Uncertainty Quantification for the DESC Stellarator System Using Optimized Perturbation Method

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Outline

Quick and Accurate Equilibria

- MD Conservation: $\mathbf{J} \times \mathbf{B} = \nabla p$
- Ampere's Law: $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$
- Gauss's Law: $\nabla \cdot \mathbf{B} = 0$

- Force Balance Equation: $\mathbf{F} = \mathbf{J} \times \mathbf{B} - \nabla p = 0$
- Plasma Potential Energy: $W = \int_V \left(\frac{B^2}{2\mu_0} + \frac{p}{\gamma - 1} dV \right)$

- $\mathbf{F} = \mathbf{F}_\rho \nabla \rho + \mathbf{F}_\beta \hat{\beta}_{desc}$ with $\hat{\beta}_{desc} = -\mathbf{B}_\theta \nabla \phi + \mathbf{B}_\phi \nabla \theta$
- $\mathbf{F}_\rho = \sqrt{g}(\mathbf{J}^\phi \mathbf{B}^\theta - \mathbf{B}^\phi \mathbf{J}^\theta) + p'$ and $\mathbf{F}_\beta = \sqrt{g}\mathbf{J}^\rho$

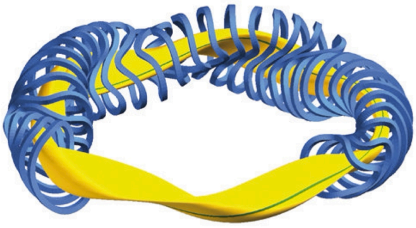


Figure: Illustration of Wendelstein 7-X Stellarator

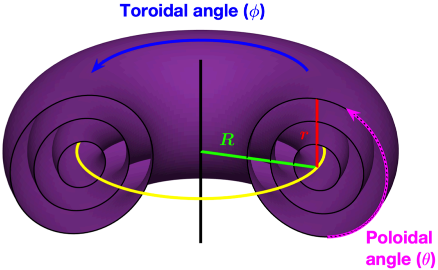
DESC: 3D equilibrium code developed to find equilibria by minimizing the MHD force balance error

Perturbations

Constraint Function

$$\mathbf{f}(\mathbf{x}, \mathbf{c}) = 0 \tag{1}$$

Output Results Input Parameters



with $c = \{R_b, Z_b, p, \iota, \Psi\}$ and $\mathbf{x} = [R_{lmn}, Z_{lmn}, \lambda_{lmn}]$

- R_b, Z_b: R, Z coordinates of the boundary surface
- p: pressure profile
- ι: rotational transform
- Ψ: toroidal flux through the torus
- $R_{lmn}, Z_{lmn}, \lambda_{lmn}$: spectral coefficients of the flux surface positions and the poloidal stream function

Task: Find how the equilibrium would change if the parameters $\mathbf{c}$ are perturbed to $\mathbf{c} + \Delta\mathbf{c}$

$$\mathbf{f}(\mathbf{x} + \Delta\mathbf{x}, \mathbf{c} + \Delta\mathbf{c}) = 0 \tag{2}$$

Perturbations Contd.

Taylor Series Approximation

$$\mathbf{f}(\mathbf{x}+\Delta\mathbf{x},\mathbf{c}+\Delta\mathbf{c}) = \mathbf{f}(\mathbf{x},\mathbf{c}) + \frac{\partial \mathbf{f}}{\partial \mathbf{x}}\Delta\mathbf{x} + \frac{\partial \mathbf{f}}{\partial \mathbf{c}}\Delta\mathbf{c} + \frac{1}{2}\frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}^2}\Delta\mathbf{x}^2 + \frac{1}{2}\frac{\partial^2 \mathbf{f}}{\partial \mathbf{c}^2}\Delta\mathbf{c}^2 + \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}\partial \mathbf{c}}\Delta\mathbf{x}\Delta\mathbf{c} + \ldots\ldots \tag{3}$$

