Computing local sensitivity & tolerances of stellarators using shape gradients



The shape gradient is a new (to fusion) way to think about derivatives involving shapes.

- Derivatives involving shapes are central to stellarator optimization.
- These derivatives also encode tolerances, which have been a leading driver of cost:

"The largest driver of the project cost growth were the accuracy requirements."

Strykowsky et al, *Engineering Cost & Schedule Lessons Learned on NCSX*, (2009).

• Compared to 'parameter derivatives', shape gradients have 2 advantages:

• Spatially local

• Independent of parameterization and discretization

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- 2 ways to represent derivatives: parameter derivatives vs. shape gradients.
- Computing shape gradients from existing codes.
- Fast computation of shape gradients via adjoint methods.
- Coil tolerances
- Magnetic sensitivity and tolerances

Historically, we have represented derivatives of shapes using parameter derivatives.

Let *f* denote any figure of merit, e.g. rotational transform $\iota = 1/q$, neoclassical transport, etc. **Parameter derivatives:** Example: $\partial f / \partial R^c_{m,n}$ and $\partial f / \partial Z^s_{m,n}$ where $R^c_{m,n}$ and $Z^s_{m,n}$ parameterize the plasma boundary shape:

$$R(\theta,\zeta) = \sum_{m,n} R_{m,n}^{c} \cos(m\theta - n\zeta),$$
$$Z(\theta,\zeta) = \sum_{m,n} Z_{m,n}^{s} \sin(m\theta - n\zeta)$$

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- Successfully used in STELLOPT to design NCSX, etc.
- Computable by finite differencing any code.

But,

- Not unique: coordinate-dependent,
- Nonlocal: awkward for engineering.



The shape gradient is a complementary way to express derivatives involving shapes.

For surfaces, the shape gradient = *S* where
$$\delta f = \int d^2 a \left(\delta \mathbf{r} \cdot \mathbf{n} \right) S$$
.
Unit normal



- Local (real-space, not Fourier-space). More useful for engineering.
- Independent of coordinates & discretization used to represent surface.

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The shape gradient representation can be expected to exist for many shape functionals.

Derivative of a function
of *n* numbers
$$f(r_1, r_2, ..., r_n)$$
:
 $\delta f = \sum_{j=1}^n \frac{\partial f}{\partial r_j} \delta r_j$
 $n \to \infty$:
 $f = f[r(\ell)], \quad \delta f = \int d\ell \frac{\delta f}{\frac{\delta f}{\delta r}} \delta r$

This is an instance of the "Riesz representation theorem":

Any linear functional can be written as an inner product with some element of the appropriate space.

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<u>Coils</u>: Discretize coil shapes: $X(\vartheta) = X_0^c + \sum_{m=1} \left[X_m^c \cos(m\vartheta) + X_m^s \sin(m\vartheta) \right] \qquad \& Y, Z$ Parameters p_j are $\left\{ X_m^c, X_m^s, Y_m^c, Y_m^s, Z_m^c, Z_m^s \right\}$.

Compute $\partial f / \partial p_i$ using finite differences, e.g. STELLOPT.

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Discretize shape gradient:

$$S_{X}(\vartheta) = S_{X,0}^{c} + \sum_{m=1} \left[S_{X,m}^{c} \cos(m\vartheta) + S_{X,m}^{s} \sin(m\vartheta) \right] \qquad \& S_{Y}, S_{Z}$$

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$$\int d\ell \, \delta \mathbf{r} \cdot \mathbf{S} = \delta f \quad \Rightarrow \quad \text{Solve } \int d\ell \, \frac{\partial \mathbf{r}}{\partial p_j} \cdot \mathbf{S} = \frac{\partial f}{\partial p_j} \text{ for } \mathbf{S}.$$

(Square linear system)

Example: Neoclassical transport $\varepsilon_{eff}^{3/2}$ at r/a=0.5



Example: Neoclassical transport $\varepsilon_{eff}^{3/2}$ at r/a=0.5



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Adjoint methods:

- You can get the derivative of a code result with respect to <u>all</u> *N* parameters with only 1 (not *N*) extra calculation.
- Requires some theory work and code modifications.

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Recently used for optimizing tokamak divertor shapes:

- W. Dekeyser, Ph.D. thesis, KU Leuven (2014).
- W. Dekeyser et al, *Nucl. Fusion* 54, 073022 (2014).
- M. Baelmans, et al, Nucl. Fusion 57, 036022 (2017).

