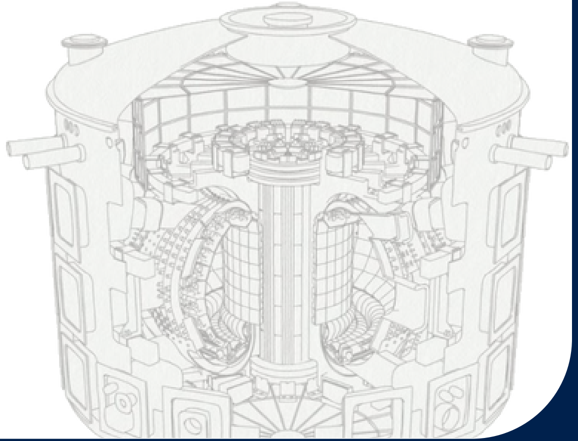
Ioannis Mavrogiannis

Surrogate Model Comparison for Uncertainty Quantification of Heating for Nuclear Fusion Plasma through Neutral Beam Injection

Joint Work With:

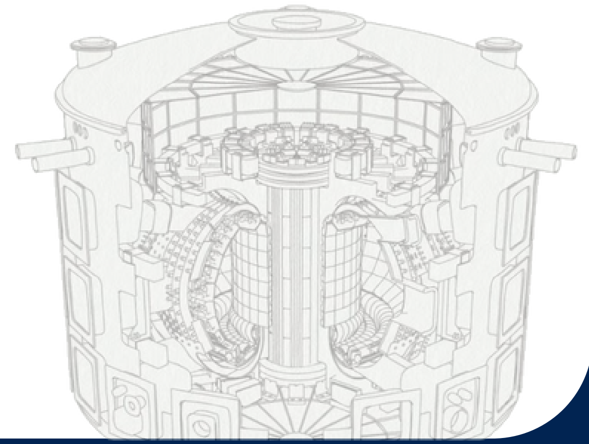
Mitra Fouladirad
David Zarzoso Fernandez



Piraeus, Greece, September 17, 2025

The Need for Uncertainty Quantification

Can we use numerical codes to *Predict Reality ?*



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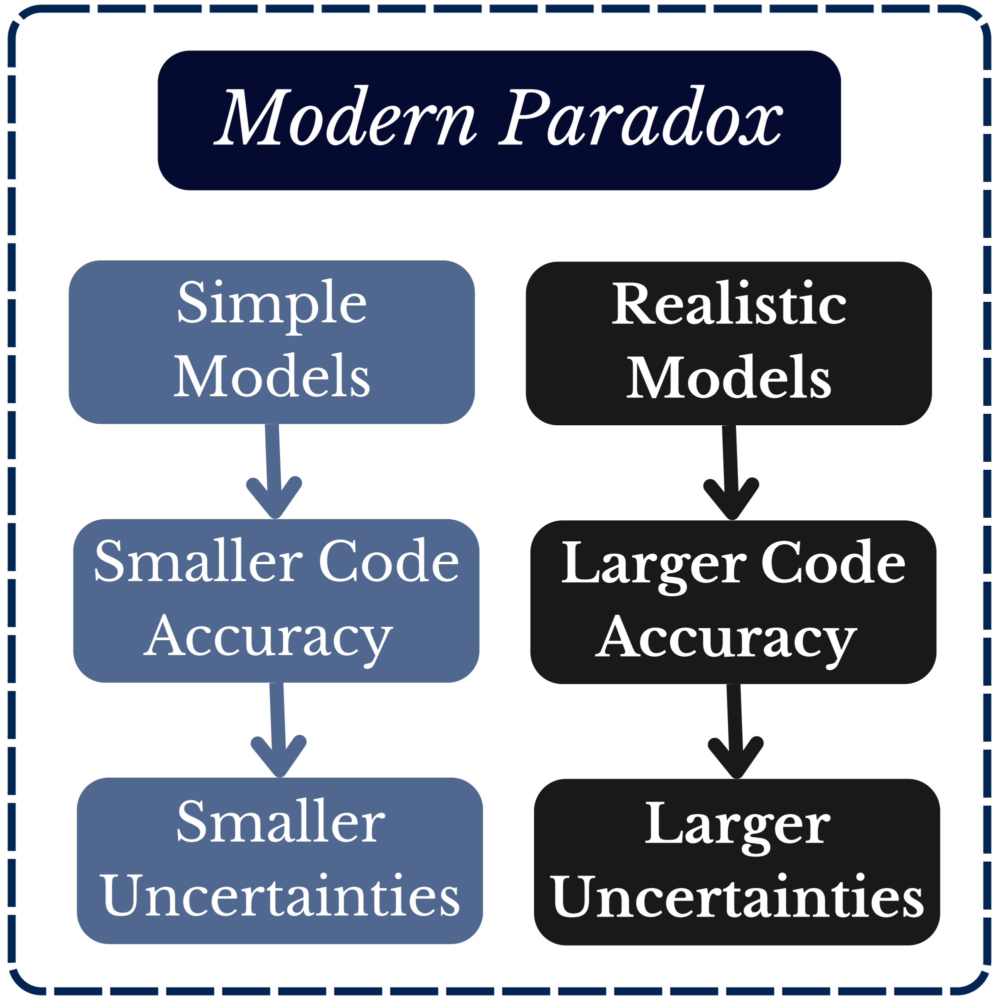
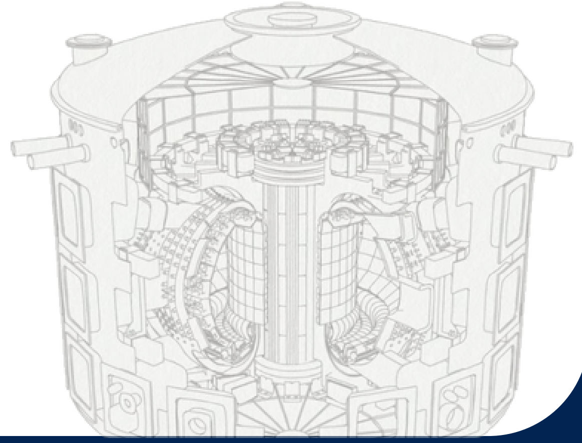




The Need for Uncertainty Quantification

Can we use numerical codes to *Predict Reality ?*

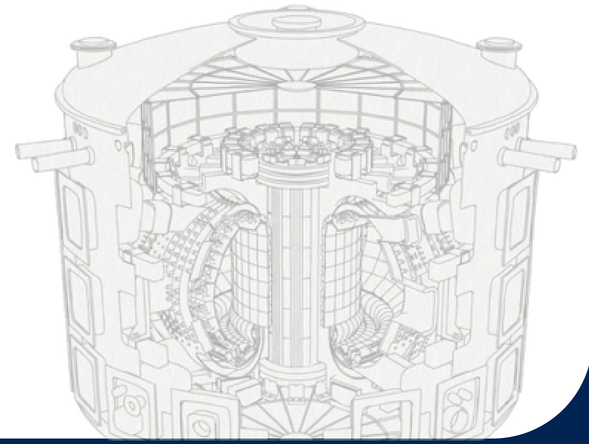
Modern Paradox

Simple Models	**Realistic Models**
↓	↓
Smaller Code Accuracy	**Larger Code Accuracy**
↓	↓
Smaller Uncertainties	**Larger Uncertainties**