Expand $\Delta\mathbf{x}$ and $\Delta\mathbf{c}$ in a perturbation series

$$\Delta\mathbf{x} = \epsilon\mathbf{x}_1 + \epsilon^2\mathbf{x}_2 + \epsilon^3\mathbf{x}_3\ldots \tag{4}$$

$$\Delta\mathbf{c} = \epsilon\mathbf{c}_1 \tag{5}$$

$$\begin{aligned}
0 = & \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\epsilon\mathbf{x}_1 + \epsilon^2\mathbf{x}_2 + \epsilon^3\mathbf{x}_3) + \frac{\partial \mathbf{f}}{\partial \mathbf{c}}\epsilon\mathbf{c}_1 \\
& + \frac{1}{2}\frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}^2}(\epsilon\mathbf{x}_1 + \epsilon^2\mathbf{x}_2 + \epsilon^3\mathbf{x}_3)^2 + \frac{1}{2}\frac{\partial^2 \mathbf{f}}{\partial \mathbf{c}^2}(\epsilon\mathbf{c}_1)^2 + \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}\partial \mathbf{c}}(\epsilon\mathbf{x}_1 + \epsilon^2\mathbf{x}_2 + \epsilon^3\mathbf{x}_3)\epsilon\mathbf{c}_1 \\
& + \frac{1}{6}\frac{\partial^3 \mathbf{f}}{\partial \mathbf{x}^3}(\epsilon\mathbf{x}_1 + \epsilon^2\mathbf{x}_2 + \epsilon^3\mathbf{x}_3)^3 + \frac{1}{6}\frac{\partial^3 \mathbf{f}}{\partial \mathbf{c}^3}(\epsilon\mathbf{c}_1)^3 \\
& + \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x}^2\partial \mathbf{c}}(\epsilon\mathbf{x}_1 + \epsilon^2\mathbf{x}_2 + \epsilon^3\mathbf{x}_3)^2(\epsilon\mathbf{c}_1) + \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x}\partial \mathbf{c}^2}(\epsilon\mathbf{x}_1 + \epsilon^2\mathbf{x}_2 + \epsilon^3\mathbf{x}_3)(\epsilon\mathbf{c}_1)^2 + h.o.t.
\end{aligned}$$

Perturbation Contd.

Collect powers of ϵ and set each order to zero. First order equation

$$0 = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \epsilon \mathbf{x}_1 + \frac{\partial \mathbf{f}}{\partial \mathbf{c}} \epsilon \mathbf{c}_1 \tag{6}$$

$$\mathbf{x}_1 = -\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^{-1} \left(\frac{\partial \mathbf{f}}{\partial \mathbf{c}} c_1\right) \tag{7}$$

Second order equation

$$0 = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \epsilon^2 \mathbf{x}_2 + \frac{1}{2} \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}^2} (\epsilon \mathbf{x}_1)^2 + \frac{1}{2} \frac{\partial^2 \mathbf{f}}{\partial \mathbf{c}^2} (\epsilon \mathbf{c}_1)^2 + \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x} \partial \mathbf{c}} (\epsilon^2 \mathbf{x}_1 \mathbf{c}_1) \tag{8}$$

$$\mathbf{x}_2 = -\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^{-1} \left(\frac{1}{2} \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}^2} \mathbf{x}_1^2 + \frac{1}{2} \frac{\partial^2 \mathbf{f}}{\partial \mathbf{c}^2} \mathbf{c}_1^2 + \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x} \partial \mathbf{c}} (\mathbf{x}_1 \mathbf{c}_1)\right) \tag{9}$$

Third order equation

$$0 = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \epsilon^3 \mathbf{x}_3 + \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}^2} (\epsilon^3 \mathbf{x}_1 \mathbf{x}_2) + \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x} \partial \mathbf{c}} (\epsilon^3 \mathbf{x}_2 \mathbf{c}_1) + \frac{1}{6} \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x}^3} (\epsilon \mathbf{x}_1)^3 + \frac{1}{6} \frac{\partial^3 \mathbf{f}}{\partial \mathbf{c}^3} (\epsilon \mathbf{c}_1)^3 + \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x}^2 \partial \mathbf{c}} (\epsilon^3 \mathbf{x}_1^2 \mathbf{c}_1) + \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x} \partial \mathbf{c}^2} (\epsilon^3 \mathbf{x}_1 \mathbf{c}_1^2) \tag{10}$$