Antonsen, Paul, & ML, PO5.00005 Wed 2:48pm

Self-adjointness of linearized MHD:

$$\int_{\Omega} \left(\boldsymbol{\xi}^{(2)} \cdot \mathbf{F}^{(1)} - \boldsymbol{\xi}^{(1)} \cdot \mathbf{F}^{(2)} \right) = \int_{\partial \Omega} \left[\left(\mathbf{n} \cdot \boldsymbol{\xi}^{(1)} \right) \left(\mathbf{B} \cdot \boldsymbol{\delta} \mathbf{B}^{(2)} \right) - \left(\mathbf{n} \cdot \boldsymbol{\xi}^{(2)} \right) \left(\mathbf{B} \cdot \boldsymbol{\delta} \mathbf{B}^{(1)} \right) \right]$$

where $\mathbf{F}^{(j)} = \mathbf{J}^{(j)} \times \mathbf{B} + \mathbf{J} \times \mathbf{B}^{(j)} - \nabla p^{(j)}$, $\mathbf{B}^{(j)} = \nabla \times \left(\boldsymbol{\xi}^{(j)} \times \mathbf{B} \right)$, $\mu_0 \mathbf{J}^{(j)} = \nabla \times \mathbf{B}^{(j)}$, $p^{(j)} + \boldsymbol{\xi}^{(j)} \cdot \nabla p = 0$.

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⇒ If perturbations to a figure of merit *f* can be written $\delta f = \int_{\Omega} \xi \cdot (\text{something})$, adjoint calculation is given by perturbing the equilibrium by the "something".

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⇒ If perturbations to a figure of merit *f* can be written $\delta f = \int_{\Omega} \xi \cdot (\text{something})$, adjoint calculation is given by perturbing the equilibrium by the "something".

Can be generalized to include perturbations that change i, & vacuum region + coils.

Adjoint calculations for several figures of merit have now been demonstrated.



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Coil tolerances can be computed from the shape gradient.

Choose an acceptable Δf & any weight $w(\ell) \ge 0$.

Let
$$T(\ell) = \frac{w \Delta f}{\sum \int d\ell w |\mathbf{S}|}$$

If $|\delta \mathbf{r}| \leq T$, $|\delta f| \leq \int d\ell |\mathbf{S} \cdot \delta \mathbf{r}| \leq \int d\ell |\mathbf{S}| |\delta \mathbf{r}| \leq \int d\ell |\mathbf{S}| T = \Delta f$.

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Conservative: a bound on the worst possible outcome.

Coil tolerances can be computed from the shape gradient.



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A magnetic sensitivity S_B can be computed from the shape gradient.

Define
$$S_{B}$$
 by $\mathbf{B}_{0} \cdot \nabla S_{B} = \langle S \rangle - S$.

Substitute into
$$\delta f = \int d^2 a \, S \delta \mathbf{r} \cdot \mathbf{n}$$
.

After some algebra ...

$$\Rightarrow \quad \delta f = \int d^2 a \, S_{B} \delta \mathbf{B} \cdot \mathbf{n}.$$



A magnetic tolerance T_B can be computed from the magnetic sensitivity.

Choose an acceptable Δf & any weight $W(\theta, \zeta) \ge 0$.

Let
$$T_{B}(\theta,\zeta) = \frac{W \Delta f}{\int d^{2}a W |S_{B}|}$$
.

If
$$\left| \delta \mathbf{B} \cdot \mathbf{n} \right| \leq T_{B}$$
,
 $\left| \delta f \right| \leq \int d^{2}a \left| S_{B} \right| \left| \delta \mathbf{B} \cdot \mathbf{n} \right|$
 $\leq \int d^{2}a \left| S_{B} \right| T_{B}$
 $\leq \Delta f$.

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Conclusions

Shape gradients provide *local* sensitivity & tolerance information which could inform

- How accurately and rigidly the coils should be built,
- Where coils should be connected to support structure,
- Where sources of error fields like coil leads should be located.

Future work:

- Shape gradients for island width.
- Develop adjoint methods for more figures of merit. Need 3D equilibrium or stability code with arbitrary pressure anisotropy.
- Target tolerances in STELLOPT to increase them.

