Multi-fidelity Monte Carlo for Uncertainty Quantification in the Free-Boundary Grad–Shafranov Equation

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Outline

- ▷ Physical Model: Grad-Shafranov Equation
- ▷ Uncertainty Quantification
- ▷ Objectives & Approaches
- ▷ Multi-fidelity Monte Carlo
- ▷ Parameter Estimation
- ▷ Numerical Results

- ▷ **Physical Model: Grad-Shafranov Equation**
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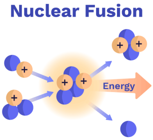
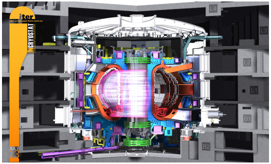
Fusion & Magnetic Confinement

- **Fusion reactor:** Focus on Tokamak – doughnut-shaped vacuum chamber.
- **Fusion mechanism:** Inject fuel gas (hydrogen isotopes) into the chamber $\rightarrow$ heated with microwave $\rightarrow$ form a plasma $\rightarrow$ particles overcome coulomb repulsion $\rightarrow$ fuse to produce energy.





- During fusion, the hot plasma tends to expand, to prevent it from contacting the reactor wall, it must be confined.
- **Magnetic confinement:** Confinement is achieved through magnetic fields generated by currents running through external coils surrounding the reactor.
- Our project focuses on studying the **impact of variations in current** on the physical properties of the confinement field. These **variations** may come from power supply, temperature fluctuations, and material impurities in the conduction wire.

Source: https://www.iter.org/mach/Tokamak

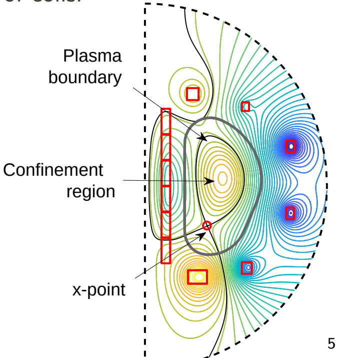
The Grad-Shafranov Free Boundary Problem

$$-\nabla \cdot \left(\frac{1}{\mu x}\nabla\psi\right) = \begin{cases} x\frac{d}{d\psi}p(\psi) + \frac{1}{2\,\mu x}\frac{d}{d\psi}g^2(\psi) & \text{in } \overline{\Omega_p(\psi)} \\ \boldsymbol{I_i}/S_i & \text{in } \Omega_{C_i} \\ 0 & \text{elsewhere} \end{cases}$$

$$\psi(0,y) = 0; \qquad \lim_{\|(x,y)\|\to\infty} \psi(x,y) = 0.$$

ψ: poloidal flux. $\mu(\psi)$: magnetic permeability. $p(\psi)$: hydrodynamic pressure. $g(\psi)$: toroidal field function. $\Omega_p(\psi)$: confinement region. I_i: current intensity. S_i: cross section area of the coils. Ω_{c_i}: locations of coils.

- **Non-linear** free boundary problem with the source of uncertainty arises from the **current intensities**.
- **Knowns:** $p(\psi), g(\psi), I_i, \Omega_{c_i}$, and μ. **Unknowns:** ψ and $\Omega_p(\psi)$.
- **Software:** MATLAB finite element package `FEEQS.M` – H. Heumann and his collaborators.



Uncertain Coil Currents

- **Source of uncertainty:** Investigate the impact of uncertainties in the current intensities on the confinement properties of a plasma.
- **Baseline current intensities:**

$$\begin{array}{lll}
I_1 : -1.40 \times 10^6\text{A} & I_5 : -9.00 \times 10^6\text{A} & I_9 : -6.43 \times 10^6\text{A} \\
I_2 : -9.50 \times 10^6\text{A} & I_6 : 3.56 \times 10^6\text{A} & I_{10} : -4.82 \times 10^6\text{A} \\
I_3 : -2.04 \times 10^7\text{A} & I_7 : 5.47 \times 10^6\text{A} & I_{11} : -7.50 \times 10^6\text{A} \\
I_4 : -2.04 \times 10^7\text{A} & I_8 : -2.27 \times 10^6\text{A} & I_{12} : 1.72 \times 10^7\text{A}
\end{array}$$