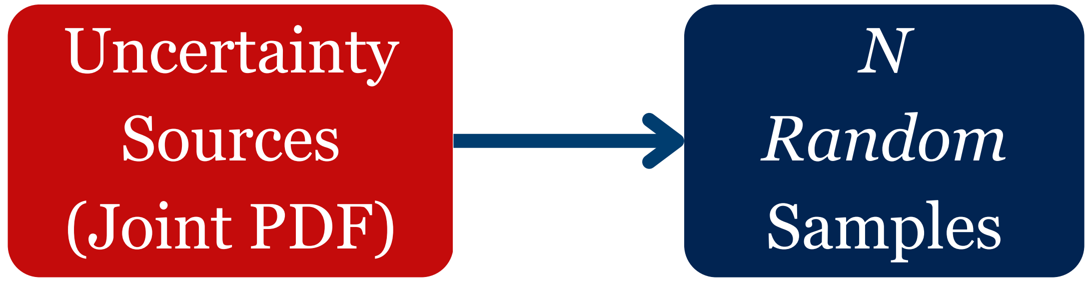
How does **Uncertainty** in

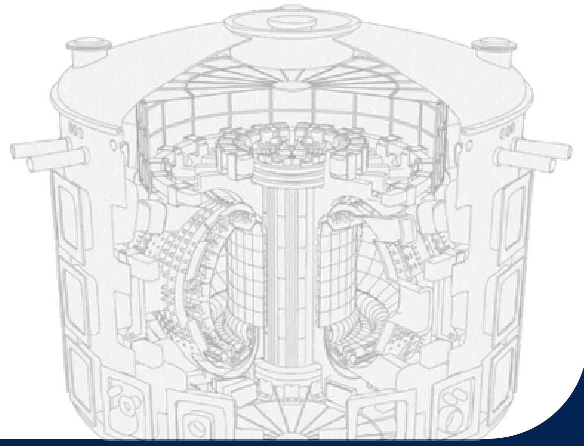
plasma structure & ionization

influence NBI shine-through losses?



Uncertainty Quantification Framework





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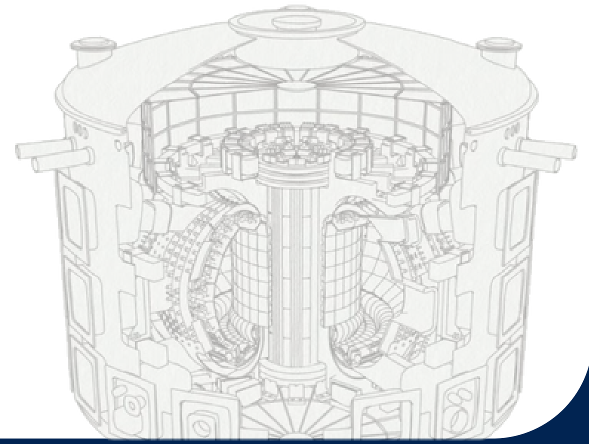

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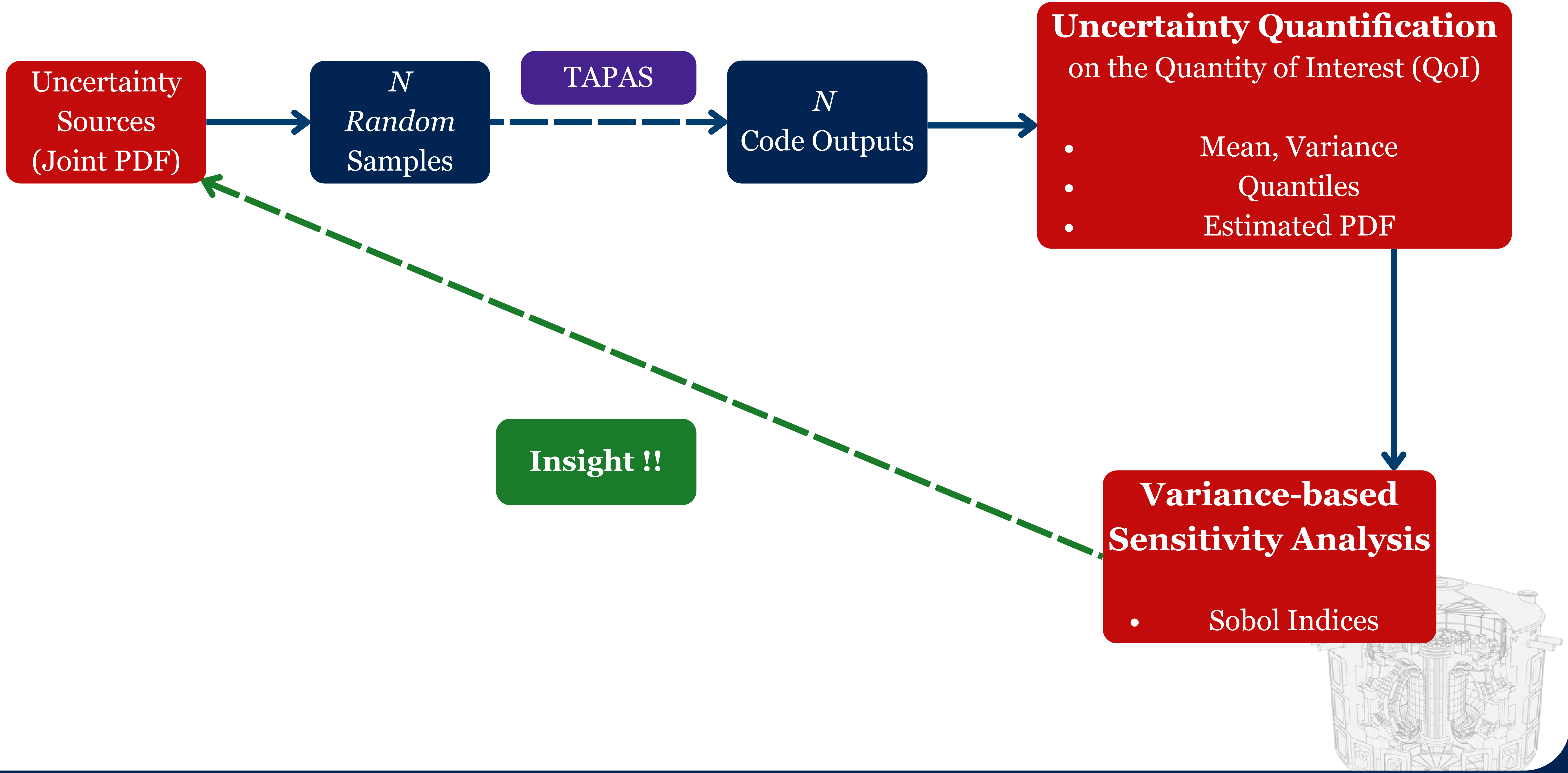