$$\mathbf{x}_3 = -\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^{-1} \left(\frac{\partial^2 \mathbf{f}}{\partial \mathbf{x}^2} (\mathbf{x}_1 \mathbf{x}_2) + \frac{\partial^2 \mathbf{f}}{\partial \mathbf{x} \partial \mathbf{c}} (\mathbf{x}_2 \mathbf{c}_1) + \frac{1}{6} \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x}^3} \mathbf{x}_1^3 + \frac{1}{6} \frac{\partial^3 \mathbf{f}}{\partial \mathbf{c}^3} \mathbf{c}_1^3 + \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x}^2 \partial \mathbf{c}} (\mathbf{x}_1^2 \mathbf{c}_1) + \frac{\partial^3 \mathbf{f}}{\partial \mathbf{x} \partial \mathbf{c}^2} (\mathbf{x}_1 \mathbf{c}_1^2)\right) \tag{11}$$

Improvements and Expectations

- Current Limitations
  - An input parameter sets for an output equilibrium solution
  - Cannot simulate the actual modeling system automatically and spontaneously
  - Lack of directional motions directed by random distributions
  - Lack of uncertainty control for the input parameter sets
- Improvements and Expectations
  - Assign distributions for input parameters
  - R_b, Z_b: 2D jointly space field, Gaussian Random Field
  - p, ι: 1D profile function, Gaussian Process
  - Ψ: Normal Distribution
  - Automatically update input equilibrium state equation to simulate a real-world model

$$P(\rho) = \sum_{i=0}^{r} p_i \rho^i \qquad (P_1, P_2, ..., P_n) \tag{12}$$

$$G(\rho) \approx \sum_{i=0}^{r} g_i \rho^i \qquad (G_1, G_2, ..., G_n) \tag{13}$$

$$\hat{P}(\rho) = P(\rho) + G(\rho) \approx \sum_{i=0}^{r} p_i (1 + \sigma g_i) \rho^i \qquad (\hat{P}_1, \hat{P}_2, ..., \hat{P}_n) \tag{14}$$

Computational model

DESC solves the equilibrium problem that is defined by the following four inputs

1. Pressure profile $p(\rho)$
2. Rotational transform profile $\iota(\rho)$
3. Last Closed Flux Surface (LCFS) Boundary Shape
4. Total toroidal magnetic flux enclosed by the LCFS

Quantities of interest include

1. Force balance error $|\mathbf{J} \times \mathbf{B} - \nabla p|$
2. Magnetic field strength
3. ...

In this study, we focus on quantifying the uncertainty of the maximum force balance error given uncertain pressure profile.

Pressure profile

1. Plasma pressure field is crucial to achieve equilibrium
2. For stellarator design, it's convenient to model the plasma pressure field using a **one-dimensional** polynomial series due to smoothness and axial-symmetry:

$$p(\rho) = \sum_{i=0}^{N} p_i \rho^i$$

3. **0 gauge pressure** at the boundary needs to be satisfied.

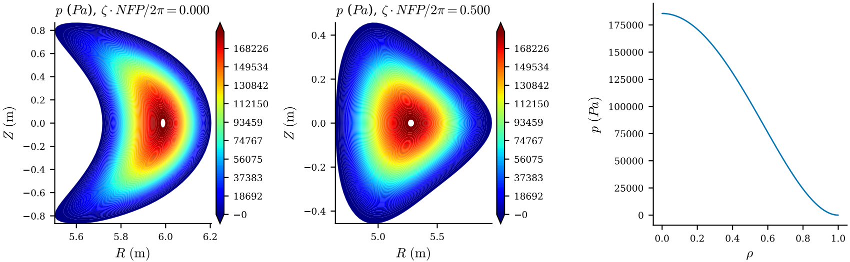


Figure: (a) Pressure field for two cross sections of the W7-X stellarator. (b) 1-dimensional pressure profile

Force balance error

1. DESC is an **equilibrium** (not dynamics) code, it tries to minimize the force balance error given predefined pressure profile
2. Such error is usually not zero