- **Uncertianty Quantification UQ:** Variations in the baseline current intensities. Each current in the array is considered to be a parameter, so we have 12-dimensional parameter space.
- **Currents uniformly distributed:**
  τ: perturbation level ($\tau = 1\%$ & 2%). I_k: current intensity in the k-th coil.
  - Joint density function: $\pi(\boldsymbol{\omega}) = \prod_{k=1}^{d} \pi_k(\omega_k) = \prod_{k=1}^{d} \frac{1}{2\tau|I_k|}$.
  - 12-d parameter space: $W := \prod_{k=1}^{d} [I_k - \tau|I_k|, I_k + \tau|I_k|]$.

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Objectives & approaches

- **Uncertainty Quantification in Plasma Equilibria**
  Quantify the **impact of variations in current intensity** on determining
  - **Expectation:** $\mathbb{E}[\psi(x, y, \boldsymbol{\omega})] = \int_W \psi(x, y, \boldsymbol{\omega})\pi(\boldsymbol{\omega})d\boldsymbol{\omega}$.
  - **Key plasma features:** presence and locations of x-points, contact points, strike points & separatrices.
  - **Geometry parameters:** elongation, triangularity etc.

- **Enhancing Sampling Efficiency**
  Use **sampling methods** to approximate the expectation efficiently
  - Multi-fidelity Monte Carlo (MFMC)
    Blending high- and low-fidelity models, where high-fidelity models provide accuracy and low-fidelity surrogates reduce computational cost.

- **Contributions**
  - Reformulation of the optimization problem for MFMC sample allocation.
  - Dynamic pilot-sampling strategy for correlation estimation.
  - Application of the MFMC framework to the plasma problem.

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Monte Carlo Sampling

- **Monte Carlo (MC)**
  Estimate $\mathbb{E}[u]$ by a finite number of i.i.d. sample average.

$$A_N^{\mathrm{MC}} := \frac{1}{N}\sum_{i=1}^{N} u_h^{(i)}$$

- **MC estimator A^{MC} for $\mathbb{E}[u]$**
  - Unbiased $\mathbb{E}[A_N^{\mathrm{MC}}] = \mathbb{E}[u_h]$.
  - Variance decays slowly: $\mathcal{O}(N^{-1/2})$,
    $\mathbb{V}[A_N^{\mathrm{MC}}] = \mathbb{V}[u_h]/N$, where $\mathbb{V}[u_h] := \mathbb{E}[\| u_h - \mathbb{E}[u_h]\|_U^2]$.

Multi-fidelity Monte Carlo Sampling

▷ **Multi-fidelity Monte Carlo (MFMC)**

A variance reduction technique that efficiently estimates statistical quantities by using low fidelity (LF) models to reduce variance of high fidelity (HF) model. HF models are used to maintaining accuracy.

B. Peherstorfer, K. Willcox, and M. Gunzburger. Optimal Model Management for Multifidelity Monte Carlo Estimation. SIAM J. SCI. COMPUT, Vol. 38, No. 5, pp. A3163–A3194.

▷ **HF and LF models**

- **High fidelity models:** Expensive but accurate
  (e.g., finite element solution of Grad-Shafranov equation).
- **Low fidelity models:** Cheap but less accurate, correlated with HF as control variates.
  (e.g., sparse grid stochastic collocation + coarser meshes).

