Computing the shape gradient of stellarator coil complexity with respect to the plasma boundary

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Coil complexity is a critical consideration in stellarator design. The traditional two-step optimization approach, in which the plasma boundary is optimized for physics properties and the coils are subsequently optimized to be consistent with this boundary, can result in plasma shapes which cannot be produced with sufficiently simple coils. To address this challenge, we propose a method to incorporate considerations of coil complexity in the optimization of the plasma boundary. Coil complexity metrics are computed from the current potential solution obtained with the REGCOIL code \cite{Landreman2017}. We compute the local sensitivity of these metrics with respect to perturbations of the plasma boundary using the shape gradient \cite{Landreman&Paul2018}. We extend REGCOIL to compute derivatives of these metrics with respect to parameters describing the plasma boundary. In keeping with previous research on winding surface optimization \cite{Paul2018}, the shape derivatives are computed with a discrete adjoint method. In contrast with the previous work, derivatives are computed with respect to the plasma surface parameters rather than the winding surface parameters. To further reduce the resolution required to compute the shape gradient, we present a more efficient representation of the plasma surface which uses a single Fourier series to describe the radial distance from a coordinate axis and a spectrally condensed poloidal angle. This representation is advantageous over the standard cylindrical representation used in the VMEC code \cite{Hirshman&Whitson1983}, as it provides a uniquely defined poloidal angle, eliminating a null space in the optimization of the plasma surface. The resulting shape gradient highlights features of the plasma boundary that are consistent with simple coils and can be used to couple coil and fixed-boundary optimization.

1. Introduction

Historically, stellarators have been optimized with a two-staged approach. In the first stage, the outer boundary of the plasma, denoted by $S_{\text{plasma}}$, is optimized based on physical properties of the magnetohydrodynamic (MHD) equilibrium. This task is performed with optimization codes such as STELLOPT \cite{Spong2001} and ROSE \cite{Drevlak2018}. During the second stage, the currents in the vacuum region must be chosen to be consistent with the boundary obtained from the first stage. This is typically formulated as obtaining the currents in the vacuum region, $J^{\text{coil}}$, given the magnetic field due to the plasma currents, $B^{\text{plasma}}$, such that the total normal magnetic field on $S_{\text{plasma}}$ vanishes,

$$B^{\text{plasma}}(r) \cdot \hat{n}(r) + \frac{\mu_0}{4\pi} \int_{\Omega_c} \frac{J^{\text{coil}}(r') \times (r - r') \cdot \hat{n}(r)}{|r - r'|^3} \, dV' = 0,$$  

(1.1)
where $\Omega_c$ is the vacuum region. This is an integral equation of the first kind, which is known to be ill-posed in the sense that a unique solution may not exist and a small change in the prescribed data, $B_{\text{plasma}} \cdot \hat{n}$, may result in a large change in the solution, $J_{\text{coil}}$ \cite{Kress1989,Imbert-Gerard2019}. Given the ill-posedness, the coils problem has been reformulated as a regularized optimization problem. Under the approximation that the coils are filamentary curves, this nonlinear optimization problem is solved with the FOCUS \cite{Zhu2018} and ONSET \cite{Drevlak1998} codes. If $J_{\text{coil}}$ is assumed to be a continuous surface current supported on a toroidal winding surface, $S_{\text{coil}}$, a convex optimization optimization problem is obtained, which is solved with the REGCOIL \cite{Landreman2017} and NESCOIL \cite{Merkel1987} codes. We refer to this technique as a current potential formulation, as the divergence-free current density can be expressed as the gradient of a potential function. Given the inherent ill-posedness in the coil design problem \eqref{eq:coil}, these coil optimization problems can be formulated to favor simple coil shapes that can be constructed at a lower cost.

Decoupling the physics and practical considerations of a design in this way is thought to have several possible advantages. By initially ignoring engineering considerations, one may obtain a configuration with enhanced confinement properties. This approach may also enable one to explore a wider space of coil designs, allowing for multiple coil topologies or the incorporation of permanent magnets. A major shortcoming of this approach is the possibility of arriving at a configuration that cannot be produced with sufficiently simple coils or magnets. For this reason, it is favorable to integrate engineering considerations of the coils with stellarator equilibrium optimization.

This priority can be addressed with several techniques. One option is to directly optimize coils based on free-boundary solutions of the MHD equilibrium equations, eliminating the need to design coils as a second step. This approach was used in the final stages of the NCSX design \cite{Hudson2002,Strickler2003} and recent developments have enabled more efficient direct optimization of coils with adjoint methods \cite{Giuliani2020}. This direct optimization approach is sometimes more challenging for several reasons. Free-boundary equilibrium calculations tend to be more expensive than fixed-boundary calculations, as they often require iterations between an equilibrium solve and vacuum field calculations. This iterative scheme will not always converge in practice, hence the historical use of the more robust fixed-boundary method. It has also been suggested that fixed-boundary optimization may yield better equilibrium properties, as the model assumes the existence of at least one magnetic surface. An algorithm has been proposed \cite{Hudson2018} to simultaneously optimize the plasma boundary and a set of coils by minimizing the coil complexity at fixed confinement properties. Another approach is to incorporate metrics of coil complexity into the fixed-boundary equilibrium design. This is possible with the ROSE code \cite{Drevlak2018}, which enables the inclusion of properties of the current potential in the objective function. In this work, we adopt a similar approach, but enable the efficient computation of shape derivatives of such metrics for gradient-based optimization.