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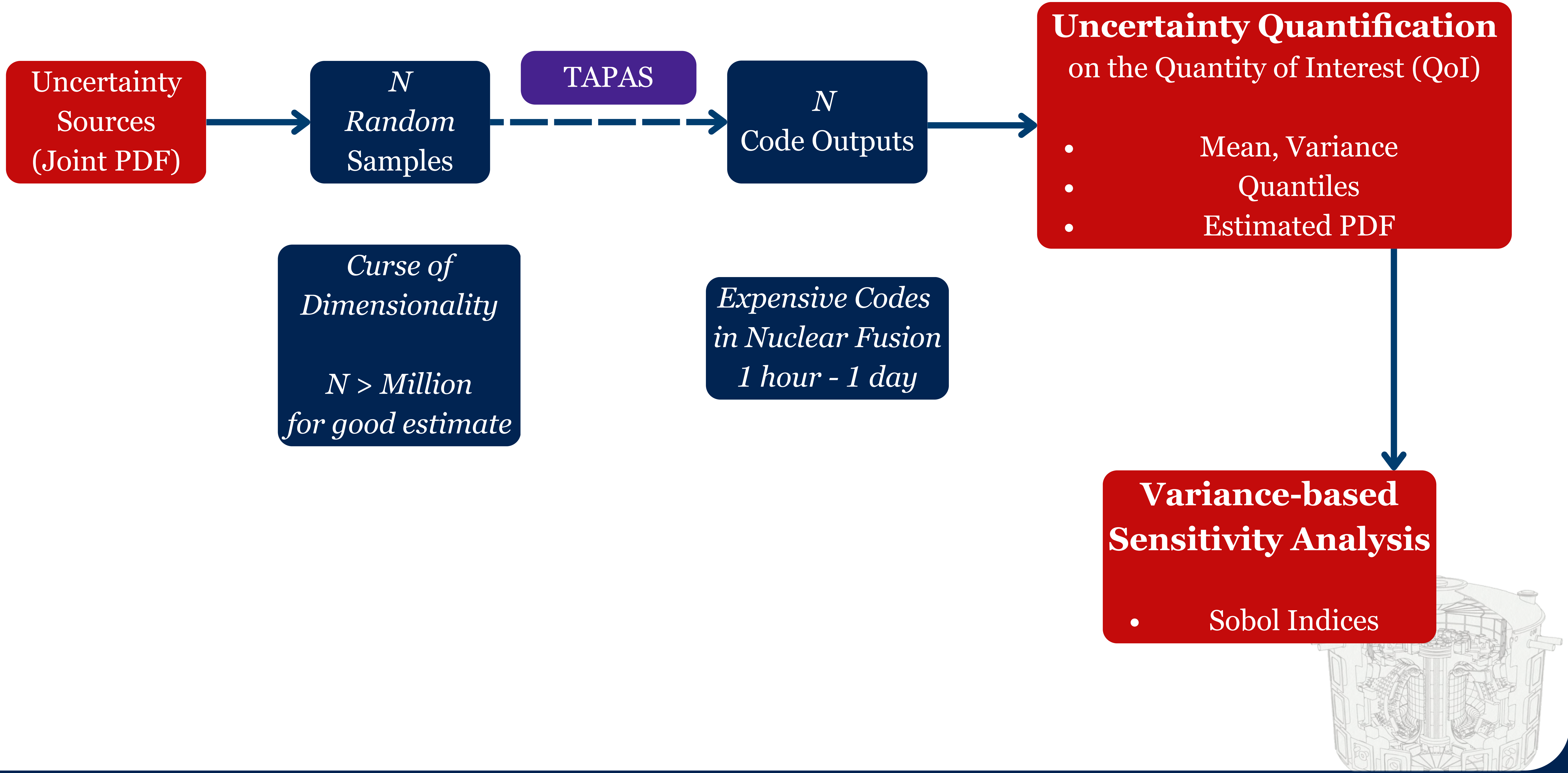

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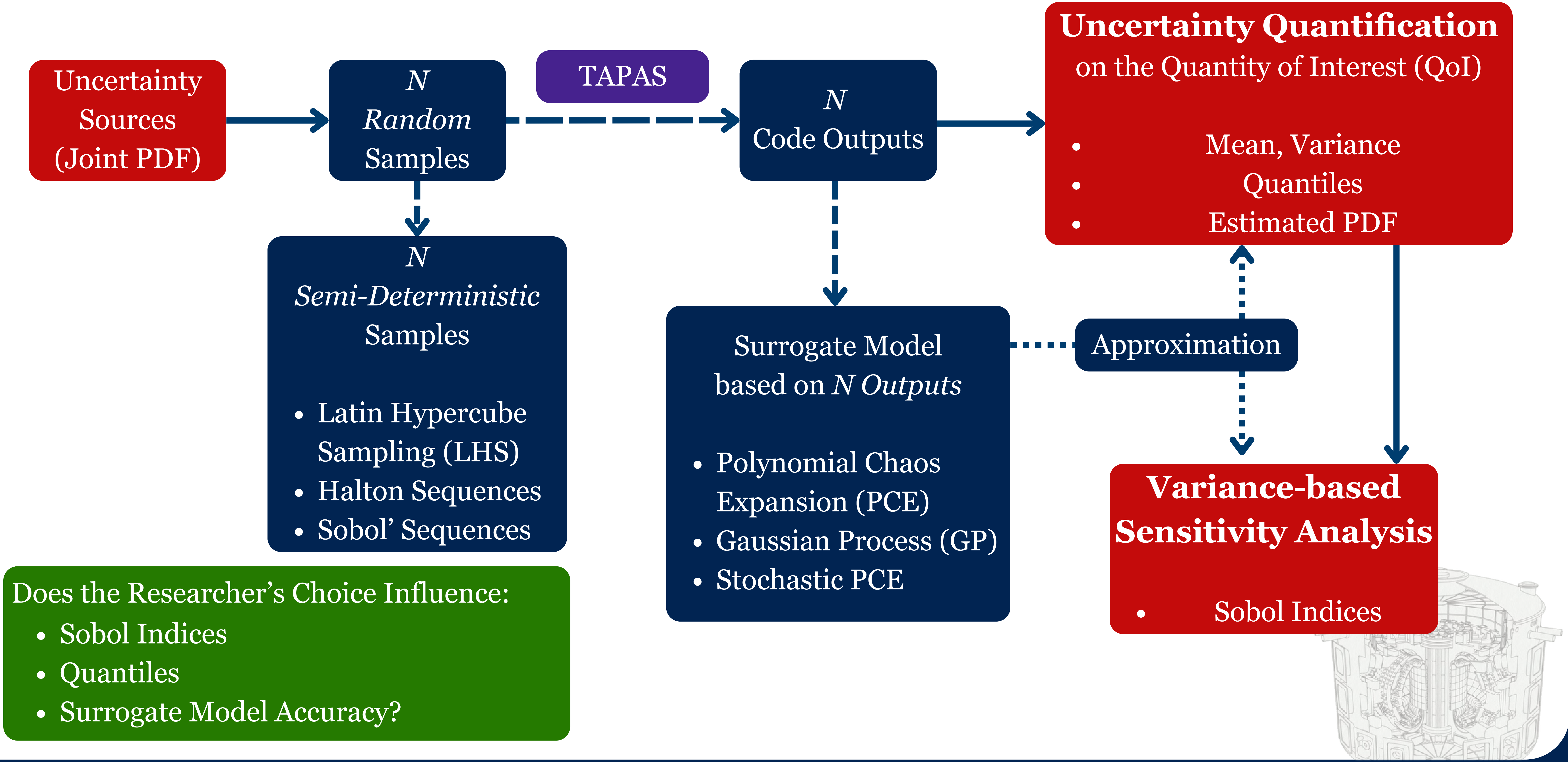


