An adjoint approach for the shape gradients of 3D MHD equilibria

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PPPL Research Seminar November 25, 2019

Outline

- Introduction
 - Stellarator shape optimization
 - Adjoint methods
- Shape gradients for MHD equilibria
- Perturbed equilibrium approach
- Conclusions

Stellarators require shape optimization (I)

Traditional two-step optimization

1. MHD equilibrium optimization (e.g. STELLOPT¹, ROSE²)

How to design boundary for optimal confinement?



¹D.A. Spong et al, *Nuclear Fusion*, 41 (2001). ²M. Drevlak et al, *Nuclear Fusion*, 59 (2019).

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MHD force balance

Stellarators require shape optimization (I)

Traditional two-step optimization

1. MHD equilibrium optimization (e.g. STELLOPT¹, ROSE²)

How to design boundary for optimal confinement?

2. Coil design (e.g. REGCOIL³, FOCUS⁴)

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

¹D.A. Spong et al, *Nuclear Fusion*, 41 (2001).
²M. Drevlak et al, *Nuclear Fusion*, 59 (2019).
³M. Landreman, *Nuclear Fusion*, 57 (2017).
⁴C. Zhu et al, *Nuclear Fusion*, 58 (2017).

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Biot-Savart

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Stellarators require shape optimization (II)

Combined one-step optimization

1. MHD equilibrium direct optimization of coils¹

How to design coils for optimal confinement and engineering feasibility?



MHD force balance

¹D. Strickler et al, *IAEA FT/P2-06* (2003).

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Stellarators require shape optimization (II)

Combined one-step optimization

1. MHD equilibrium direct optimization of coils¹

How to design coils for optimal confinement and engineering feasibility?



MHD force balance

"The highest priority for technology is to better integrate the engineering design with the physics design at the earliest possible stage." -Report from the National Stellarator Coordinating Committee²

¹D. Strickler et al, *IAEA FT/P2-06* (2003). ²D.Gates et al, *J. Fusion Energy*, 37 (2018).

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Analytic gradients are valuable in high-dimensional spaces (I)



Minimization of 2D Rosenbrock function

Z. Lyu et al, *Proc. Inter. Conf. Comp. Fluid Dyn.*, *11* (2014).

Analytic gradients are valuable in high-dimensional spaces (II)

Minimization of ND Rosenbrock function



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Adjoint method for analytic derivatives

- Figure of merit $f(\mathbf{x})$ s.t. $L(\mathbf{x}) = 0$
- Goal: compute $\partial f(\mathbf{x})/\partial \Omega$ for $\Omega = \{\Omega_i\}_{i=1}^{N_\Omega}$

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Adjoint methods widely used in computational fluid dynamics



Inward for smaller drag Outward for smaller drag

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

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• Goal: compute $\partial f(\mathbf{x}) / \partial \Omega$ for $\Omega = \{\Omega_i\}_{i=1}^{N_{\Omega}} (\geq N_{\Omega} + 1 \text{ solves with finite differences})$ $f(\mathbf{x}) = \mathbf{c}^T \mathbf{x} \text{ s.t. } \overleftrightarrow{\mathbf{A}} \mathbf{x} = \mathbf{b}$

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- Compute perturbations of linear system

$$\frac{\partial \vec{A}}{\partial \Omega_i} x + \vec{A} \frac{\partial x}{\partial \Omega_i} = \frac{\partial b}{\partial \Omega_i} \longrightarrow \frac{\partial x}{\partial \Omega_i} = \left(\vec{A}\right)^{-1} \left(\frac{\partial b}{\partial \Omega_i} - \frac{\partial \vec{A}}{\partial \Omega_i} x\right)$$

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• Compute derivative with chain rule

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• Solve adjoint equation

 $\overleftarrow{A}^T z = c$

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Solve adjoint equation

$$\overrightarrow{A}^T \boldsymbol{z} = \boldsymbol{c}$$

• Get derivative with respect to all Ω_i with 2 solutions of linear system (x, z)

$$\frac{\partial f}{\partial \Omega_i} = \mathbf{z}^T \left(\frac{\partial \mathbf{b}}{\partial \Omega_i} - \frac{\partial \vec{\mathbf{A}}}{\partial \Omega_i} \mathbf{x} \right)$$