The goal of this work is to understand which plasma boundary shapes are consistent with simple coils using the shape gradient, a scalar functional defined on the plasma boundary that quantifies the local sensitivity of an objective to perturbation of the surface. Specifically, we will consider an objective which quantifies coil complexity using the current potential solution on a uniformly offset winding surface. Other approaches have been used to understand the relationship between the complexity of external currents and magnetic surface shapes. A singular value decomposition of the matrix coupling external fields and the normal field on the plasma boundary can quantify the “efficiency” of an external magnetic field on a control surface in producing a given plasma
Shape gradient of stellarator coil complexity with respect to the plasma boundary. This analysis highlights certain characteristics that are difficult to produce with external magnetic fields, such as boundaries with small-wavelength features and concavity. By considering a two-parameter family of magnetic surfaces near the magnetic axis with fixed rotational transform, it has also been observed that ellipticity of the boundary tends to increase the coil complexity more than the torsion of the axis. We present a different approach to put plasma surface and coil design on a similar footing. By determining how the coil complexity metrics computed from REGCOIL depend on perturbations of the plasma boundary, plasma shapes can be designed which give rise to simpler coils.

Using the derivatives of the objective function with respect to the shaping parameters, or the shape derivatives, we can construct the shape gradient by solving a linear system. The shape gradient can be used for efficient gradient-based optimization of the shape. Furthermore, the evaluation of the shape gradient enables the identification of features of the plasma boundary that are amenable to simpler coils. Using techniques similar to those presented in this work, the shape gradient of coil complexity metrics with respect to $S_{\text{coil}}$ has previously been computed. This analysis highlighted features of the winding surface which allow for more accurate reproduction of the desired plasma surface, and gradient-based optimized of the winding surface was demonstrated.

Stellarators typically require a large set of parameters to fully describe their three-dimensional geometry. The optimization in REGCOIL introduces an implicit dependence of the metrics on the plasma surface parameters through the linear least-squares system. This means that taking these derivatives with a finite-difference method would ordinarily require solving a linear system similar to the one solved by REGCOIL corresponding to the perturbation of each surface parameter; however, this can be avoided using the adjoint method. A variable, called the adjoint variable, can be computed by solving a similar linear system. However, the adjoint variable is common to all the surface parameters, so the system only needs to be solved one additional time for all the parameters. With the application of an adjoint method, we furthermore eliminate the noise associated with the finite-difference step size. The adjoint method has recently been applied to several problems in stellarator design and is commonly implemented in the field of fluid dynamics and aerodynamic engineering.

In §2, we will give an overview of the current potential method used in the REGCOIL code. We provide some background on the theory of shape gradients and their application to stellarator optimization in §3. We compute the shape gradient with a specific choice of poloidal angle described in §4, which is chosen for its spectral condensation. To construct the shape gradients, the derivatives of the REGCOIL metrics with respect to the plasma surface parameters are described in §5. In §6, benchmarks of these derivatives and shape gradients computed from them are shown. Finally, the shape gradients of the figures of interest are also shown in §6 for the W7-X and QHS46 configurations.

2. Overview of the current potential method

A balance must be reached between a simple coil design and accuracy in reproducing the desired plasma shape. REGCOIL uses a current potential approximation to formulate this optimization as a linear least-squares system with a regularization factor balancing the coil complexity and plasma surface accuracy. The
surface current on the coil winding surface is taken to be of the form,

\[ \mathbf{K} = \hat{n}' \times \nabla \Phi, \]

where \( \Phi \) is the current potential and \( \hat{n}' \) is the unit normal vector to the coil surface. The surface current is then divergence-free and tangential to the coil surface. Since the gradient and level curves of the current potential are perpendicular and on the coil surface, the surface current flows along the level curves of the current potential. The discrete coil shapes are then determined by taking a selection of level curves of the current potential, or streamlines of \( \mathbf{K} \). These level curves will be closer together in regions of high current density, implying a reduction of the discrete coil-coil separation.

This current potential has secular terms and a single valued term. The single valued component of the current potential can be expanded as a sine series over the coil surface under the assumption of stellarator symmetry (Dewar & Hudson 1998). The current potential then has the form,

\[ \Phi = G \frac{\zeta'}{2\pi} + I \frac{\theta'}{2\pi} + \sum_j \Phi_j \sin(m_j \theta' - n_j \zeta'), \]

where \( G \) and \( I \) are currents which link the coil surface poloidally and toroidally, \( \theta' \) is a poloidal angle, and \( \zeta' \) is a toroidal angle.

We consider two figures of merit,

\[ \chi_B^2 = \int_{S_{\text{plasma}}} (\mathbf{B}(\theta, \zeta) \cdot \hat{n}(\theta, \zeta))^2 \, da \]

\[ \chi_K^2 = \int_{S_{\text{coil}}} |\mathbf{K}(\theta', \zeta')|^2 \, da', \]

where \( \mathbf{B} \) is the magnetic field and \( \hat{n} \) is the unit normal vector to the plasma surface. In this work, we make the approximation that the normal field from the plasma current is negligible such that only the vacuum field from the coils is included. In keeping with Landreman (2017), primed coordinates refer to the coil surface while unprimed coordinates refer to the plasma surface. Similarly, primed and unprimed quantities are used to refer to those of the coil and plasma surface respectively when a distinction is necessary. The integral for \( \chi_B^2 \) is over the desired magnetic surface, \( S_{\text{plasma}} \), and the integral for \( \chi_K^2 \) is over the coil winding surface, \( S_{\text{coil}} \). The goal is for \( S_{\text{plasma}} \) to be a magnetic surface, so the normal component of the magnetic field will vanish if the plasma surface is properly reconstructed and, thus, so will \( \chi_B^2 \). Large values of \( \chi_K^2 \) are correlated with increased coil complexity (Paul et al. 2018). Regions of higher surface current density require reduced coil-coil spacing; thus, the coil-coil separation is increased by reducing \( \chi_K^2 \). When comparing configurations, it is also useful to consider normalized quantities,

\[ \| \mathbf{B}_n \|^2 = \sqrt{\frac{\chi_B^2}{B_0^2 a_{\text{plasma}}}} \]

\[ \| K \|^2 = \sqrt{\frac{\chi_K^2}{a_{\text{coil}}}}, \]

where \( a_{\text{plasma}} \) and \( a_{\text{coil}} \) are the plasma and coil surface areas respectively, and \( B_0 \) is a constant with the dimensions of magnetic field. In this work, we take it to be the root-mean-squared average of the magnetic field strength from the equilibrium.