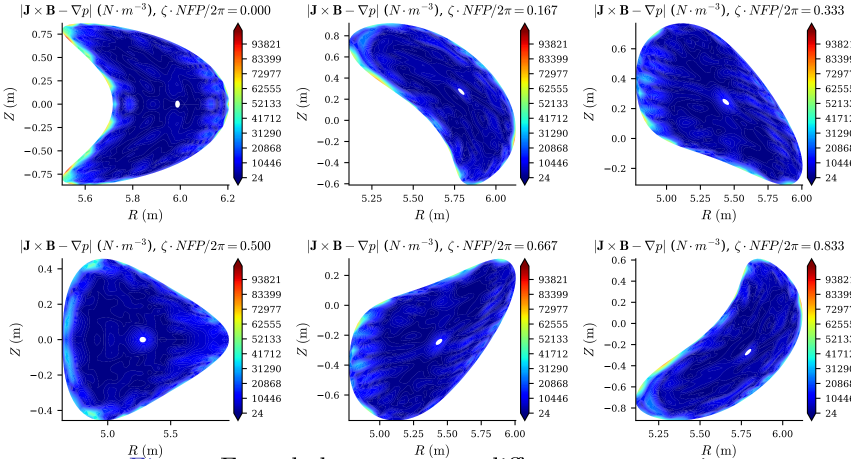


Figure: Force balance error at different cross sections

Monte Carlo: direct coefficient perturbation

1. First, we define the prior by directly perturbing the coefficients of the power series:

$$\Delta p(\rho) = \Delta p_0 + \Delta p_2 \rho^2 + \Delta p_4 \rho^4 + \cdots + \Delta p_{10} \rho^{10}, \quad \Delta p_i \sim U(-25, 25)$$

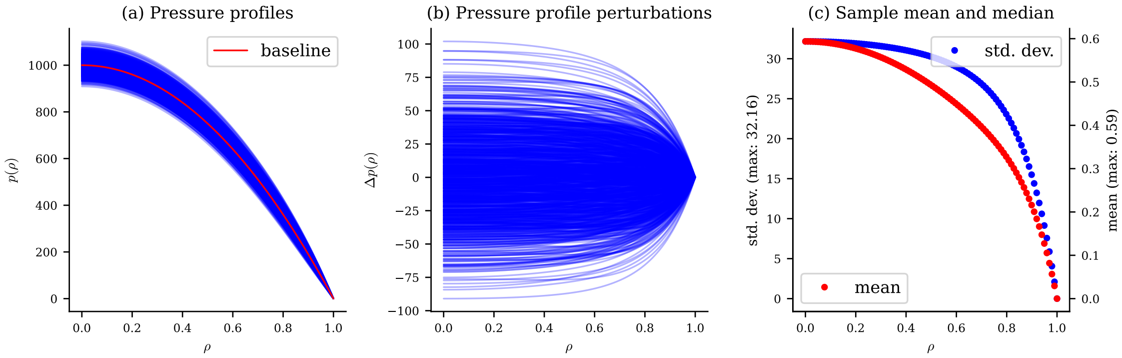


Figure: Pressure profile perturbations

Monte Carlo: direct coefficient perturbation

1. Here we present the distribution of the output using histogram and kernel density estimation
2. Convergence study shows that as number of samples grows, distribution becomes smoother

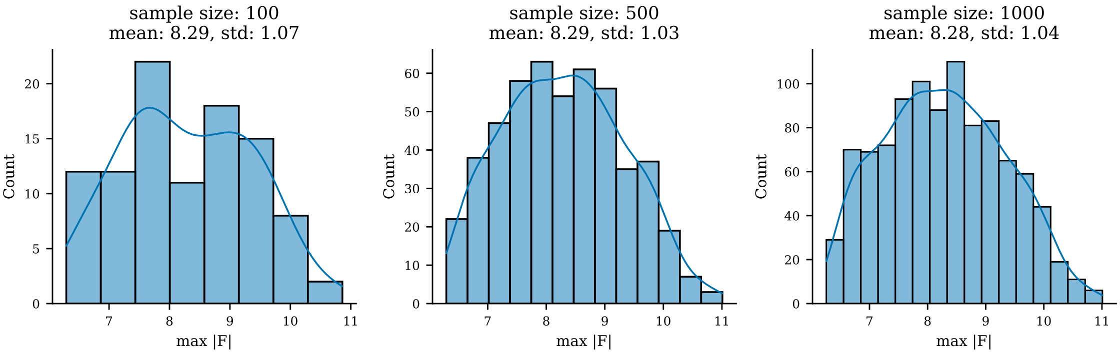


Figure: Distribution of $|F|$ for different sample size N

Monte Carlo: Gaussian process

1. Next, we define the prior by sampling from a Gaussian process $\Delta p(\rho) \sim \mathrm{GP}$.
2. Radial basis function (RBF) kernel is used:

$$k(\rho_i, \rho_j) = \exp\left(\frac{d(\rho_i, \rho_j)^2}{2l^2}\right)$$

where l controls the length scale, here we use $l = 0.5$ (recall that $\rho \in [0, 1]$)