Outline

- Introduction
- Shape gradients for MHD equilibria
 - Introduction to shape gradients
 - Fixed-boundary relation
 - Free-boundary relation
- Perturbed equilibrium approach
- Conclusions



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- f(S) = physics objective depending on equilibrium field
- Surface is displaced by vector field δr

 $S_{\epsilon} = \{r_0 + \epsilon \delta r : r_0 \in S\}$



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- Surface is displaced by vector field δr $S_{\epsilon} = \{r_0 + \epsilon \delta r : r_0 \in S\}$
- Shape derivative of f(S) $\delta f(\delta r) = \lim_{\epsilon \to 0} \frac{f(S_{\epsilon}) - f(S)}{\epsilon}$



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- Shape derivative of f(S) $\delta f(\delta r) = \lim_{\epsilon \to 0} \frac{f(S_{\epsilon}) - f(S)}{\epsilon}$
- Under assumption of smoothness

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

• For any δr , shape gradient, G, provides change to figure of merit, δf



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- Under assumption of smoothness $\delta f(\delta \mathbf{r}) = \int_{S} d^{2}x \, \delta \mathbf{r} \cdot \mathbf{n} \, \mathcal{G}$
- For any δr , shape gradient, G, provides change to figure of merit, δf

Why is the shape gradient (G) useful?

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

Computing MHD shape gradient directly is expensive

- *S* described by parameters $\{\Omega_i\}_1^{N_{\Omega}}$
- $\partial f / \partial \Omega$ computed from finite differences
 - $\geq N_{\Omega} + 1$ non-linear equilibrium evaluations

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- $\partial f / \partial \Omega$ computed from finite differences
 - $\geq N_{\Omega} + 1$ non-linear equilibrium evaluations
- Fourier solution for shape gradient

$$\mathcal{G} = \sum_{j} S_j \cos(m_j \theta - n_j \phi)$$

• Shape gradient computed from linear system $\frac{\partial f}{\partial \Omega_i} = \int_S d^2 x \, S_j \cos(m_j \theta - n_j \phi) \frac{\partial \boldsymbol{r}}{\partial \Omega_i} \cdot \boldsymbol{n}$

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¹M. Landreman & E.J. Paul, *Nuclear Fusion*, 58 (2018).

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

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

Note: magnetic surfaces assumed (variational solution¹)

¹M. Kruskal & R.M. Kulsrud, *Phys. Fluids*, 1 (1958).

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Note: magnetic surfaces assumed (variational solution¹)

• Perturbation with fixed $\iota(\psi)$ and $p(\psi)$ determined from ξ_1

$$\delta \boldsymbol{B}_1 = \nabla \times (\boldsymbol{\xi}_1 \times \boldsymbol{B}) \\ \delta p(\boldsymbol{\xi}_1) = -\boldsymbol{\xi}_1 \cdot \nabla p$$

Unperturbed boundary

¹M. Kruskal & R.M. Kulsrud, *Phys. Fluids*, 1 (1958).

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Perturbed

boundary

Displacement

 $(\delta \boldsymbol{r} \cdot \boldsymbol{n})$

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• Perturbation with fixed $\iota(\psi)$ and $p(\psi)$ determined from ξ_1

$$\delta \boldsymbol{B}_1 = \nabla \times (\boldsymbol{\xi}_1 \times \boldsymbol{B})$$
$$\delta p(\boldsymbol{\xi}_1) = -\boldsymbol{\xi}_1 \cdot \nabla p$$

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

$$\boldsymbol{F}(\boldsymbol{\xi}_{1}) = \frac{(\nabla \times \boldsymbol{B}) \times \delta \boldsymbol{B}_{1} + \nabla \times (\delta \boldsymbol{B}_{1}) \times \boldsymbol{B}}{4\pi} - \nabla \delta \boldsymbol{p}(\boldsymbol{\xi}_{1}) = 0$$
$$\boldsymbol{\xi}_{1} \cdot \boldsymbol{n} \Big|_{S_{\text{plasma}}} = \delta \boldsymbol{r} \cdot \boldsymbol{n} \Big|_{S_{\text{plasma}}}$$

Unperturbed boundary

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Perturbed

boundary

Displacement $(\delta r \cdot n)$



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¹T. Antonsen Jr., E.J. Paul, M. Landreman, *J. Plasma Phys.* 85 (2019). ²I.B. Bernstein et al, *Proc. Royal Society A*, 244 (1958).