REGCOIL minimizes the quantity \( \chi_B^2 + \lambda \chi_K^2 \) by solving a linear least-squares system.
for the Fourier modes of the single valued current potential, $\Phi_j$ defined in (2.2). Here $\lambda$ is the regularization parameter which sets the relative importance of $\chi^2_B$ and $\chi^2_K$ in the optimization. A fixed value of $\lambda$ can be chosen, or the freedom in $\lambda$ can be used to fix a certain target function, such as $\chi^2_K$ or $\|K\|_2$. We employ the notation $\Phi$ to represent the vector of unknowns, $\{\Phi_j\}$. The linear least-squares system takes the form,

$$A\Phi = b,$$

(2.5)

with,

$$A = A^B + \lambda A^K,$$

$$b = b^B + \lambda b^K,$$

(2.6)

where the $B$ matrix and vector are associated with the system that optimizes only $\chi^2_B$, and the $K$ matrix and vector are associated with the system that optimizes only $\chi^2_K$. Expressions for these quantities are given in Appendix A of (Landreman 2017).

3. Shape gradients

The shape gradient describes the local dependence of a functional on a surface and is independent of the choice of basis or parameterization. Consider a functional $F$ of the plasma surface, such as $\chi^2_B$, $\chi^2_K$, $\|B_n\|_2$, or $\|K\|_2$. Assuming sufficient smoothness, the Hadamard-Zolésio structure theorem (Delfour & Zolésio 2011) states that the change in $F$ due to a vector field of infinitesimal displacements $\delta r$ to the plasma surface is given by,

$$\delta F(S_{\text{plasma}}; \delta r) = \int_{S_{\text{plasma}}} S_F \delta r \cdot \hat{n} \, da,$$

(3.1)

where $S_F$ is the shape gradient and $\delta F$ is called the shape derivative. This gives information about how the plasma surface can be deformed to alter a functional of the surface. For the case that the functional $F$ is $\chi^2_K$ or $\|K\|_2$, its shape gradient enables the plasma surface to be deformed to obtain simpler coils.

Given a parameterization of the plasma surface with a set of parameters $\Omega$, (3.1) can be expressed as,

$$\frac{\partial F}{\partial \Omega_j} = \int_{S_{\text{plasma}}} S_F \frac{\partial r}{\partial \Omega_j} \cdot \hat{n} \, da.$$  

(3.2)

The shape gradient can be expanded as a Fourier series, assuming stellarator symmetry, as,

$$S_F = \sum_i S^i_F \cos(m_i \theta - n_i \zeta),$$

(3.3)

such that the linear system for the shape gradient Fourier coefficients, $\{S^i_F\}$, is,

$$\frac{\partial F}{\partial \Omega_j} = \sum_i S^i_F \int_{S_{\text{plasma}}} \cos(m_i \theta - n_i \zeta) \frac{\partial r}{\partial \Omega_j} \cdot \hat{n} \, da.$$  

(3.4)

If the same number of modes are used to discretize $S_F$ as the number of modes retained in $\{\partial F/\partial \Omega_j\}$, then the system is square, and the shape gradient can then be constructed from a local parameterization of the surface with a linear solve. If the system is not square, it can still be solved (Landreman & Paul 2018) using a pseudoinverse or QR factorization. Details of the chosen parameterization of the plasma boundary are provided in the following Section.
4. Efficient Fourier representation of the plasma boundary

A toroidal surface such as $S_{\text{plasma}}$ can be specified by two Fourier series in the cylindrical coordinates $R$ and $Z$,

$$R(\theta, \zeta) = \sum_{m,n} R_{c,m,n} \cos(m\theta - n\zeta)$$

$$Z(\theta, \zeta) = \sum_{m,n} Z_{s,m,n} \sin(m\theta - n\zeta).$$  \hfill (4.1)

Here $\zeta$ is taken to be the cylindrical toroidal angle and $\theta$ is a poloidal angle. This representation is used in the VMEC (Hirshman & Whitson 1983) and SPEC (Hudson et al. 2012) equilibrium codes. Here we have assumed stellarator symmetry such that,

$$R(-\theta, -\zeta) = R(\theta, \zeta)$$

$$Z(-\theta, -\zeta) = -Z(\theta, \zeta).$$  \hfill (4.2)

Because this representation does not constrain the poloidal angle, the Fourier amplitudes could be altered corresponding to a redefinition of the poloidal angle, while the surface is left unchanged. This freedom in the choice of poloidal angle has been used to condense the Fourier spectrum using a variational method (Hirshman & Meier 1985; Hirshman & Breslau 1998). In the context of fixed-boundary optimization, a uniquely defined poloidal angle may eliminate a null space in the parameter space.

To eliminate such a null space, we consider a new representation which requires only one series representation of a radial distance, $l$, from a fixed coordinate axis. In this work, we take the coordinate axis to coincide with the magnetic axis from the equilibrium, although this assumption is not necessary. We define a unique poloidal angle $\vartheta$ using the arctangent in the poloidal plane,

$$l = \sqrt{(R - R_0)^2 + (Z - Z_0)^2}$$

$$\vartheta = \arctan \left( \frac{Z - Z_0}{R - R_0} \right),$$  \hfill (4.3)

where $R_0(\zeta)$ and $Z_0(\zeta)$ are the cylindrical coordinates of the axis. Note that a representation of this form assumes that each cross-section in the poloidal plane is a star domain, indicating that there exists a coordinate axis $(R_0, Z_0)$ such that the line segment connecting the axis and any point on the boundary is contained within the boundary.