Nuclear Fusion Powers the Stars

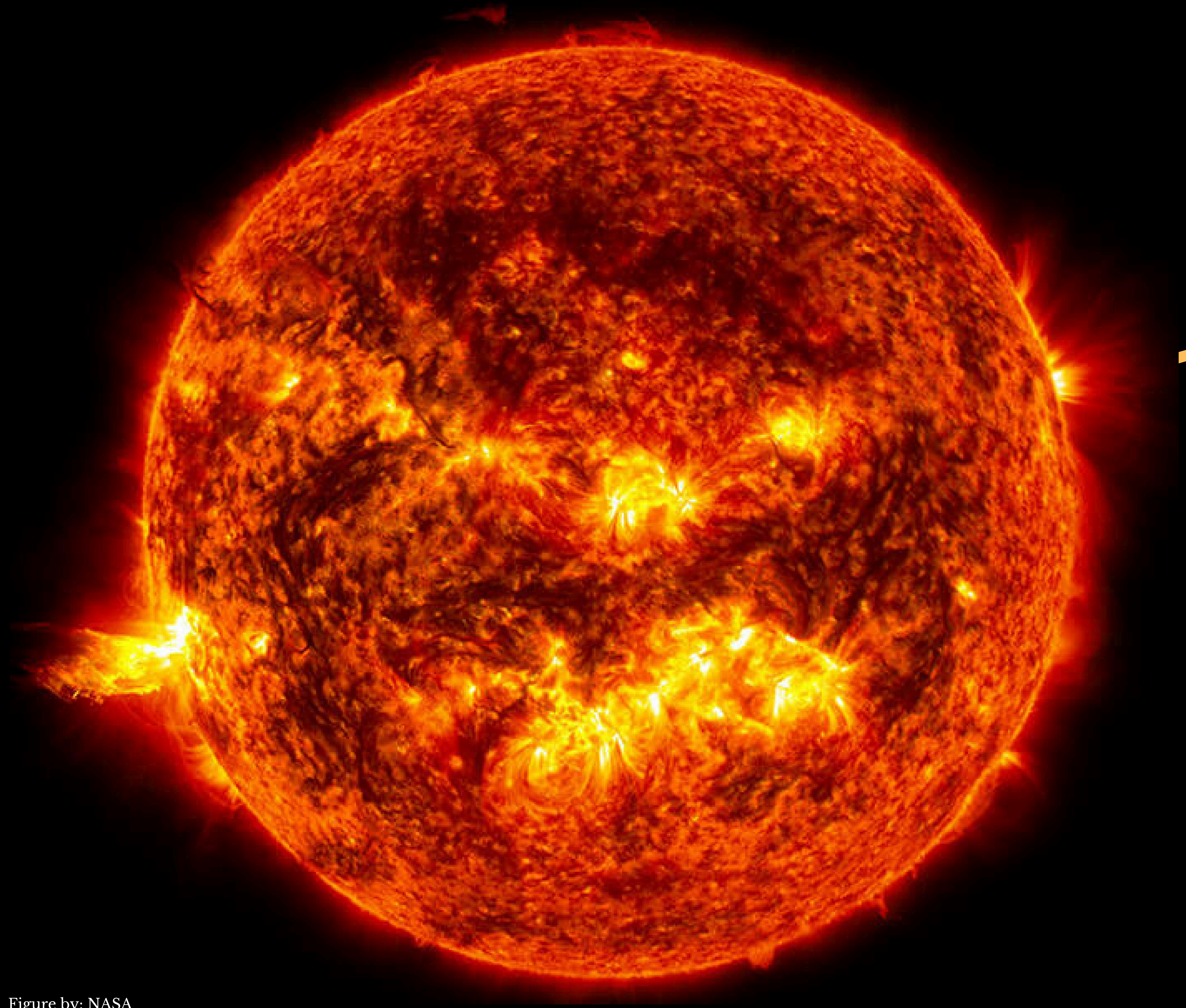


Figure by: NASA

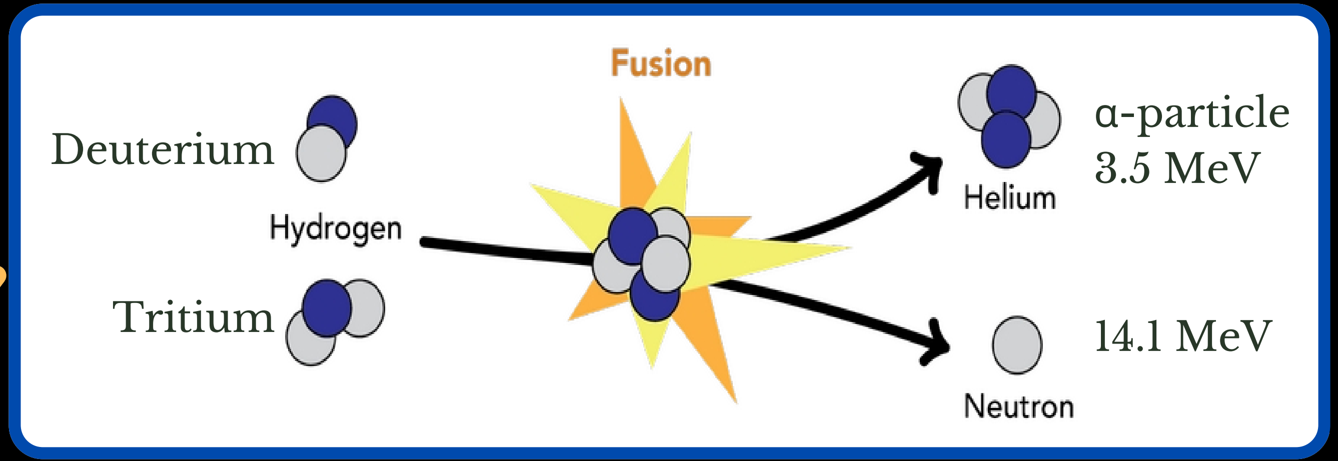


Figure by: Aparna Nathan

Sun Core Temperature = 15 Million C°

Tokamak: a “different” kind of sun on Earth

Tokamak

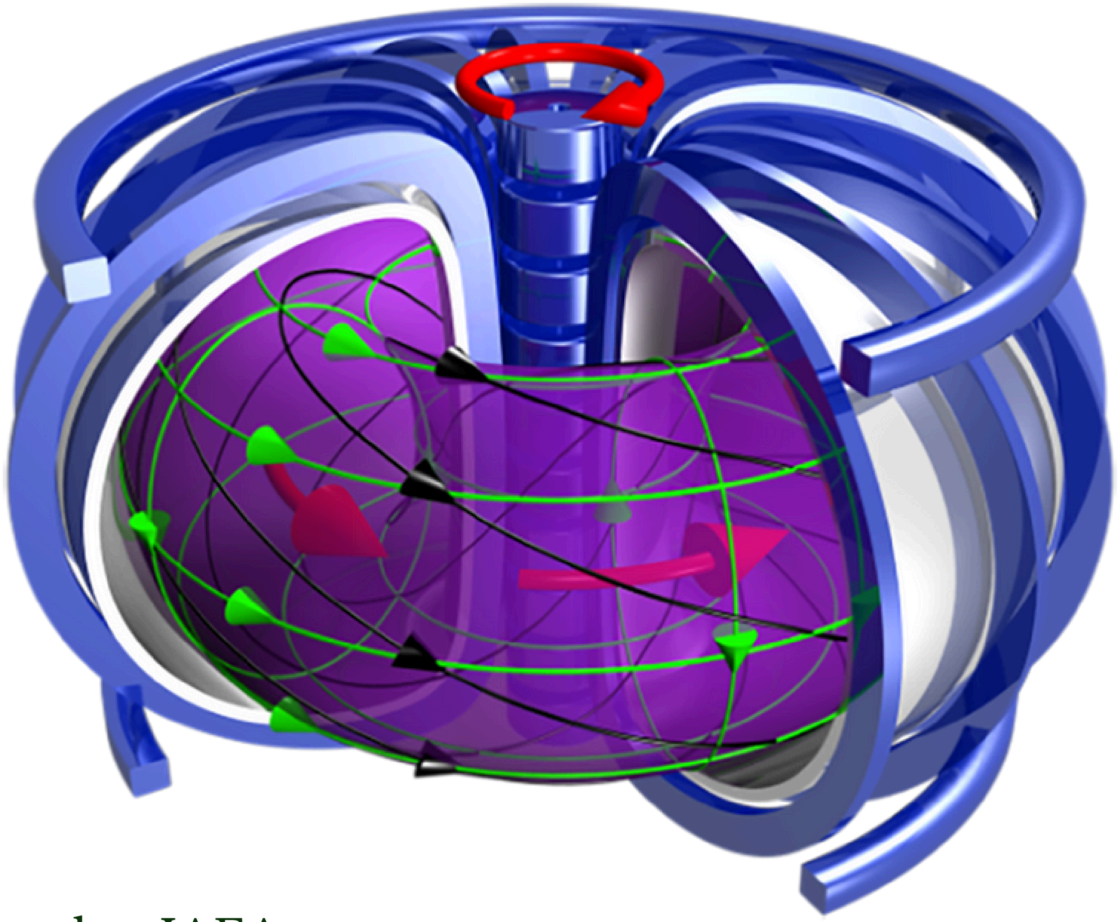


Figure by: IAEA

- Vacuum Chamber