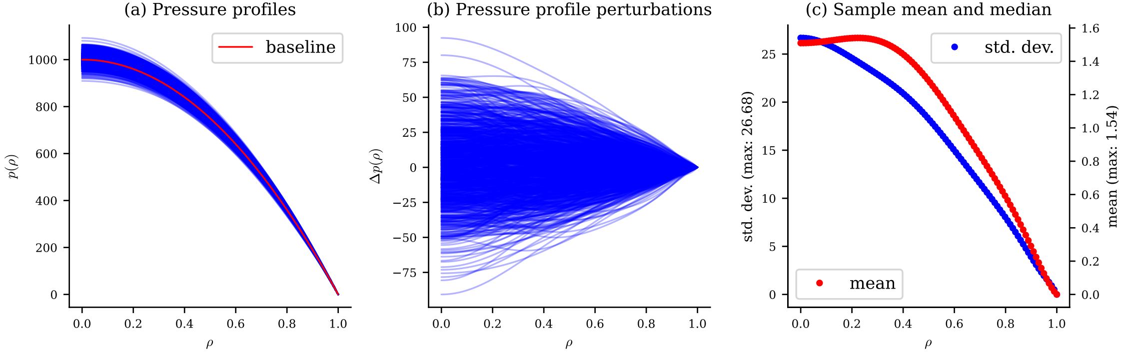


Figure: Pressure profile perturbations, length scale $l = 0.5$

Monte Carlo: Gaussian process ($l = 0.5$)

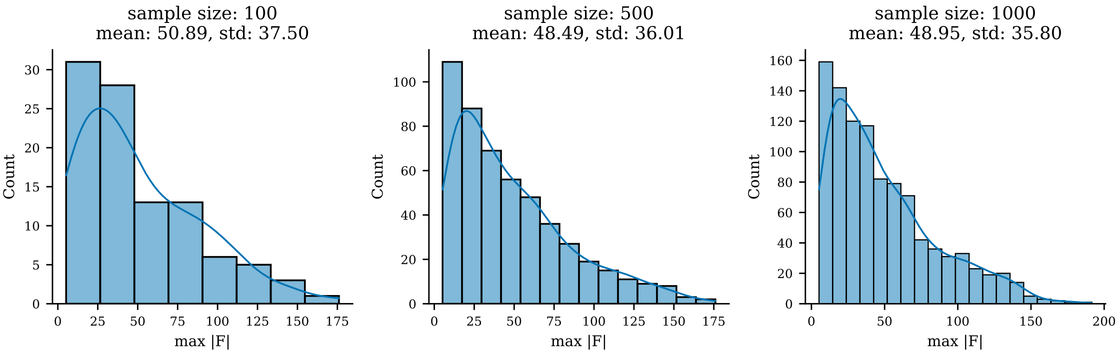


Figure: Distribution of $|F|$ for different sample size N

Monte Carlo: Gaussian process ($l = 0.1$)

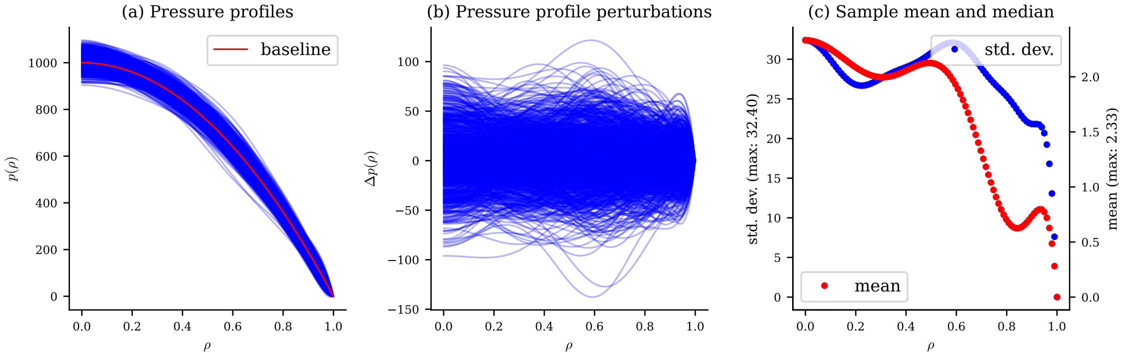


Figure: Pressure profile perturbations, length scale $l = 0.1$

Monte Carlo: Gaussian process ($l = 0.1$)