The variable $l$ then admits a Fourier representation as,

$$l(\vartheta, \zeta) = \sum_{m,n} l_{c,m,n} \cos(m\vartheta - n\zeta).$$  \hfill (4.4)

This representation uses a Fourier expansion in only a single quantity $l$ rather than in both $R$ and $Z$. The cylindrical coordinates can now be expressed in the new representation as,

$$R(\vartheta, \zeta) = R_0(\zeta) + l(\vartheta, \zeta) \cos(\vartheta)$$

$$Z(\vartheta, \zeta) = Z_0(\zeta) + l(\vartheta, \zeta) \sin(\vartheta).$$  \hfill (4.5)

In practice, the Fourier series in (4.4) may decay rather slowly for relevant stellarator boundaries with widely varying curvature, as equally-spaced grid points in $\vartheta$ accumulate in concave regions of the surface and become sparse near the convex regions (Figure 1).

To improve the efficiency of this representation, a second unique poloidal angle can be
defined by the arclength along the plasma surface at constant toroidal angle,

$$\bar{\theta}(\vartheta, \zeta) = 2\pi \frac{\int_0^\vartheta \sqrt{\left(\frac{\partial R}{\partial \vartheta'}\right)^2 + \left(\frac{\partial Z}{\partial \vartheta'}\right)^2} \, d\vartheta'}{\int_0^{2\pi} \sqrt{\left(\frac{\partial R}{\partial \vartheta'}\right)^2 + \left(\frac{\partial Z}{\partial \vartheta'}\right)^2} \, d\vartheta'}.$$  \tag{4.6}

This choice of poloidal angle has been shown to correspond to the minimum of a spectral width functional \cite{Hirshman & Breslau 1998}. The Hirshman-Breslau technique can be used to obtain improved spectral convergence over the arclength angle by minimizing an energy functional with a nonlinear conjugate gradient method. In contrast, we present a method for improving the spectral convergence by computing an arclength angle on a uniform offset surface. This simply requires a Fourier transform to compute the coefficients in the new representation rather than the solution of a nonlinear optimization problem. We define a uniform offset surface by,

$$r_{\text{arclength}} = r + a_{\text{arclength}} \hat{n},$$  \tag{4.7}

where $a_{\text{arclength}}$ is a constant offset distance. This parameterization is particularly important for constraining the coil winding surface as described in \cite{5.3}. It is important that the offset distance $a_{\text{arclength}}$ is not too large; otherwise, the offset surface will self-intersect. The maximum offset distance is constrained by the principal curvatures, $\kappa_1$ and $\kappa_2$, of $S_{\text{plasma}}$. Here we use the convention that $\kappa_{1,2} < 0$ indicates concavity. The maximum curvature in the outwardly concave regions of the plasma surface ($\kappa_{1,2} < 0$) determines the minimum outward radius of curvature, and thus the maximum outward ($a_{\text{arclength}} > 0$) offset distance. Conversely, the maximum curvature in the outwardly convex regions of the plasma surface ($\kappa_{1,2} > 0$) determines the maximum inward ($a_{\text{arclength}} < 0$) offset distance \cite{Farouki 1986}. The constraint on the offset distance is therefore given by,

$$-\frac{1}{\max\{\kappa_1, \kappa_2\}} < a_{\text{arclength}} < \frac{1}{\min\{\kappa_1, \kappa_2\}}.$$  \tag{4.8}

Note that for any closed toroidal surface, the surface integral of the Gaussian curvature ($\int \kappa_1 \kappa_2 \, d^2a$) must vanish, indicating that the minimum of the principal curvatures must always be negative and maximum of the principal curvatures must be positive.

In this case, rather than using the arclength on the plasma surface to define $\bar{\theta}$, the arclength is computed on a surface uniformly offset from the plasma boundary as defined in \cite{4.7} with the restriction on outward offsets as in \cite{4.8}. In this way, the poloidal angle can be tuned to accommodate a particular offset of the coil surface from the plasma surface or to increase resolution in regions of large (positive or negative) curvature.

We define $\omega$ to be the difference between the arclength and arctangent angles,

$$\omega(\vartheta, \zeta) = \bar{\theta}(\vartheta, \zeta) - \vartheta.$$  \tag{4.9}

The quantities $l$ and $\omega$ can now be expressed as Fourier series in $\bar{\theta}$,

$$l(\bar{\theta}, \zeta) = \sum_{m,n} l_{m,n}^c \cos(m\bar{\theta} - n\zeta)$$

$$\omega(\bar{\theta}, \zeta) = \sum_{m,n} \omega_{m,n}^s \sin(m\bar{\theta} - n\zeta).$$  \tag{4.10}

Note that while we express $\omega$ in a Fourier series to describe the relationship between the arctangent angle $\vartheta$ and the arclength angle $\bar{\theta}$, it is only necessary to differentiate with respect to $l_{m,n}^c$ when constructing shape gradients. In this way, the poloidal angle is fixed.
as the plasma boundary is perturbed, and the corresponding null space is eliminated. The cylindrical coordinates can now be expressed in the new representation as,

\[ R(\bar{\theta}, \zeta) = R_0(\zeta) + l(\bar{\theta}, \zeta) \cos(\bar{\theta} - \omega(\bar{\theta}, \zeta)) \]
\[ Z(\bar{\theta}, \zeta) = Z_0(\zeta) + l(\bar{\theta}, \zeta) \sin(\bar{\theta} - \omega(\bar{\theta}, \zeta)). \] (4.11)

The arclength angle is advantageous over the arctangent angle because it allows for a more efficient representation of the plasma surface with a uniform sampling of the poloidal angle. This is particularly useful for representing plasma boundaries with regions of large curvature. In Figure 1, we compare the distribution of poloidal grid points on the bean-shaped cross-section of the W7-X boundary, which features both concave and convex regions. While the grid points in the arclength angle are equally-spaced along the cross-section, the points in the arctangent angle accumulate in the concave region. Observe that in highly convex regions of the plasma surface, the normal vector is changing rapidly, causing points on the offset surface to diverge from each other. By fixing the points on the offset surface to be spaced by uniform arclength increments, the points on the plasma surface tend to accumulate in the highly convex regions. Extra resolution in these regions is beneficial for improved convergence of REGCOIL calculations as well as a more efficient Fourier series representation. Alternatively, for surfaces which feature highly concave regions, it may be more advantageous to use an inward offset when computing the arclength angle. In this case, the maximum inward offset is set by the maximum curvature in the outwardly convex regions as in (4.8).