Landreman & Paul, Nuclear Fusion **58** 076023 (2018), Antonsen, Paul, & Landreman, PO5.00005 Wed 2:48pm

Extra slides

For some shape functionals, the shape gradient can be computed analytically. Example: Given $\mathbf{B}(\mathbf{r})$, vary surface to minimize $f = \frac{1}{2} \left[\int d^2 a (\mathbf{B} \cdot \mathbf{n})^2 \right] + \lambda \int d^3 x$ Volume "Quadratic flux" [1] Perturb position vector $\mathbf{r}(\theta, \zeta)$. 0.2 After some algebra... Poincare plot 0.15 S=0 surfaces $\delta f = \int d^2 a \, S \, \delta \mathbf{r} \cdot \mathbf{n}$ 0.1 0.05 where $S = (\mathbf{B} \cdot \mathbf{n})^2 H + \mathbf{B} \cdot \nabla (\mathbf{B} \cdot \mathbf{n}) + \lambda$, N H = mean curvature. -0.05 -0.1 S = 0 at the optimum. -0.15 -0.2 0.7 0.9 1.1 1.2 1.3 0.8 [1] Dewar, Hudson, Price (1994).

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The algorithm for computing shape gradients can be verified by comparison to analytic theory.

Consider f = area. Analytic result: $S = -2 \times (\text{mean curvature})$



Example: Rotational transform at r/a=0.5

Shape gradient for boundary surface:

Parameter derivatives from STELLOPT/VMEC:



$$\delta f = \int d^2 a \Big(\delta \mathbf{r} \cdot \mathbf{n} \Big) S$$



Example: Rotational transform at r/a=0.5





Shape gradient on a current surface for $f = \int d^2 a (\mathbf{B} \cdot \mathbf{n})^2$ given a fixed plasma boundary



Plasma boundary shape:

Parameters p_{j} are $\left\{R_{m,n}^{c}, Z_{m,n}^{s}\right\}$. Compute $\frac{\partial f}{\partial p_{j}}$ using finite differences, e.g. STELLOPT. Discretize shape gradient: $S(\theta, \zeta) = \sum_{q} S_{q} \cos\left(m_{q}\theta - n_{q}\zeta\right)$ $\int d^{2}a \left(\delta \mathbf{r} \cdot \mathbf{n}\right) S = \delta f \implies \text{Solve } \int d^{2}a \frac{\partial \mathbf{r}}{\partial p_{j}} \cdot \mathbf{n} S = \frac{\partial f}{\partial p_{j}} \text{ for } S.$ (1)

Linear system, not square.

Check that $\frac{\partial f}{\partial p_j}$ is in the column space of matrix. If so, (1) can be solved for S_q using pseudo-inverse of matrix.

In some cases, shape gradients can be computed analytically.

Integrals over a curve:

If
$$f[C] = \int_{C} d\ell Q$$
 for some $Q(\mathbf{r})$ and space curve C ,
 $\Rightarrow \delta f = \int_{C} d\ell \delta \mathbf{r} \cdot \left[(\mathbf{\ddot{I}} - \mathbf{tt}) \cdot \nabla Q - q\kappa \mathbf{n} \right]$
where $\kappa = \text{curvature}$, $\mathbf{t} = \text{tangent}$.

Integrals over a surface:

If
$$f[\partial\Omega] = \int_{\partial\Omega} d^2 a Q$$
 for some $Q(\mathbf{r})$ and surface $\partial\Omega$,
 $\Rightarrow \delta f = \int_{\partial\Omega} d^2 a (\delta \mathbf{r} \cdot \mathbf{n}) \underbrace{(\mathbf{n} \cdot \nabla Q - 2QH)}_{S}$
where $H =$ mean curvature.