- Helical Magnetic Field Confines the Plasma
- Plasma requires Extreme Temperatures for Fusion to occur

Tokamak: a “different” kind of sun on Earth

Tokamak Plasma Temperature = 10 X 

How to increase the plasma temperature?

Tokamak

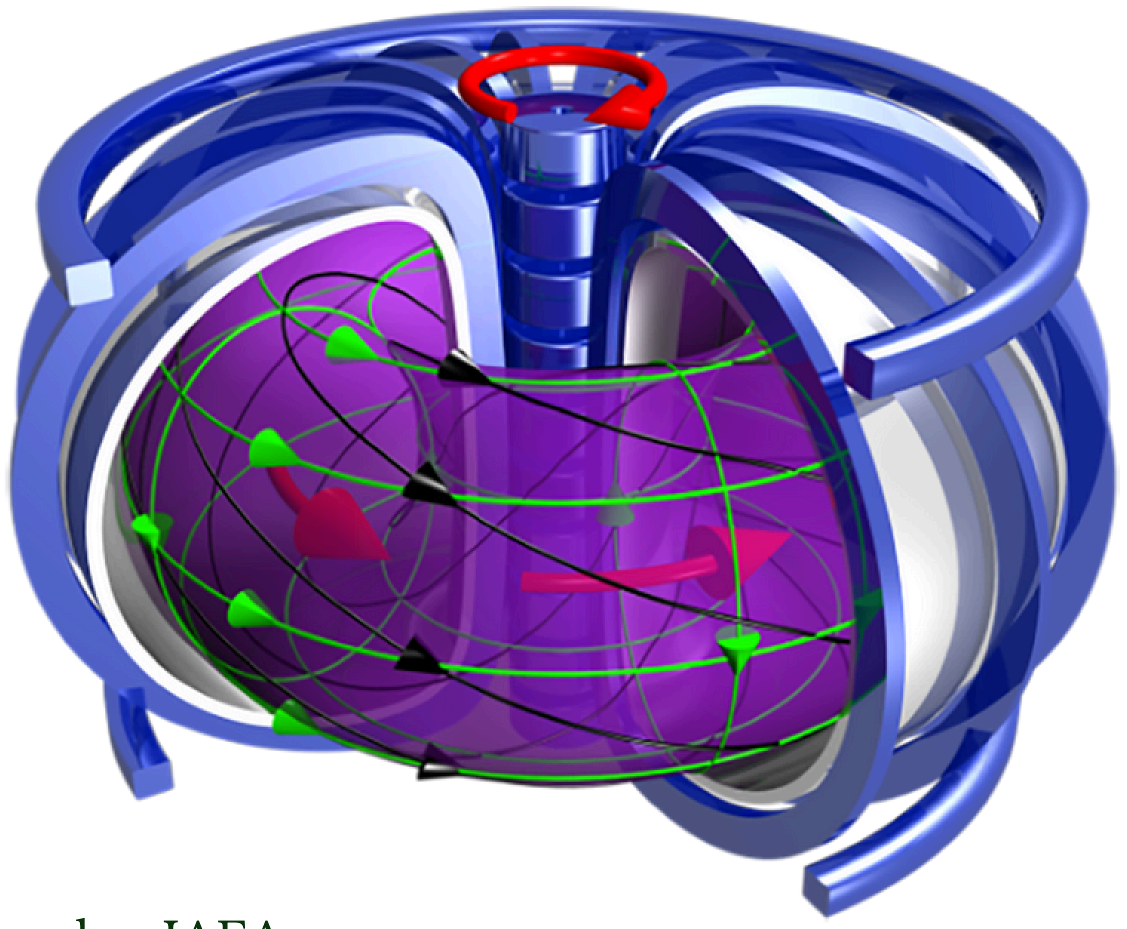
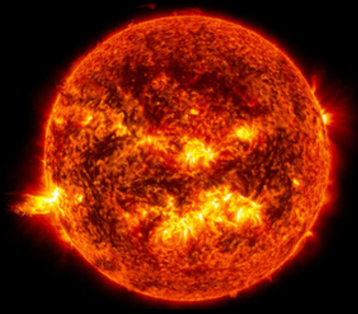
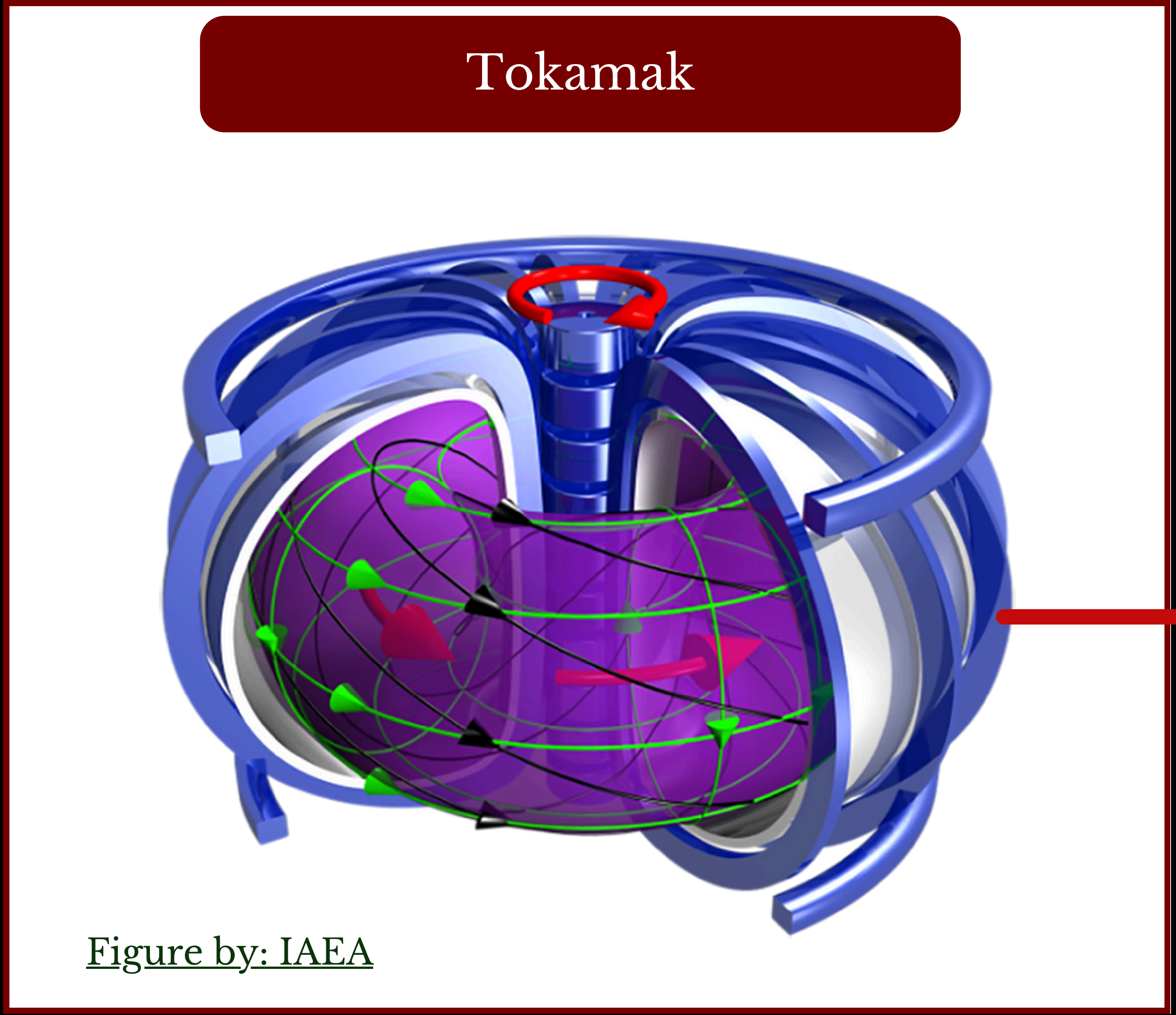