Multi-fidelity Monte Carlo

- **MFMC estimator A^{MF} for $\mathbb{E}[u]$**

$$
\begin{aligned}
A^{\mathrm{MF}} &= A^{\mathrm{MC}}_{1,N_1} + \sum_{k=2}^{K} \alpha_k \left(\overline{A}_{k,N_k} - \overline{A}_{k,N_{k-1}} \right) \\
&= A^{\mathrm{MC}}_{1,N_1} + \sum_{k=2}^{K} \alpha_k \left(\frac{N_{k-1}}{N_k} - 1 \right) \left(A^{\mathrm{MC}}_{k,N_{k-1}} - A^{\mathrm{MC}}_{k,N_k \setminus N_{k-1}} \right)
\end{aligned}
$$

  - $\overline{A}_{k,N_{k-1}}$ reuses the first N_{k-1} samples from $\overline{A}_{k,N_k}$, $N_k \geq N_{k-1}$.
  - $A^{\mathrm{MC}}_{k,N_k \setminus N_{k-1}}$: MC estimator of $N_k - N_{k-1}$ samples not included in $A^{\mathrm{MC}}_{k,N_{k-1}}$.
  - Unbiased $\mathbb{E}[A^{\mathrm{MF}}] = \mathbb{E}[u_h]$.
  - $\mathbb{V}[A^{\mathrm{MF}}] = \frac{\sigma_1^2}{N_1} + \sum_{k=2}^{K} \left(\frac{1}{N_{k-1}} - \frac{1}{N_k} \right) \left(\alpha_k^2 \sigma_k^2 - 2\alpha_k \rho_{1,k} \sigma_1 \sigma_k \right)$.
  - Efficiency depends on correlation $\rho_{1,k}$ between HF and LF.
  - Requires estimating optimal weights α_k and sample sizes N_k.

Multi-fidelity Monte Carlo

- **The original optimization problem – Constraint on budget**

$$
\begin{aligned}
\text{min} \quad & \mathbb{V}\left[A^{\mathrm{MF}}\right] \\
\text{subject to} \quad & \sum_{k=1}^{K} C_k N_k = p, \\
& -N_1 \le 0, \quad N_{k-1} - N_k \le 0, \;\; k = 2\dots, K, \\
& N_1, \dots, N_K \in \mathbb{R}, \\
& \alpha_2, \dots, \alpha_K \in \mathbb{R}.
\end{aligned}
$$

- **Our formulation – Constraint on variance**

$$
\begin{aligned}
\text{min} \quad & \sum_{k=1}^{K} C_k N_k, \\
\text{subject to} \quad & \mathbb{V}\left[A^{\mathrm{MF}}\right] = \epsilon_{\mathrm{tar}}^2, \\
& -N_1 \le 0, \quad N_{k-1} - N_k \le 0, \;\; k = 2\dots, K, \\
& N_1, \dots, N_K \in \mathbb{R}, \\
& \alpha_2, \dots, \alpha_K \in \mathbb{R}.
\end{aligned}
$$

MFMC Optimal Sample Allocation

Theorem (Original problem – Constraint on budget)

Consider an ensemble of K models $\{u_{h,k}\}_{k=1}^{K}$ each characterized by the standard deviation σ_k of its output, the correlation coefficient $\rho_{1,k}$ with the highest-fidelity model $u_{h,1}$, and the computational cost per sample evaluation C_k. Define $\Delta_k = \rho_{1,k}^2 - \rho_{1,k+1}^2$ for $k = 1, \ldots, K$, with $\rho_{1,K+1} = 0$. Assume the following conditions hold

$$(i)\quad \textit{Correlation monotonicity}: \quad |\rho_{1,1}| > \cdots > |\rho_{1,K}|,$$

$$(ii)\quad \textit{Cost-correlation ratio}: \quad \frac{\Delta_k}{C_k} > \frac{\Delta_{k-1}}{C_{k-1}}, \quad k = 2, \ldots, K.$$

Under these assumptions, the solution to the original optimization problem yields optimal weights $\alpha_k^* = \frac{\rho_{1,k}\sigma_1}{\sigma_k}$. define an intermediate vector $\boldsymbol{r}^* = [r_1, \ldots, r_k]^T$, then $\boldsymbol{r}^*$ and the real-valued sample sizes N_k^*

$$r_k^* = \sqrt{\frac{C_1\Delta_k}{C_k\Delta_1}}, \quad N_1^* = \frac{p}{\sum_{k=1}^{K} C_k r_k^*}, \quad N_k^* = N_1^* r_k^*, \quad \Rightarrow \quad N_k^* = \sqrt{\frac{\Delta_k}{C_k}} \frac{p}{\sum_{j=1}^{K} \sqrt{C_j\Delta_j}}.$$