A magnetic sensitivity S_B can be computed from the shape gradient.

$$\mathbf{B} \cdot \nabla \boldsymbol{\psi} = 0 \qquad \Rightarrow \qquad \mathbf{B}_{0} \cdot \nabla \delta \boldsymbol{\psi} + \delta \mathbf{B} \cdot \nabla \boldsymbol{\psi}_{0} = 0.$$
Also $0 = d\boldsymbol{\psi} = \delta \boldsymbol{\psi} + \delta \mathbf{r} \cdot \nabla \boldsymbol{\psi}_{0}.$

$$\Rightarrow \qquad \mathbf{B}_{0} \cdot \nabla \left(\delta \mathbf{r} \cdot \nabla \boldsymbol{\psi}_{0} \right) = \delta \mathbf{B} \cdot \nabla \boldsymbol{\psi}_{0}. \qquad (1)$$
Define S_{B} by $\mathbf{B}_{0} \cdot \nabla S_{B} = \langle S \rangle - S. \qquad (2)$
Substitute $(2) \& (1)$ into $\delta f = \int d^{2}a \ S \delta \mathbf{r} \cdot \mathbf{n}$

$$\Rightarrow \qquad \delta f = \langle S \rangle \delta V + \int d^{2}a \ S_{B} \delta \mathbf{B} \cdot \mathbf{n}.$$

Perturbation to volume

3D MHD Toroidal Equilibrium

$$-\nabla p + \frac{\mathbf{J} \times \mathbf{B}}{c} = 0$$
$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{J}$$

In vacuum $\nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{J}_{c}$ coil current

Assume good flux surfaces in plasma

Poloidal flux $\mathbf{B} = \nabla \alpha \times \nabla \theta - \nabla \Phi_p(\alpha) \times \nabla \zeta$ $= \nabla \alpha \times \nabla \left(\theta - \iota(\alpha) \zeta \right)$ Toroidal Flux $\int_{\iota(\alpha)}^{\iota(\alpha)} = d\Phi_p(\alpha) / d\alpha$ Rotational transform

Linear Perturbations to Equilibrium

$$\mathbf{J}_{c} \Rightarrow \mathbf{J}_{c} + \delta \mathbf{J}_{c}$$
$$\nabla p \Rightarrow \nabla p + \nabla \cdot \delta \mathbf{P}$$
$$\Phi_{p}(\alpha) \Rightarrow \Phi_{p}(\alpha) + \delta \Phi_{p}(\alpha)$$
$$\iota(\alpha) = d\Phi_{p}(\alpha) / d\alpha$$

Generalized Forces:

Changes in current/shape/location of coils

Added pressure tensor

Change in poloidal flux profile

Generalized responses:

Changes in vacuum fields

Changes in magnetic field

Change in toroidal current profile

$$\mathbf{A}_{v} \Rightarrow \mathbf{A}_{v} + \delta \mathbf{A}_{v}$$
$$\mathbf{B} \Rightarrow \mathbf{B} + \nabla \times (\xi \times \mathbf{B} - \delta \Phi_{p} \nabla \zeta)$$
$$I_{T} \Rightarrow I_{T} + \delta I_{T}(\alpha)$$

Generalized Forces and Responses



More generically, for two different persugert Synsmetry Give $\sum_{j} \left\{ \delta x_{i}^{(1)} \delta F_{i}^{(2)} - \delta x_{i}^{(2)} \delta F_{i}^{(1)} \right\} = 0$

Onsager Symmetry for MHD Equilibria (free boundary)

$$\int_{VP} d^3x \left(-\boldsymbol{\xi}^{(1)} \cdot \nabla \cdot \left(\boldsymbol{\delta} \underline{\underline{P}}^{(2)} + \boldsymbol{\xi}^{(2)} \cdot \nabla p \underline{\underline{1}} \right) + \boldsymbol{\xi}^{(2)} \cdot \nabla \cdot \left(\boldsymbol{\delta} \underline{\underline{P}}^{(1)} + \boldsymbol{\xi}^{(1)} \cdot \nabla p \underline{\underline{1}} \right) \right)$$

Pressure - Displacement

$$+\frac{2\pi}{c}\int_{VP}d\alpha\left(\frac{\delta\Phi_{p}^{(1)}}{d\alpha}\frac{d}{d\alpha}\delta I_{T}^{(2)}-\delta\Phi_{p}^{(2)}\frac{d}{d\alpha}\delta I_{T}^{(1)}\right)$$

Rotational transform – Toroidal current

$$+\frac{1}{c}\int_{V-ext} d^3x \left(\delta \mathbf{J}_C^{(1)} \cdot \mathbf{A}_V^{(2)} - \delta \mathbf{J}_C^{(2)} \cdot \mathbf{A}_V^{(1)} \right) = 0$$