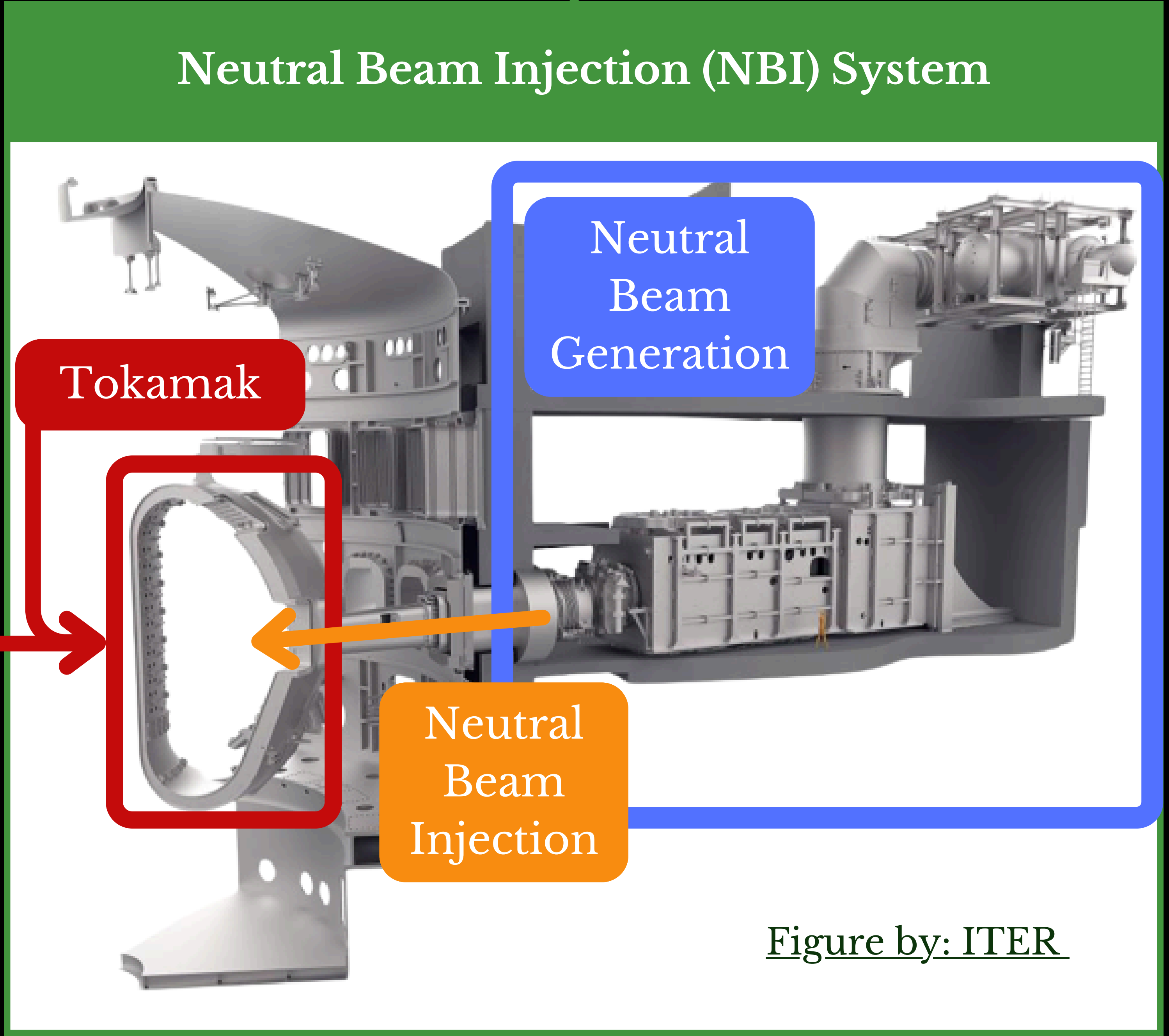
Figure by: IAEA

Neutral Beam Injection : Heating the Plasma

Tokamak Plasma Temperature = 10 X 

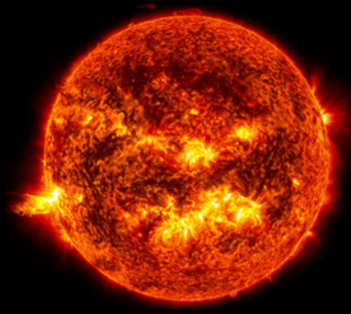
How to increase the plasma temperature?