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¹T. Antonsen Jr., E.J. Paul, M. Landreman, J. Plasma Phys. 85 (2019).

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$$\int_{V_{\text{plasma}}} d^3x \left(-F(\xi_1) \cdot \xi_2 + F(\xi_2) \cdot \xi_1\right) + \frac{1}{4\pi} \int_{S_{\text{plasma}}} d^2x \, \mathbf{n} \cdot \left(\xi_1 \delta \mathbf{B}_2 \cdot \mathbf{B} - \xi_2 \delta \mathbf{B}_1 \cdot \mathbf{B}\right)$$
$$-\frac{2\pi}{c} \int_{V_{\text{plasma}}} d\psi \left(\delta I_{T,2}(\psi) \delta \iota_1(\psi) - \delta I_{T,1}(\psi) \delta \iota_2(\psi)\right) = 0$$
1. Compute shape derivative for figure of merit
$$\delta f(\xi_1) = \int_{V_{\text{plasma}}} d^3x \, \xi_1 \cdot \mathbf{A}_1 + \int_{S_{\text{plasma}}} d^2x \, \mathbf{n} \cdot \xi_1 \mathbf{A}_2$$
2. Adjoint displacement ξ_2 satisfies
$$F(\xi_2) = -\mathbf{A}_1$$
$$\xi_2 \cdot \mathbf{n}|_{S_{\text{plasma}}} = 0$$

¹T. Antonsen Jr., E.J. Paul, M. Landreman, J. Plasma Phys. 85 (2019).

$$\int_{V_{\text{plasma}}} d^3x \left(-F(\xi_1) \cdot \xi_2 + F(\xi_2) \cdot \xi_1\right) + \frac{1}{4\pi} \int_{S_{\text{plasma}}} d^2x \, \mathbf{n} \cdot \left(\xi_1 \delta \mathbf{B}_2 \cdot \mathbf{B} - \xi_2 \delta \mathbf{B}_1 \cdot \mathbf{B}\right)$$
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Magnetic well shape gradient requires pressure perturbation



 ψ/ψ_0

Magnetic well shape gradient requires pressure perturbation



Magnetic well shape gradient requires pressure perturbation



Magnetic well shape gradient computed with VMEC¹

 \approx

Linearization approximated with $\Delta_P \ll 1$

$$F(\xi_2) = \nabla w(\psi)$$

$$\xi_2 \cdot n \Big|_{S_{\text{plasma}}} = 0$$

$$\delta I_{T,2}(\psi) = 0$$

$$0 = \frac{(\nabla \times \boldsymbol{B}) \times \boldsymbol{B}}{4\pi} - \nabla (p(\psi) + \Delta_{\boldsymbol{P}} w(\psi))$$

S_{plasma}, $I_T(\psi)$, $p(\psi)$ prescribed

¹S. Hirshman & J.C. Whitson, *Phys. Fluids*, 26 (1983).

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Magnetic well shape gradient computed with VMEC¹

Linearization approximated with $\Delta_P \ll 1$



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Magnetic well shape gradient computed with VMEC¹

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Magnetic ripple shape gradient requires anisotropic pressure



Magnetic ripple shape gradient requires anisotropic pressure

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Variational principle for equilibria with anisotropic pressure

Equilibrium with anisotropic pressure

$$\frac{\boldsymbol{J} \times \boldsymbol{B}}{c} = \nabla \cdot \left(p_{||} (\boldsymbol{\psi}, B) \boldsymbol{b} \boldsymbol{b} + p_{\perp} (\boldsymbol{\psi}, B) (\boldsymbol{\vec{I}} - \boldsymbol{b} \boldsymbol{b}) \right)$$