The resulting MFMC estimator achieves a variance of

$$\mathbb{V}\left[A^{MF}\right] = \frac{\sigma_1^2}{p} \left(\sum_{k=1}^{K} \sqrt{C_k\Delta_k} \right)^2.$$

MFMC Optimal Sample Allocation

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\end{aligned}
$$

Under these assumptions, the solution to the original optimization problem yields optimal weights $\alpha_k^* = \frac{\rho_{1,k}\sigma_1}{\sigma_k}$. The real-valued sample sizes N_k^* and cost are

$$
N_k^* = \frac{\sigma_1^2}{\epsilon_{tar}^2}\sqrt{\frac{\Delta_k}{C_k}}\sum_{j=1}^{K}\sqrt{C_j\Delta_j}, \qquad \mathcal{W}^{MF} = \frac{\sigma_1^2}{\epsilon_{tar}^2}\left(\sum_{k=1}^{K}\sqrt{C_k\Delta_k}\right)^2.
$$

- Our formulation yields the **same real-valued solution** as the original problem when using the same budget p or variance constraint ϵ_{tar}^2.

Summary for MFMC formulations

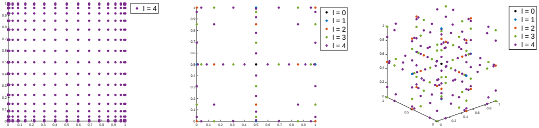
	Original	Modified MFMC (due to decimal sample size btw $0 \sim 1$)	Ours
$\mathbb{V}\left[A^{\mathrm{MF}}\right]$	$\frac{\sigma_1^2}{p}\left(\sum_{k=1}^{K}\sqrt{C_k\Delta_k}\right)^2$	$\sigma_1^2\sum_{k=1}^{K}\frac{\Delta_k}{N_k}$	$\epsilon_{\mathrm{tar}}^2$
$\mathcal{W}^{\mathrm{MF}}$	p	$\leq p$	$\frac{\sigma_1^2}{\epsilon_{\mathrm{tar}}^2}\left(\sum_{k=1}^{K}\sqrt{C_k\Delta_k}\right)^2$
N_k	$\sqrt{\frac{\Delta_k}{C_k}}\frac{p}{\sum_{j=1}^{K}\sqrt{C_j\Delta_j}}$	While there is $1 \leq j \leq K-1$ such that $N_j < 1$, set $N_j \leftarrow 1$ and update $\sqrt{\frac{\Delta_k}{C_k}}\frac{p-\sum_{i=1}^{j}C_i}{\sum_{i=j+1}^{K}\sqrt{C_i\Delta_i}}, \quad j+1 \leq k \leq K.$	$\frac{\sigma_1^2}{\epsilon_{\mathrm{tar}}^2}\sqrt{\frac{\Delta_k}{C_k}}\sum_{j=1}^{K}\sqrt{C_j\Delta_j}$
Rounding	Floor	Ceil+Floor	Ceil

Anthony Gruber, Max Gunzburger, Lili Ju, Zhu Wang. A multifidelity Monte Carlo method for realistic computational budgets. Journal of Scientific Computing, 94(1):Paper No. 2, 18, 2023.

- Build surrogate via **Sparse Grid Stochastic Collocation**.
  - **Idea:** Select a special set of current $\{\boldsymbol{\omega}^{(k)}\}_{1\leq k\leq n_{sc}}$ in the parameter space. For each $\boldsymbol{\omega}^{(k)}$, evaluate the nonlinear solver to yield the realization $\{\psi_h^{(k)}\}$. An interpolation (surrogate) is then constructed to mimic the original nonlinear function with

$$\widehat{\psi_h}(\cdot,\boldsymbol{\omega}) = \sum_k \psi_h^{(k)}(\cdot) L_{\boldsymbol{\omega}^{(k)}}(\boldsymbol{\omega}).$$

  - **Sparse grids**:



Left to right: Full tensor grid 2d, level 4. Chebyshev sparse grids for 2d and 3d from level 0 to level 4.