Neutral Beam Injection : Heating the Plasma

Tokamak Plasma Temperature = 10 X



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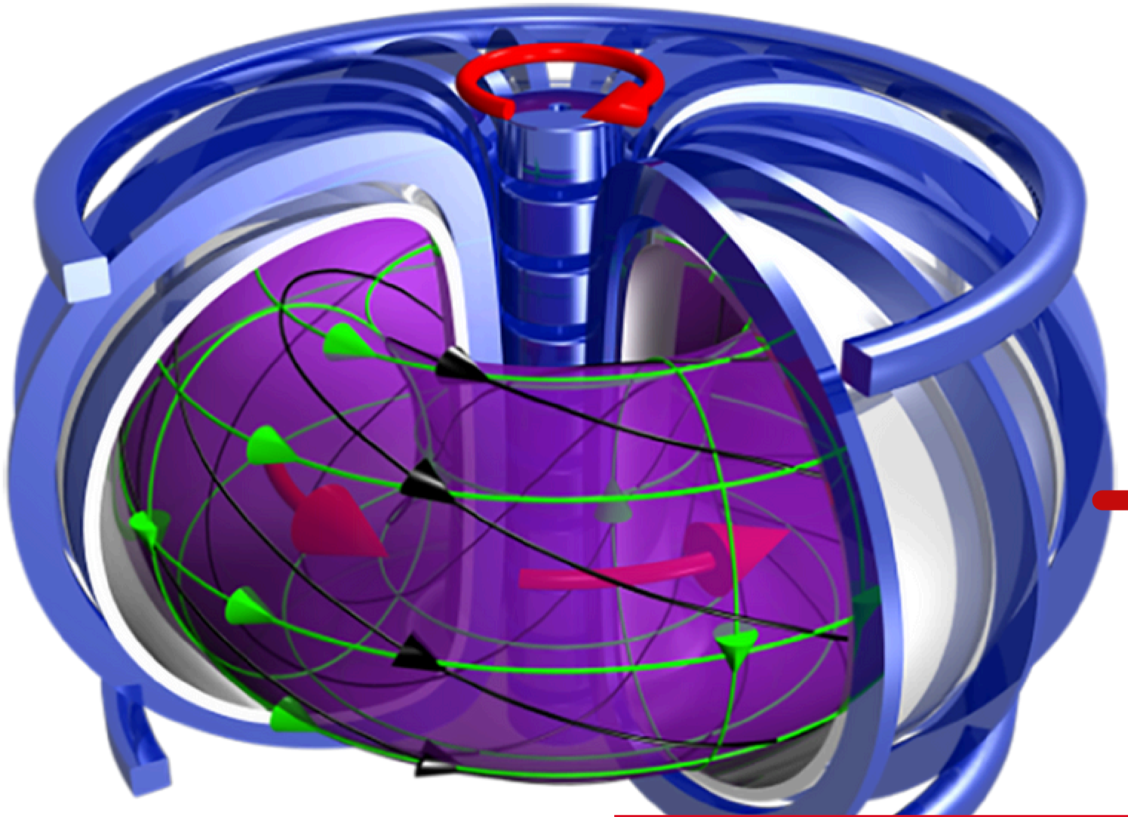
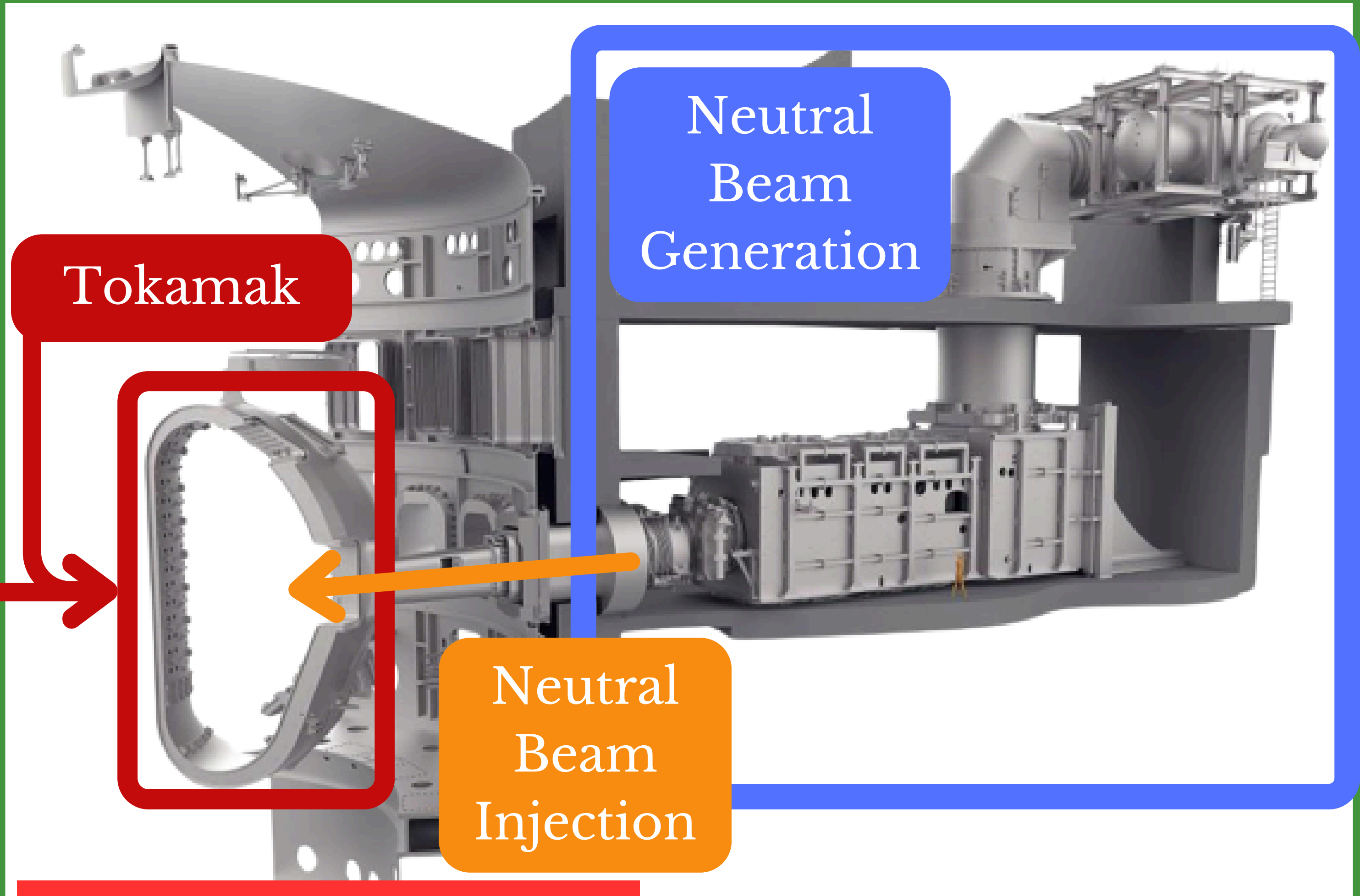


Figure by: IAEA

How to Simulate with a Computer ?