 $\frac{p_{\perp}(\psi, B)}{\partial B} = \frac{p_{\parallel}(\psi, B) - p_{\perp}(\psi, B)}{B}$

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Variational principle for equilibria with anisotropic pressure

Equilibrium with anisotropic pressure

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 $\frac{p_{\perp}(\psi, B)}{\partial B} = \frac{p_{\parallel}(\psi, B)}{B}$

Stationary points of *W*[*B*, *p*]

$$W[B,p] = \int_{V_P} d^3x \, \frac{B^2}{8\pi} - p_{||}$$

Subject to:

- 1. Prescribed $p_{\parallel}(\psi, B)$
- 2. Fixed $\iota(\psi)$
- 3. Magnetic surfaces

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Variational principle for equilibria with anisotropic pressure

Equilibrium with anisotropic pressure

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- Solutions computed with ANIMEC¹ code
- Used for analysis of energetic particle contributions to equilibria

¹W.A. Cooper et al, *Computer Phys. Comm.*, 72 (1992).

Magnetic ripple shape gradient computed with ANIMEC¹

Linearization approximated with $\Delta_P \ll 1$

$$F(\xi_2) = \nabla \cdot P$$

$$\xi_2 \cdot n \Big|_{S_{\text{plasma}}} = 0$$

$$\delta \iota_2(\psi) = 0$$

$$0 = \frac{(\nabla \times \boldsymbol{B}) \times \boldsymbol{B}}{4\pi} - \nabla (p(\psi)) - \Delta_{\boldsymbol{P}} \nabla \cdot \boldsymbol{P}$$

S_{plasma}, $\iota(\psi)$, $p(\psi)$, $p_{||}(\psi, B)$ prescribed

¹W.A. Cooper et al, *Computer Phys. Comm.*, 72 (1992).

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Magnetic ripple shape gradient computed with ANIMEC¹

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Magnetic ripple shape gradient computed with ANIMEC¹

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Many other applications of adjoint approach possible¹ Effective Ripple² ($\epsilon_{eff}^{3/2}$)

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- Proxy for low-collisionality neoclassical confinement
- Adjoint approach requires bulk force $\mathcal{F} = \nabla \cdot \mathbf{P}(\psi, \alpha)$ $f_{OS} = \int d^3x \, \epsilon_{eff}^{3/2}(\psi) w(\psi)$

¹E.J. Paul et al, *submitted to J. Plasma Phys.*, (arXiv:1910.14144).
²V.V. Nemov et al, *Phys. Plasmas*, 6 (1999).
³P. Helander, *Rep. Prog. Phys.*, 77 (2014).

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Many other applications of adjoint approach possible¹ Effective Ripple² ($\epsilon_{eff}^{3/2}$)

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Cannot be implemented with ANIMEC

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³P. Helander, *Rep. Prog. Phys.*, 77 (2014).



Many other applications of adjoint approach possible¹ Departure from quasi-symmetry

• Quasi-symmetry → guiding center confinement, reduced neoclassical transport

 $f_{QS} = \int d^3x \, w(\psi) (\boldsymbol{B} \times \nabla B \cdot \nabla \psi - F(\psi) \boldsymbol{B} \cdot \nabla B)^2$

Does not require Boozer coordinate transformation





¹E.J. Paul et al, *submitted to J. Plasma Phys.*, (arXiv:1910.14144). ²L.M. Imbert-Gerard, E.J. Paul, A. Wright, (arXiv:1908.05360).

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Does not require Boozer coordinate transformation

• Adjoint approach requires bulk force, $\mathcal{F}(r)$





¹E.J. Paul et al, *submitted to J. Plasma Phys.*, (arXiv:1910.14144). ²L.M. Imbert-Gerard, E.J. Paul, A. Wright, (arXiv:1908.05360).

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Adjoint approach for coil shape gradient



¹T. Antonsen Jr., E.J. Paul, M. Landreman, J. Plasma Phys., 85 (2019).

