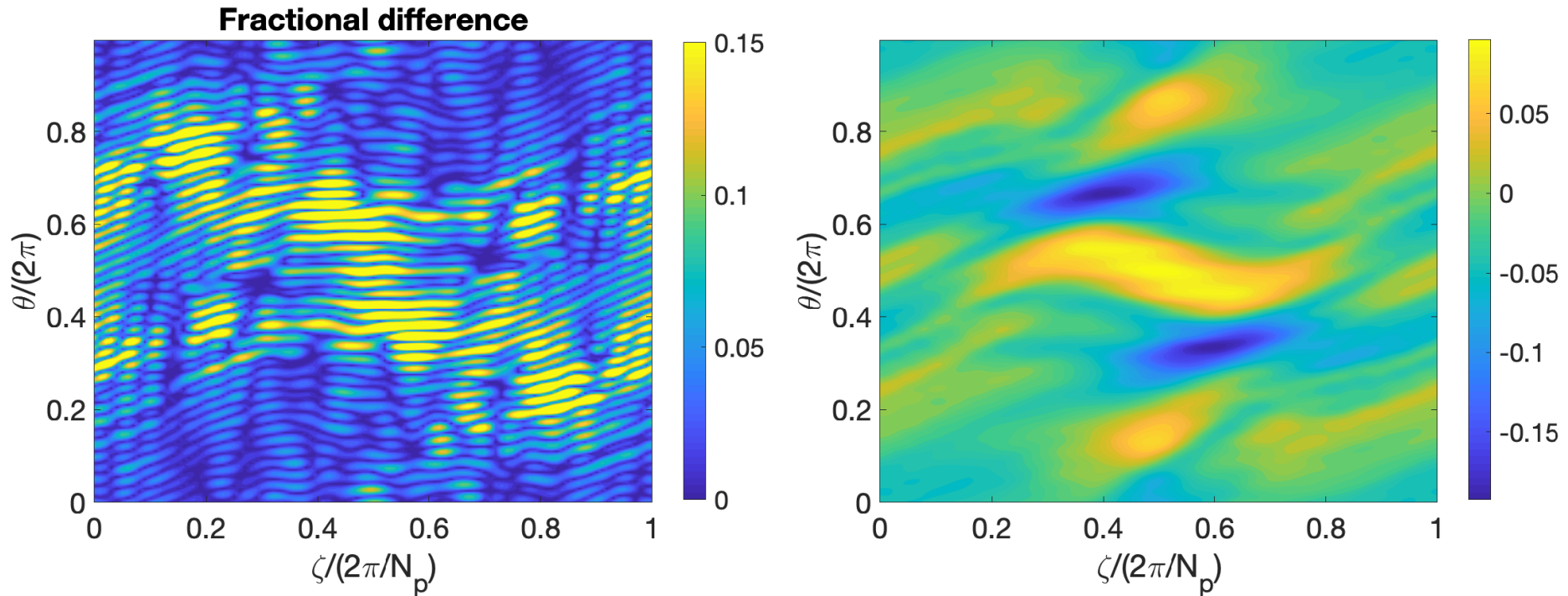
$$\begin{aligned} \delta J_{C_2} &= 0 \\ \mathbf{F}(\xi_2) &\neq 0 \\ \delta I_{T,2} &\neq 0 \end{aligned}$$