To further evaluate these representations, we compare the convergence of the Fourier series for the W7-X surface. The double Fourier series representation (4.1) is compact in both \( m \) and \( n \) as shown in Figures 2a and 2b, as the surface was optimized with a truncated spectrum. (The surface is from a fixed-boundary equilibrium which predated the coil optimization.) For the other representations, the modes form a tilted band which is thin in the \( n \) direction and decays slowly in the \( m \) direction as shown in Figure 3a. With the arctangent representation, many modes must be retained in the Fourier series to accurately reconstruct the plasma surface. With the arclength angle defined on the plasma boundary, the magnitude of the Fourier modes decreases more rapidly in \( m \). This decay is enhanced when the arclength angle is computed on a surface displaced by the plasma by 0.25 m. This offset surface will be used in Section 6.3 for computation of the shape gradients.

5. Differentiation with respect to the Fourier coefficients

To take the derivative of \( \chi_2^2 \), where \( I \in \{ B, K \} \), with respect to some parameter of the plasma surface, one must consider the explicit and implicit dependence of the functional on the parameters. We will call the set of parameters of the plasma surface \( \Omega \) and a particular one \( \Omega_j \). The derivative of \( \chi_2^2 \) with respect to \( \Omega_j \) is computed using the chain rule,

\[ \frac{\partial \chi_2^2(\Omega, \Phi(\Omega))}{\partial \Omega_j} = \left. \frac{\partial \chi_2^2}{\partial \Omega_j} \right|_{d\Phi=0} + \frac{\partial \chi_2^2}{\partial \Phi} \cdot \frac{\partial \Phi}{\partial \Omega_j}. \] (5.1)

The bar notation here means that the first derivative on the right hand side of (5.1) is taken with \( d\Phi = 0 \). The derivatives involving \( \Phi \) are taken to indicate element-wise operation; thus \( \partial \chi_2^2 / \partial \Phi \) are vectors of the same dimension as \( \Phi \). The dot product between these vectors in the second term of (5.1) indicates contraction over \( \Phi \).
Figure 1: The bean-shaped cross-section of the W7-X configuration with a 0.25 m uniformly offset coil surface sampled at 32 values of the poloidal using (a) the initial VMEC representation, (b) the single Fourier representation with an arctangent angle, (c) the single Fourier representation with an arclength angle on the plasma surface, and (d) the single Fourier representation with an arclength angle on a surface uniformly offset from the plasma surface by 0.25 m.

Figure 2: Magnitude of (a) $R_{m,n}$ and (b) $Z_{m,n}$ on a grid of mode numbers $m$ and $n/N_p$. 
Figure 3: (a) Magnitude of $l_{m,n}^c$ for the arctangent poloidal angle on a grid of mode numbers $m$ and $n/N_P$ where $N_P$ is the number of field periods. The dominant $l_{m,n}^c$ lie on a long, tilted band. Magnitudes of (b) $l_{m,n}^c$ and (c) $\omega_{m,n}^s$ for the arclength poloidal angle on the plasma surface. The amplitudes are more localized to the smaller mode numbers than with the arctangent angle, but still lie on a long, tilted band. Magnitudes of (d) $l_{m,n}^c$ and (e) $\omega_{m,n}^s$ for the arclength poloidal angle on a surface uniformly offset from the plasma surface by 0.25 m. The amplitudes are even more localized to the smaller mode numbers.

5.1. Optimal Solution Constraint

To take this derivative such that the current potential satisfies the linear least-squares system given in (2.5), we differentiate the constraint given by (2.5) with respect to the Fourier coefficients to obtain,

$$\frac{\partial \Phi}{\partial \Omega_j} = A^{-1} \left( \frac{\partial b}{\partial \Omega_j} - \frac{\partial A}{\partial \Omega_j} \Phi \right),$$

(5.2)
where the second expression uses the transpose to perform the inner product between
the vectors of the first expression as a matrix multiplication. The quantity on the left
side of this product is a row vector while the quantity in parenthesis on the right is a
column vector. Note that,

\[
\left( \frac{\partial \chi^2_I}{\partial \Phi} \right)^T (A^{-1})^T \frac{\partial \chi^2_I}{\partial \Phi} = \frac{\partial \chi^2_I}{\partial \Phi},
\]

meaning that the operation \( A^{-1} \) can be moved to the left side of the inner product by
taking its transpose. By defining an adjoint variable \( q_I \) using,

\[
A^T q_I = \frac{\partial \chi^2_I}{\partial \Phi},
\]

the inner product term becomes

\[
q_I^T \left( \frac{\partial b}{\partial \Omega_j} - \frac{\partial A}{\partial \Omega_j} \Phi \right) = q_I \cdot \left( \frac{\partial b}{\partial \Omega_j} - \frac{\partial A}{\partial \Omega_j} \Phi \right);
\]

thus, a linear system involving the matrix \( A \) only needs to be solved once for all \( \Omega_j \)
to get the adjoint variable in addition to the linear solve to get the solution \( \Phi \). Then (5.1)
becomes,

\[
\left. \frac{\partial \chi^2_I(\Phi(\Omega))}{\partial \Omega_j} \right|_{A\Phi=b} = \left. \frac{\partial \chi^2_I(\Phi)}{\partial \Omega_j} \right|_{d\Phi=0} + q_I \cdot \left( \frac{\partial b}{\partial \Omega_j} - \frac{\partial A}{\partial \Omega_j} \Phi \right).
\]