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Adjoint approach for coil shape gradient

Generalization of self-adjointness of MHD force operator¹ $\int_{V_{\text{plasma}}} d^3x \left(-F(\xi_1) \cdot \xi_2 + F(\xi_2) \cdot \xi_1 \right) + \frac{1}{c} \sum_k \left(I_{C_k} \int_{C_k} dl \left(\delta r_{C_{1,k}} \cdot t \times \delta B_2 - \delta r_{2,k} \cdot t \times \delta B_1 \right) \right)$ $- \frac{2\pi}{c} \int_{V_{\text{plasma}}} d\psi \left(\delta I_{T,2}(\psi) \delta \iota_1(\psi) - \delta I_{T,1}(\psi) \delta \iota_2(\psi) \right) = 0$

1. Compute shape derivative for figure of merit $\delta f(\xi_1) = \int_{V_{\text{plasma}}} d^3x \ \xi_1 \cdot A_1$ 2. Adjoint displacement ξ_2 satisfies $F(\xi_2) = -A_1$ $\delta r_{2,k} = 0$

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Adjoint approach for coil shape gradient

Generalization of self-adjointness of MHD force operator¹ $\int_{V_{\text{plasma}}} d^3x \left(-\mathbf{F}(\boldsymbol{\xi}_1) \cdot \boldsymbol{\xi}_2 + \mathbf{F}(\boldsymbol{\xi}_2) \cdot \boldsymbol{\xi}_1 \right) + \frac{1}{c} \sum_{\nu} \left(I_{C_k} \int_{C_{\nu}} dl \left(\delta \mathbf{r}_{C_{1,k}} \cdot \mathbf{t} \times \delta \mathbf{B}_2 - \delta \mathbf{r}_{2,k} \cdot \mathbf{t} \times \delta \mathbf{B}_1 \right) \right)$ $-\frac{2\pi}{c} \int d\psi \left(\delta I_{T,2}(\psi) \delta \iota_1(\psi) - \delta I_{T,1}(\psi) \delta \iota_2(\psi) \right) = 0$ V_{plasma} 1. Compute shape derivative for figure of merit $\delta f(\boldsymbol{\xi}_{1}) = \sum_{k} \int_{C_{k}} dl \, \delta \boldsymbol{r}_{C_{1,k}} \cdot \boldsymbol{t} \times \boldsymbol{\delta B}_{2} \, \frac{I_{C_{k}}}{c}$ $\delta f(\boldsymbol{\xi}_1) = \int_{V_{\text{plasma}}} d^3 x \ \boldsymbol{\xi}_1 \cdot \boldsymbol{A}_1$ 2. Adjoint displacement ξ_2 satisfies $F(\xi_2) = -A_1$ S_k = coil shape gradient $\delta \mathbf{r}_{2k} = 0$

¹T. Antonsen Jr., E.J. Paul, M. Landreman, J. Plasma Phys., 85 (2019).

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Rotational transform coil shape gradient with VMEC



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Rotational transform coil shape gradient with VMEC



Rotational transform coil shape gradient with VMEC



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Outline

- Introduction
- Shape gradients for MHD equilibria
- Perturbed equilibrium approach
 - Variational principle for linear MHD
 - Euler-Lagrange solutions
- Conclusions

Variational principle for perturbed MHD equilibria

Perturbed equilibrium with bulk force $F(\xi) + \delta F = \frac{(\nabla \times B) \times \delta B + (\nabla \times (\delta B)) \times B}{4\pi} - \nabla \delta p(\xi) + \delta F = 0$ $\delta B(\xi) = \nabla \times (\xi \times B)$ $\delta p = -\xi \cdot \nabla p$ $\xi \cdot \nabla \psi \mid_{\psi=0} = \xi \cdot \nabla \psi \mid_{\psi=\psi_0} = 0$

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Stationary points of $W[\xi]$ $W[\xi] = \int_{V_P} d^3x \left(-\frac{\delta B \cdot \delta B}{4\pi} + \frac{\xi \cdot J \times \delta B}{c} - \xi \cdot \nabla p(\nabla \cdot \xi) - 2\xi \cdot \delta F \right)$ $\delta \xi \cdot \nabla \psi \mid_{\psi=0} = \delta \xi \cdot \nabla \psi \mid_{\psi=\psi_0} = 0$