Comparison between adjoint and direct iota shape gradient



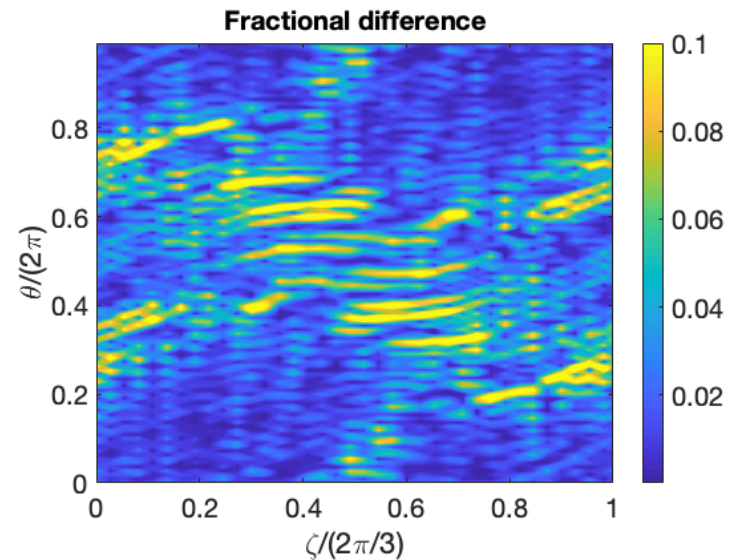
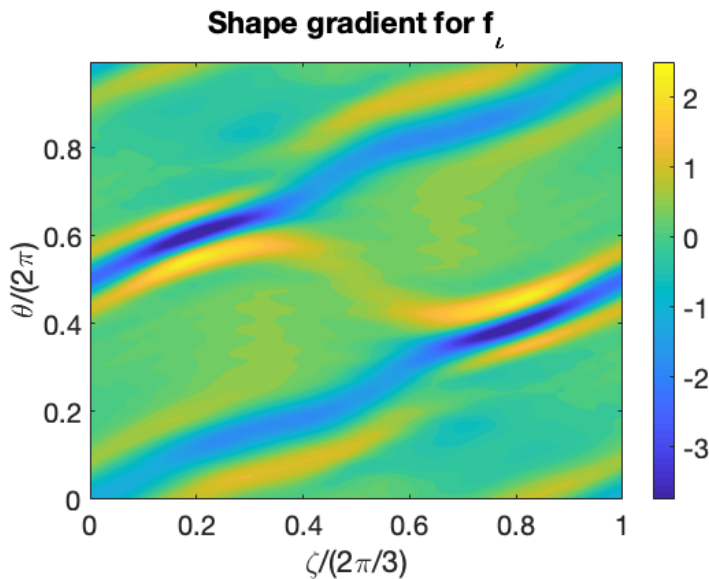
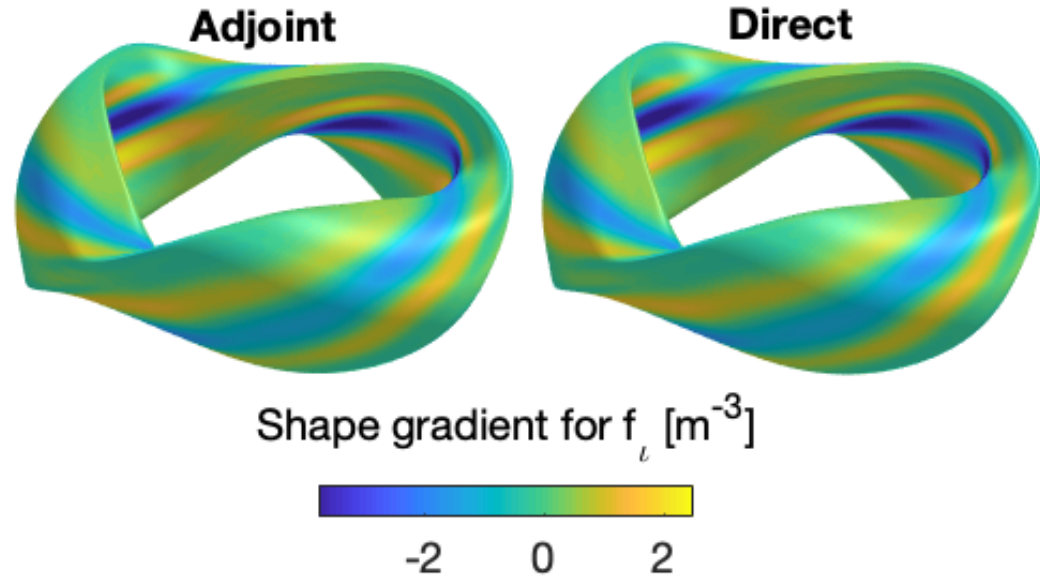
Comparison between adjoint and direct well shape gradient

$$f_W = \int_{V_{\text{plasma}}} d\psi V'(\psi) w(\psi)$$



Comparison between adjoint and direct iota shape gradient

$$f_l = \int_{V_{\text{plasma}}} w(\psi) \iota(\psi)$$



Many applications of MHD shape gradients possible

Magnetic well

- S for finite pressure magnetic well requires anisotropic pressure tensor

$$f_W = \int_{V_P} d^3x w(\psi) \frac{d}{d\psi} \left\langle \frac{B^2}{2} + \mu_0 p \right\rangle_\psi$$

Confinement

- **Neoclassical transport**

- S for particle flux in $1/\nu$ regime requires anisotropic pressure
- S for particle flux computed with solution of drift kinetic equation computed with “double adjoint” and addition of bulk force to equilibrium

$$f_{NC} = \int_{V_P} d^3x w(\psi) \langle \mathbf{\Gamma} \cdot \nabla \psi \rangle_\psi$$

- S for **breaking of quasi-symmetry** requires addition of bulk force

$$f_{QS} = \int_{V_P} d^3x w(\psi) F(\psi) \qquad F(\psi) = \frac{\left(\frac{M}{N}\right) G(\psi) + I(\psi)}{\left(\frac{M}{N}\right) \iota(\psi) - 1}$$

Magnetic well figure of merit

- Average radial curvature appears in ballooning mode potential energy¹
 - $\kappa_\psi > 0$ associated with stability

$$\kappa_\psi = \left\langle \boldsymbol{\kappa} \cdot \frac{\partial \mathbf{r}}{\partial \psi} \right\rangle_\psi = \left\langle \frac{1}{2B^2} \frac{\partial}{\partial \psi} (2\mu_0 p + B^2) \right\rangle_\psi$$

- In a vacuum magnetic field, this reduces to

$$\kappa_\psi = - \frac{V''(\psi)}{V'(\psi)}$$

- $V''(\psi) < 0$ associated with MHD stability of stellarators

¹Friedberg, *Ideal MHD* (2014).