This equation applies to both \( \chi^2_B \) and \( \chi^2_K \), so both adjoint variables \( q_B \) and \( q_K \) are
computed from (5.5). Since the quantity \( \chi^2_B + \lambda \chi^2_K \) is minimized with respect to \( \Phi \) by
REGCOIL,

\[
\frac{\partial \chi^2_B}{\partial \Phi} + \lambda \frac{\partial \chi^2_K}{\partial \Phi} = 0.
\]

This means that these adjoint variables are related by the equation,

\[
q_B + \lambda q_K = 0.
\]

5.2. Fixed Norm Constraint

In the previous Section, differentiation was performed at fixed \( \lambda \). In order to evaluate
different magnetic configurations on the same footing, we will use the freedom in \( \lambda \) to fix
a quantity such as \( \|K\|_2 \), which is related to the engineering complexity of the coils. To
account for this constraint, we define the following quantity,

\[
G = \|K\|_2 - \|K\|_2^{\text{target}},
\]

where \( \|K\|_2^{\text{target}} \) is the fixed value desired for \( \|K\|_2 \). In effect, this constraint allows the
coil complexity to be fixed to an acceptable level. Let the optimal solution constraint be
described by,

\[
F = A\Phi - b.
\]
Now $\lambda$ must be allowed to vary unlike in the previous Section. By taking the total differentials of $F$ and $G$, we obtain,

$$
dF = \sum_j \left( \frac{\partial A}{\partial \Omega_j} \Phi - \frac{\partial b}{\partial \Omega_j} \right) d\Omega_j + A d\Phi + \left( A^K \Phi - b^K \right) d\lambda = 0
$$

$$
dG = \sum_j \frac{\partial G}{\partial \Omega_j} d\Omega_j + \frac{\partial G}{\partial \Phi} \cdot d\Phi = 0.
$$

(5.12)

The differential of $\lambda$ can be eliminated from these equations, and $\partial \Phi / \partial \Omega_j$ subject to the constraints $F = 0$ and $G = 0$ is obtained,

$$
\left. \frac{\partial \Phi}{\partial \Omega_j} \right|_{F=0, \ G=0} = -A^{-1} \left[ \left( \frac{\partial A}{\partial \Omega_j} \Phi - \frac{\partial b}{\partial \Omega_j} \right) + \frac{(A^K \Phi - b^K)}{\tilde{q} \cdot (A^K \Phi - b^K)} \left[ \frac{\partial G}{\partial \Omega_j} - \tilde{q} \cdot \left( \frac{\partial A}{\partial \Omega_j} \Phi - \frac{\partial b}{\partial \Omega_j} \right) \right] \right],
$$

(5.13)

where an additional adjoint variable $\tilde{q}$ is chosen to satisfy,

$$
A^T \tilde{q} = \frac{\partial G}{\partial \Phi}.
$$

(5.14)

For the case of $G$ given by (5.10), $\partial G / \partial \Omega_j = 0$ and $\partial G / \partial \Phi$ is proportional to $\partial \chi^2 / \partial \Phi$. These conditions cause the implicit dependence in (5.1) to cancel, leaving only the explicit dependence,

$$
\left. \frac{\partial \chi^2(I(\Omega, \Phi(\Omega)))}{\partial \Omega_j} \right|_{\Phi=b, \ \|K\|_2=\|K\|^{\text{target}}_2} = \left. \frac{\partial \chi^2}{\partial \Omega_j} \right|_{d\Phi=0}.
$$

(5.15)

### 5.3. Uniform Offset Constraint

Up to this point, the derivatives have been computed with a fixed winding surface. Without placing an additional constraint on the winding surface, the plasma boundary may move uniformly toward the winding surface in order to minimize the coil-plasma distance, as the shaping components of the magnitude decay with distance from coils (Boozer 2000; Landreman & Boozer 2016). For this reason, we instead compute derivatives with respect to the plasma surface parameters while maintaining the constraint that the coil winding surface is uniformly offset a distance $a$ from the plasma surface. The coil surface is then defined by,

$$
r' = r + a \hat{n}.
$$

(5.16)

The coil offset distance must similarly be constrained by the principal curvatures as,

$$
0 < a < \frac{1}{\min \{\kappa_1, \kappa_2\}}.
$$

(5.17)

Unlike the restriction on the offset surface that defines the poloidal angle (4.8), the coil offset distance is constrained by (5.17) to be greater than zero since the coils must lie in the vacuum region. As concavity of the plasma boundary has been shown to be correlated with coil complexity (Paul et al. 2018), placing such a constraint on the curvature of the boundary is reasonable.

This constraint couples the geometry of the winding surface to that of the plasma surface and therefore introduces additional derivatives with respect to the plasma surface.
Fourier amplitudes. For example, $A$ gains additional dependence through the $A^K$ term (2.6).

No new adjoint variables are needed to impose this constraint. With the combination of this and the fixed $\|K\|_2$ constraint, $G$ given by (5.10) now has explicit dependence on the plasma surface parameters; however, $\partial G/\partial \Phi$ is still proportional to $\partial \chi^2_K/\partial \Phi$. The derivatives of $\chi^2_B$ and $\chi^2_K$ are then given by

$$\frac{\partial \chi^2_B(\Omega, \Phi(\Omega))}{\partial \Omega_j} \bigg|_{A\Phi=b, \|K\|_2=\|K\|_2^{\text{target}}, \ r'=r+a\hat{n}} = \frac{\partial \chi^2_B}{\partial \Omega_j} \bigg|_{d\Phi=0}$$

$$-\lambda \left( \frac{\chi^2_K}{a_{\text{coil}}} \frac{\partial a_{\text{coil}}}{\partial \Omega_j} - \frac{\partial \chi^2_K}{\partial \Omega_j} \bigg|_{d\Phi=0} \right) \quad (5.18)$$

Note that the implicit dependence of $\chi^2_B$ is $-\lambda$ times the implicit dependence of $\chi^2_K$, and the total dependence of $\chi^2_K$ is such that $\|K\|_2$ vanishes.