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 $\xi \cdot B = 0 \rightarrow$ 2 independent components

$$W[\boldsymbol{\xi}^{\boldsymbol{\psi}}, \boldsymbol{\xi}^{\boldsymbol{\alpha}}] = \int_{V_P} d^3 x \left(-\frac{\delta \boldsymbol{B} \cdot \delta \boldsymbol{B}}{4\pi} + \frac{\boldsymbol{\xi} \cdot \boldsymbol{J} \times \delta \boldsymbol{B}}{c} - \boldsymbol{\xi} \cdot \nabla p(\boldsymbol{\nabla} \cdot \boldsymbol{\xi}) - 2\boldsymbol{\xi} \cdot \delta \boldsymbol{F} \right)$$
$$\boldsymbol{\xi}^{\boldsymbol{\psi}} = \boldsymbol{\xi} \cdot \nabla \boldsymbol{\psi}$$
$$\boldsymbol{\xi}^{\boldsymbol{\alpha}} = \boldsymbol{\xi} \cdot \nabla \boldsymbol{\theta} - \iota(\boldsymbol{\psi}) \boldsymbol{\xi} \cdot \nabla \boldsymbol{\phi}$$
$$\boldsymbol{\xi}^{\boldsymbol{\psi}}|_{\boldsymbol{\psi}=0} = \boldsymbol{\xi}^{\boldsymbol{\psi}}|_{\boldsymbol{\psi}=\psi_0} = 0$$

Variation w.r.t. Ξ^{α}

$$2\overleftarrow{A^{\alpha\alpha}}\Xi^{\alpha}(\psi) = \left(\overleftarrow{A^{\alpha\psi}}\Xi^{\psi}(\psi) + \overleftarrow{A^{\alpha\psi'}}\Xi^{\psi'}(\psi) + C^{\alpha}\right)$$

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• 2nd order coupled 2-point BVP solved with finite difference

• Similar to Euler-Lagrange eqn. solved by DCON¹

¹A. Glasser, *Phys. Plasmas*, 23 (2016).

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Preliminary perturbed equilibrium results



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Outline

- Introduction
- Shape gradients for MHD equilibria
- Perturbed equilibrium approach
- Conclusions

Conclusions (I)

Open questions

- How to extend linearized MHD approach to 3D (e.g. Frobenius analysis as in DCON¹)?
- Can we prevent flux surface overlap in linearized approach?
- Can adjoint approach be generalized to avoid assumption of surfaces?

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Conclusions (I)

Open questions

- How to extend linearized MHD approach to 3D (e.g. Frobenius analysis as in DCON)?
- Can we prevent flux surface overlap in linearized approach?
- Can adjoint approach be generalized to avoid assumption of surfaces?

Future work

- Application of adjoint approach for fixed and free-boundary optimization (e.g. incorporation in STELLOPT).
- Demonstration for other important figures of merit (e.g. energetic particle confinement)

Conclusions (II)

- Adjoint methods allow efficient computation of geometric derivatives
 - Gradient-based optimization
 - Sensitivity and tolerance analysis
- Adjoint approach for MHD equilibria used to compute shape gradient for plasma boundary and coil shapes
 - ✓ Magnetic well
 - ✓ Magnetic ripple
 - ✓ Rotational transform
 - \Box Effective ripple ($\epsilon_{eff}^{3/2}$)
 - **Quasisymmetry**
 - ? Energetic particles

Conclusions (II)

- Adjoint methods allow efficient computation of geometric derivatives
 - Gradient-based optimization
 - Sensitivity and tolerance analysis
- Adjoint approach for MHD equilibria used to compute shape gradient for plasma boundary and coil shapes

References for this work

- T.M. Antonsen, E.J. Paul, M. Landreman, J. *Plasma Phys.*, 85 (2019).
- E.J. Paul et al, *submitted to J. Plasma Phys.*, (arXiv:1910.14144).

Other adjoint methods for stellarators

- Optimization of coil shapes E.J. Paul et al, *Nuclear Fusion*, 58 (2018).
- Optimization of neoclassical quantities E.J. Paul et al, *J. Plasma Phys.*, 85 (2019).

Thank you for your attention