Theorem: Interpolation error bound in L_∞ norm

$$\|f - \mathscr{S}(f)\|_\infty = \mathscr{O}\left(N^{-k}\cdot|\log N|^{(k+2)(d-1)+1}\right)$$

N: # of collocation nodes, d: dimension, k: measure of smoothness of ψ wrt $\boldsymbol{\omega}$.

  - **Software:** MATLAB SPINTERP package – A.Klimke.

SPINTERP, piecewise multilinear hierarchical sparse grid interpolation, http://people.math.sc.edu/burkardt/msrc/spinterp/spinterp.html, 2007.

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Parameter Estimation

- Parameters to estimate: C_k, σ_k, $\rho_{1,k}$.
- Sample standard deviation σ_k and cost C_k: unbiased, converge quickly.
- **Sample correlation coefficient** $\rho_{1,k}$: biased, skewed distribution mean $|\rho_{1,k}| \to 1$. Requires careful pilot sampling to avoid efficiency loss.

$$\widehat{\rho}_{1,k} = \frac{\sum_{i=1}^{Q} \left\langle u_1^{(i)} - A_{1,Q}^{\mathrm{MC}},\ u_k^{(i)} - A_{k,Q}^{\mathrm{MC}} \right\rangle_U}{\sqrt{\sum_{i=1}^{Q} \left\| u_1^{(i)} - A_{1,Q}^{\mathrm{MC}} \right\|_U^2} \sqrt{\sum_{i=1}^{Q} \left\| u_k^{(i)} - A_{k,Q}^{\mathrm{MC}} \right\|_U^2}}$$

Q: number of pilot samples,
$u_k^{(i)}$: i-th realization of the k-th model.

- **Dynamic Pilot Sampling Strategy**
    - Sequentially increase the pilot sample size based on cost sensitivity until the relative update falls below a prescribed threshold.
    - Ensures accuracy and efficiency comparable to fixed large sample-size pilot run.

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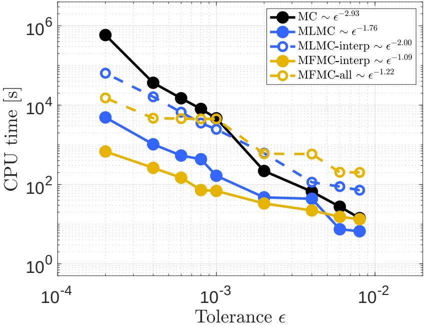
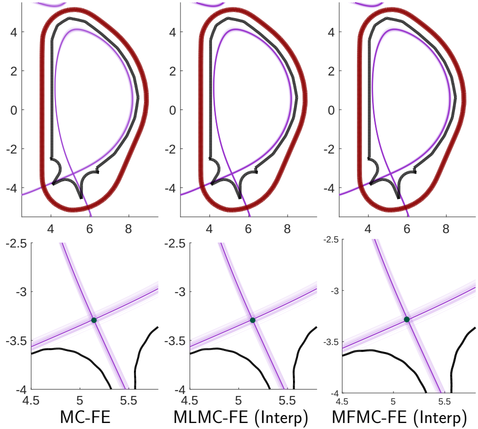
▷ **Numerical Results**

- **Efficiency:** Multi-fidelity Monte Carlo reduces the computational cost of Monte Carlo with direct non-linear solve by up to $\mathbf{10^3}$ ($\sim \epsilon^{-1}$). However, when accounting for **upfront costs** such as surrogate construction and parameter estimation, the overall gain is limited to a factor of **50**.



Numerical results

- **Accuracy:** Plasma boundary and geometric descriptors from MFMC sampling exhibit behavior consistent with those from MC and MLMC when interpolated onto a common mesh.



Thank You $|\neg\_\neg|$