Since higher order derivatives of the position vector are needed to compute the normal vector and its derivatives, any high-frequency noise in the surface representation is amplified with this constraint. For this reason, the poloidal angle defined with respect to the arclength on the winding surface as described in §4 greatly improves the numerical performance with this constraint.

6. Benchmarks and demonstrations

In this Section, we present several benchmark calculations to verify the derivatives and constraints from the previous Section.

6.1. Finite-difference derivatives

The derivatives of $\chi^2_I$ are implemented analytically as described in the previous Section rather than with a finite-difference approximation. The former is advantageous over the later in that it takes far less computation time for a high-dimensional derivative; however, the finite-difference result should converge to the analytic result as the step size is reduced. This is used to check the accuracy of the analytic derivatives. Consider a numerical forward-difference approximation of $\partial \chi^2_I/\partial \Omega_j$,

$$\left( \frac{\partial \chi^2_I}{\partial \Omega_j} \right)_{\text{num.}} = \frac{\chi^2_I(\Omega_j + \Delta \Omega) - \chi^2_I(\Omega_j)}{\Delta \Omega}.$$

When doing this calculation, the perturbation of the current potential corresponding to the perturbation of $\Omega_j$ is included in order to account for the implicit dependence of $\chi^2_I$ on the plasma surface. This expression is a first order approximation, so it should agree with the analytic expression to $O(\Delta \Omega)$.

We now define the fractional difference between the analytic and numerical derivatives as

$$\text{fractional difference} = \left( \frac{\partial \chi^2_I}{\partial \Omega_j} - \left( \frac{\partial \chi^2_I}{\partial \Omega_j} \right)_{\text{num.}} \right) \left( \frac{\partial \chi^2_I}{\partial \Omega_j} \right)^{-1}.$$  

The following results were generated using the QHS46 equilibrium (Shohet et al. 1991) with a 0.25 m uniformly offset coil winding surface which was constrained during the
A. Carlton-Jones, E. J. Paul, and W. Dorland

Figure 4: Modes with \( m \) up to 2 and \( n \) up to \( \pm 2N_p \) are displayed with lines on the red end of the spectrum corresponding to larger magnitudes of the derivative and lines on the blue end of the spectrum corresponding to smaller magnitudes. We present the fractional difference between analytic and numerical calculations of (a) \( \partial \|B_n\|_2/\partial l_{m,n}^c \), (b) \( \partial \|K\|_2/\partial l_{m,n}^c \), and (c) \( \partial \|B_n\|/\partial l_{m,n}^c \) while holding \( \|K\|_2 \) fixed.

calculation of derivatives with respect to the plasma parameters. A plot of the fractional difference for the derivatives of \( \|B\|_2 \) with only the optimal solution constraint and uniform offset constraint imposed is given in Figure 4a. The surface is described by the single Fourier representation given in (4.10) with the arclength angle define on a surface chosen to have the same 0.25 m uniform offset as the coil winding surface. A similar fractional difference plot is given for \( \|K\|_2 \) in Figure 4b. We find that the fractional difference scales linearly with \( \Delta \Omega \) for \( 10^{-7} \lesssim \Delta \Omega \lesssim 10^{-2} \). For \( \Delta \Omega \lesssim 10^{-7} \), the round-off error begins to dominate, and the linear relationship is no longer observed (Sauer 2012). Similar trends are also observed in the fractional difference for \( \|B\|_2 \) with the addition of the fixed \( \|K\|_2 \) constraint, presented in Figure 4c. For this and other QHS46 calculations with the fixed \( \|K\|_2 \) constraint, \( \|K\|_2^{\text{target}} = 1.6 \text{ MA m}^{-1} \) was used.

6.2. Area shape gradient benchmark

As a benchmark for calculating shape gradients with the modified REGCOIL code, the shape gradient of the plasma surface area is computed. There is an analytic expression for this shape gradient (Landreman & Paul 2018), which is given by,

\[
S_{a^\text{plasma}} = 2H,
\]  

(6.3)

where \( H = \frac{1}{2}(\kappa_1 + \kappa_2) \) is the mean curvature of the plasma surface. Again, we assume the convention that positive \( H \) indicates convexity. The shape gradient of the plasma area calculated using (3.4) is given in Figure 5a. The calculation is performed for the
W7-X boundary. The shape gradient is computed on a grid of \( N_\theta = 100 \) grid points in the poloidal angle and \( N_\zeta = 100 \) grid points in the toroidal angle. The derivatives of the area are computed for \( m \leq 25 \) and \( |n/N_P| \leq 25 \), and the shape gradient is discretized with a Fourier series with the same set of modes, so (3.4) is a square linear system. We compare this to the expected result, given in Figure 5b. The average error in the shape gradient,

\[
\text{error} = \frac{\int_{S_{\text{plasma}}} d^2x \left| S_{\text{plasma}} - 2H \right|}{\int_{S_{\text{plasma}}} d^2x \left| 2H_{\text{plasma}} \right|},
\]

is computed to be \( 1.59 \times 10^{-3} \). We obtain good agreement between our numerical result and the expected analytic result.

### 6.3. Shape gradients of \( \|B_n\|_2 \) and \( \|K\|_2 \)

In this Section, (3.4) is used to obtain the shape gradients of \( \|B_n\|_2 \) and \( \|K\|_2 \) for the QHS46 and W7-X configurations using the derivatives obtained from the adjoint method. For both configurations, we choose the winding surface to be uniformly offset from the plasma boundary (5.16). In the case of W7-X we choose \( a = 0.25 \) m, and for QSH46 we choose \( a = 0.143 \) m such that the offset distance is scaled according to the minor radius of the plasma boundary. Note that the chosen offset distance is somewhat smaller than the minimum coil-plasma spacing of the actual W7-X winding surface, which is 0.37 m (Paul et al., 2018). For the QHS46 calculations, a fixed value of \( \|K\|_2^{\text{target}} = 1.6 \) MA m\(^{-2}\) was used while for W7-X it was taken to be 2.2 MA m\(^{-2}\).