Coil current – Vector potential

Onsager Symmetry for MHD Equilibria (given or fixed boundary)

$$\int_{VP} d^{3}x \left(-\boldsymbol{\xi}^{(1)} \cdot \nabla \cdot \left(\boldsymbol{\delta} \underline{\underline{P}}^{(2)} + \boldsymbol{\xi}^{(2)} \cdot \nabla p \underline{\underline{1}} \right) + \boldsymbol{\xi}^{(2)} \cdot \nabla \cdot \left(\boldsymbol{\delta} \underline{\underline{P}}^{(1)} + \boldsymbol{\xi}^{(1)} \cdot \nabla p \underline{\underline{1}} \right) \right)$$

Pressure - Displacement

$$-\frac{2\pi}{c}\int_{VP}d\alpha\left(\delta I_{T}^{(2)}\frac{d}{d\alpha}\delta\Phi_{p}^{(1)}-\delta I_{T}^{(1)}\frac{d}{d\alpha}\delta\Phi_{p}^{(2)}\right)$$

Rotational transform – Toroidal current

$$+\frac{1}{4\pi}\int_{S} d^{2}x \mathbf{n} \cdot \left(\boldsymbol{\xi}^{(1)} \boldsymbol{\delta} \mathbf{B}^{(2)} \cdot \mathbf{B} - \boldsymbol{\xi}^{(2)} \boldsymbol{\delta} \mathbf{B}^{(1)} \cdot \mathbf{B}\right) = 0$$

Surface displacement

Fixed boundary shape

$$\mathbf{Figure of merit}F = \int_{VP} d^3x \, p(\alpha)$$

$$dF(\boldsymbol{\xi}^{(1)}) = -\int_{VP} d^3x \, \boldsymbol{\xi}^{(1)} \cdot \nabla p + \int_{SP} d^2x \, (\boldsymbol{\xi}^{(1)} \cdot \boldsymbol{n})p$$

$$\mathbf{Forward (hard) problem}$$

$$\begin{pmatrix} \boldsymbol{\xi}^{(1)} \cdot \boldsymbol{n} \end{pmatrix}_{SP} \neq 0 \quad \delta \Phi_P^{(1)} = 0$$

$$\delta \underline{P}^{(1)} = -\boldsymbol{\xi}^{(1)} \cdot \nabla p \underline{1}$$

$$\mathbf{Forward}(\boldsymbol{\xi}^{(1)} \cdot \nabla p \underline{1})$$

Use fixed boundary Onsager relation $\int_{VP} d^3x \, \left(-\boldsymbol{\xi}^{(1)} \cdot \nabla \delta p \right) = \frac{1}{4\pi} \int_{SP} d^2x \, \left(\boldsymbol{n} \cdot \boldsymbol{\xi}^{(1)} \right) \delta \boldsymbol{B}^{(2)} \cdot \boldsymbol{B}$

$$dF(\boldsymbol{\xi^{(1)}}) = \int_{SP} d^2 x \, (\boldsymbol{\xi^{(1)}} \cdot \boldsymbol{n}) \left(\frac{\delta \boldsymbol{B^{(2)}} \cdot \boldsymbol{B}}{4\pi\delta} + p \right)$$
Shape gradient (S) computed

Computing the shape

gradient the hard way



¹HIrshman and Whitman, 1983 Phys. Fluids 25 3553 ²Landreman and Paul, 2018 Nucl. Fusion 58 076023

Computing the shape

gradient the adjoint $VV^{-1}_{\times 10^4}$

- NCSX LI383 equilibrium computed with VMEC¹
- Requires $\approx 1\%$ CPU hours in comparison with djoine piceblem $(\xi^{(2)})$ at ive $\delta \Phi_P^{(2)} = 0$

 $\delta \underline{\underline{P}}^{(2)} = \left(-\boldsymbol{\xi}^{(2)} \cdot \nabla p + \delta p\right) \underline{\underline{1}}$



$$F = \int_{VP} d^3x \, p(\alpha) \quad dF(\boldsymbol{\xi^{(1)}}) = \int_{SP} d^2x \, (\boldsymbol{\xi^{(1)}} \cdot \boldsymbol{n}) \left(\frac{\delta \boldsymbol{B^{(2)}} \cdot \boldsymbol{B}}{4\pi\delta} + p\right)$$

Free boundary shape



Free boundary shape gradient



¹H.J. Gardner 1990 Nucl. Fusion 30 1417