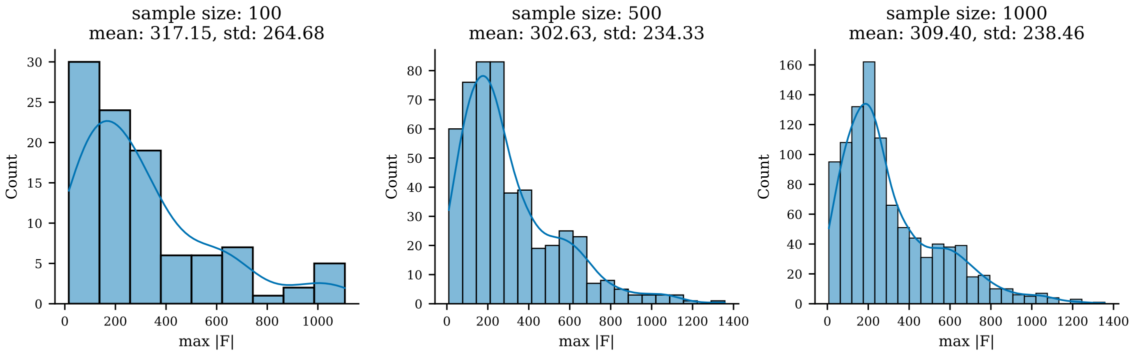


Figure: Distribution of $|F|$ for different sample size N

Summary and Further Studies

- Perturbation Method
  - Find how the equilibrium of constraint function would change for perturbed input parameters $\mathbf{f}(\mathbf{x} + \Delta\mathbf{x}, \mathbf{c} + \Delta\mathbf{c}) = 0$
  - Extend in Taylor series and find force error balance in different order
  - Improve the current perturbation method by assigning GP and MC distributions to input parameter p
- Takeaways
  - Perturbation method and continuation technique allow efficient Monte Carlo simulation
  - Assumptions of prior distribution have significant impact on the output distribution
- Future work
  - Examine other higher-dimensional input functionals including R_b, Z_b and ι
  - Study distributions of other quantities of interest, such as magnetic field
  - Employ polynomial chaos expansion
    1. Pseudo-spectral projection
    2. Point allocation method

References

[1] DESC: A Stellarator Equilibrium Solver, D. Dudt and E. Kolemen, Phys. Plasmas 27, 102513 (2020)

[2] The DESC Stellarator Code Suite Part I: Quick and Accurate Equilibria Computations, D. Panici and R. Conlin (2022)

[3] The DESC Stellarator Code Suite Part II: Perturbation and Continuation Methods, Rory Conlin and Daniel W. Dudt (2022)

[4] An Introduction to Stellarators: From Magnetic Fields to Symmetries and Optimization, Lise-Marie Imbert-Gérard (2020)

[5] Proof of concept of a fast surrogate model of the VMEC code via neural networks in Wendelstein 7- X scenarios, Andrea Merlo et al (2021)

Questions and Discussions

- Why do we need so much samples? How can we analyze our result graphs?
  Answer: We chose to use a sample size of up to 1000 to demonstrate a more comprehensive perturbed distribution of the input pressure profile. This is not an optimization problem, but rather a distribution problem, and having more sample data helps us to effectively observe how the next-step distribution will be generated. The resulting graphs illustrate how the perturbation performance affects the pressure profile distribution. However, if we were to conduct an actual numerical analysis to optimize the system, we would need to gather additional information, which could lead to another project idea such as quasi-symmetry optimization.
- How do you choose the value of parameter l in your RBF kernel equation?
  Answer: There is no exact, accurate value for the parameter l, which determines the degree of perturbation for the curves. It is usually determined based on experience. In this study, we tested two different values for l: 0.5 and 0.1, to see how they affect the resulting graphs. However, there is no one correct answer for the value of l, as it depends on the specific application and the level of perturbation desired.