In Figure 6, results are shown on the three dimensional shape of the QHS46 plasma surface. The parameter derivatives with respect to modes with \( m \leq 25 \) and \( |n/N_P| \leq 20 \) are computed on a grid with \( N_\theta = N_\zeta = 100 \). The shape gradient of \( \|B_n\|_2 \) for only the optimal solution constraint is shown in Figure 6a, and similarly for \( \|K\|_2 \) in Figure 6b. We see that for both of these quantities, the shape gradient is large and positive in the regions of convex curvature and strongly negative in the nearby regions where the surface curvature is locally reduced. This indicates that in order to reduce both of these figures of merit, the sharp ridge features on the boundary must be locally rounded. Similar features are present when the shape gradient of \( \|B_n\|_2 \) is computed with the fixed
Figure 6: The shape gradient of (a) $\|B_n\|_2$, (b) $\|K\|_2$, (c) $\|B_n\|_2$ with fixed $\|K\|_2$, and (d) $\|B_n\|_2$ with fixed $\|K\|_2$ and fixed offset distance is computed for the QHS46 boundary with a uniform offset winding surface of 0.143 m. The shape gradient is computed using a linear solve of (3.4) for a square system.

$\|K\|_2$ constraint as shown in Figure 6c, though the magnitude is slightly increased. In Figure 6d, the shape gradient with the additional uniform offset constraint is qualitatively similar, but an additional feature is present near the triangle-shaped cross-section.

In Figure 7, we present the results for the W7-X boundary. The shape gradient is computed with the same resolution used for the benchmark in Section 6.2. We see that the shape gradient for $\|B_n\|_2$ is again peaked in the region of large convexity and slightly negative in the region of concavity. This indicates that the normal field could be reduced by pushing the surface inward in the sharp convex regions and outward in the concave regions. We see that the shape gradient for $\|K\|_2$ similarly has a large magnitude in the convex region. Considering the shape gradient of $\|B_n\|_2$ with the additional constraints, we see that the trends are qualitatively similar.

Finally, we mention that the calculations presented in this Section rely on the choice of the offset distance, $a$. We find that the trends presented here do not strongly vary with this choice. This is consistent with the observations in (Paul et al. 2018).
Shape gradient of stellarator coil complexity with respect to the plasma boundary

Figure 7: The shape gradient of (a) $\|B_n\|_2$, (b) $\|K\|_2$, (c) $\|B_n\|_2$ with fixed $\|K\|_2$, and (d) $\|B_n\|_2$ with fixed $\|K\|_2$ and fixed offset distance is computed for the W7-X boundary with a uniform offset winding surface of 0.25 m. The shape gradient is computed using a linear solve of (3.4) for a square system.

7. Conclusion

We have presented a new approach to stellarator design which differs from the traditional approach of choosing a plasma shape for its MHD properties and then optimizing the coils to be consistent with the boundary. To assess a given plasma boundary, we evaluate metrics obtained from the current potential on a uniformly offset winding surface, namely the normal field error and current density. Derivatives of these objectives with respect to the Fourier series coefficients used to parameterize the plasma surface are computed with an adjoint method in order to reduce the number of linear solves required. Moreover, we present a new parameterization of the plasma boundary which improves the convergence of the Fourier series by choosing a fixed poloidal angle to be an arclength angle on a uniformly offset surface. This choice furthermore eliminates the non-uniqueness of the poloidal angle that is present in the standard cylindrical representation and the related null space in the optimization of the boundary.

With these parameter derivatives, we construct the shape gradient with respect to displacements of the plasma boundary. This provides information on how to deform the plasma surface in order to reduce the normal field error or coil complexity. Several constraints are enforced in order to ensure that the regularization parameter used in the REGCOIL code is chosen to target engineering constraints and that the winding surface
maintains a uniform displacement from the plasma surface. This shape gradient provides intuition about what kinds of plasma shapes are consistent with simpler coils. The results presented in Section 6.3 indicate that both convex and concave curvature of the plasma boundary are associated with coil complexity.

The shape gradient obtained with this method could be used within the optimization of the MHD equilibrium to avoid arriving at a configuration that requires overly-complex coils. With a slight modification, a similar technique could be utilized to compute the shape gradient of objectives related to the permanent magnets (Helander et al. 2020; Zhu et al. 2020; Landreman & Zhu 2020) required to confine a given equilibrium. Under the assumption that a continuous surface magnetization lies on the winding surface with an orientation in the normal direction, an equivalent linear least-squares problem can be formulated in which the current potential is related to the magnitude of the magnetization. Thus in computing the shape gradient with respect to the plasma boundary, the norm of the current potential rather than the norm of the current density could be fixed to choose the regularization parameter.

The new parameterization of the plasma boundary utilizes the distance from a fixed coordinate axis. In this work, we have taken this coordinate axis to coincide with the magnetic axis, although this assumption is not required. Other possible choices for the coordinate axis may be favorable. In the stellarator equilibrium code VMEC, the initial coordinate axis is taken to maximize the minimum value of the flux coordinate Jacobian (Hirshman & Whitson 1983), and in the SPEC code (Hudson et al. 2011) the coordinate axis is chosen to minimize the variation of the Jacobian over a poloidal cross-section (Qu et al. 2020). Although a three-dimensional Jacobian is not necessary for current potential calculations, a similar analysis could be performed to minimize the variation of the surface Jacobian \( \left| \frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \zeta} \right| \) with a cleverly chosen axis.

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