Neutral Beam Injection (NBI) System



How to Simulate with a Computer ?

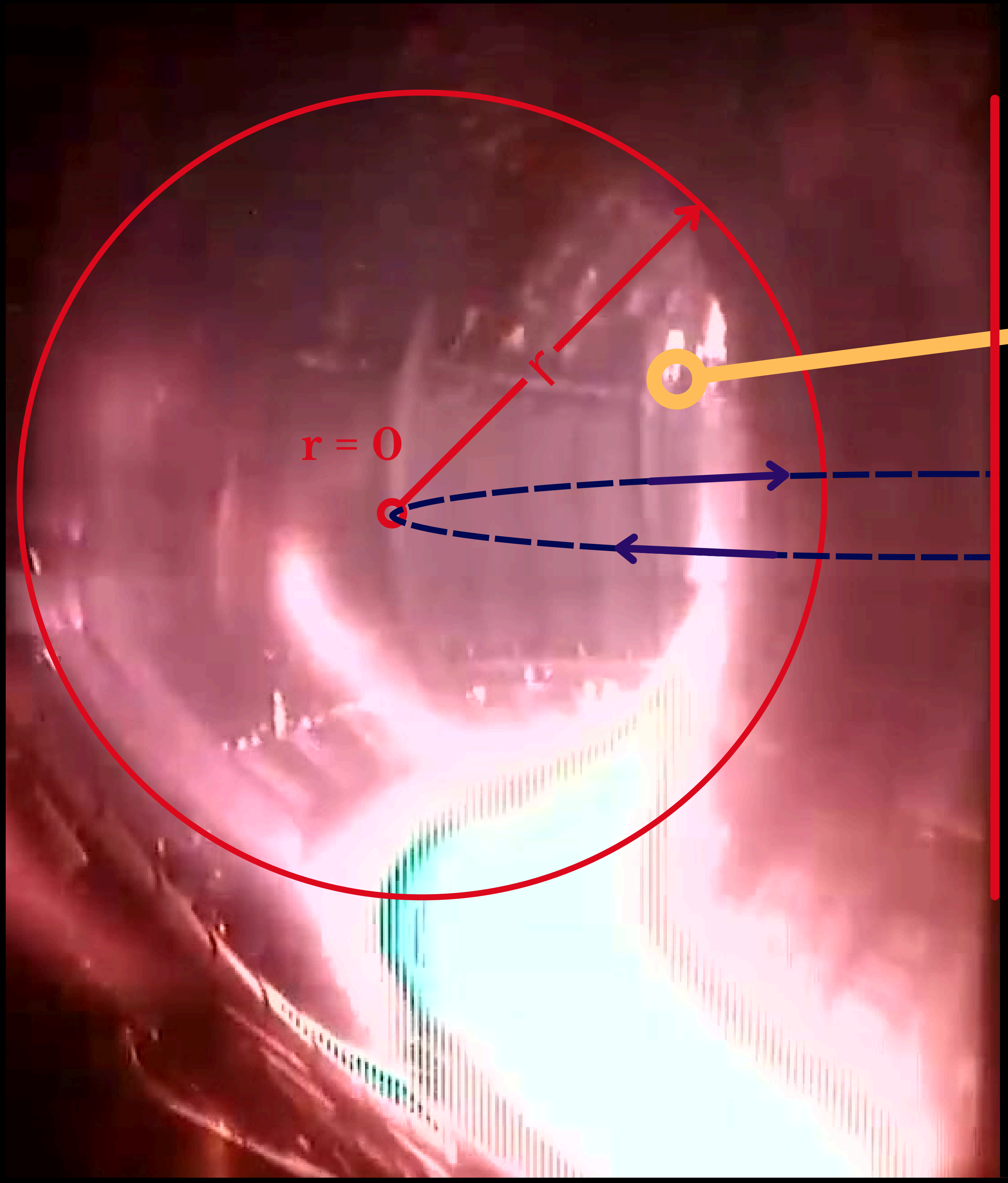
Figure by: ITER

Tokamak Plasma Modeling from Data

A pulse of plasma in the JET machine

Video by: UK Atomic Energy Authority

Tokamak Plasma Modeling from Data



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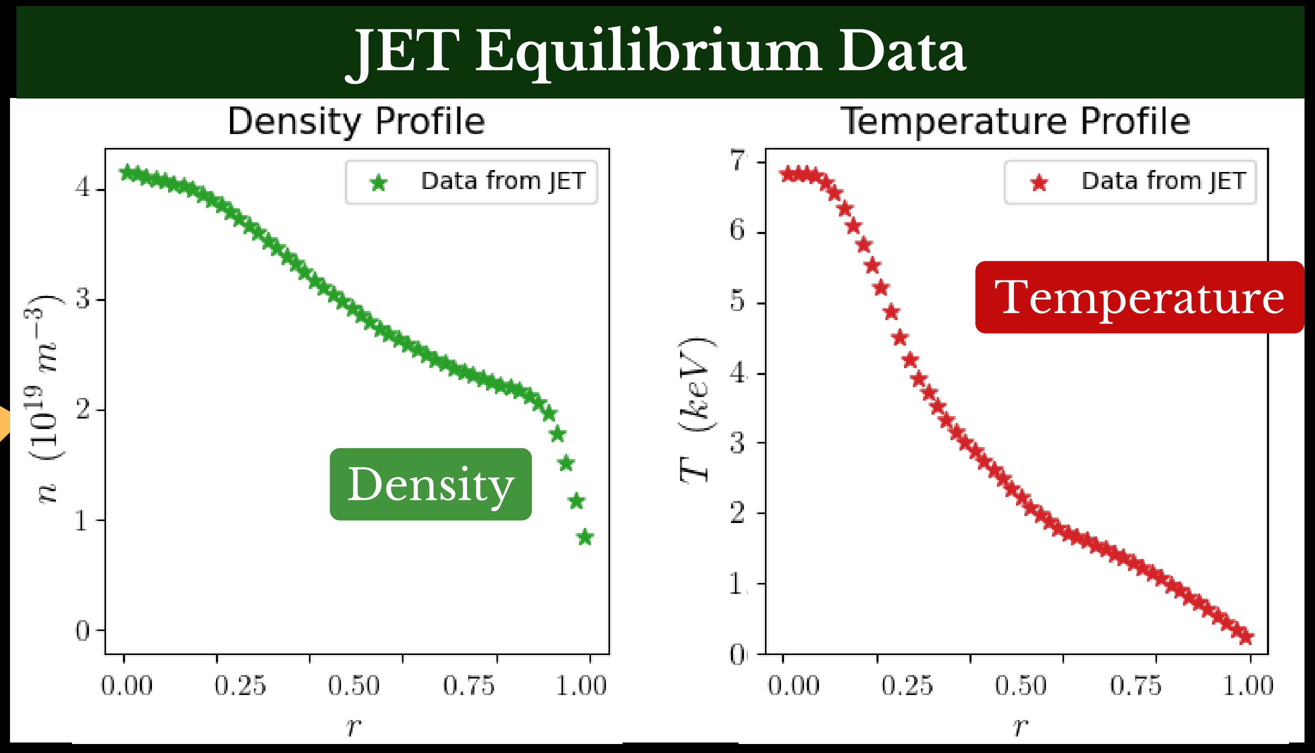
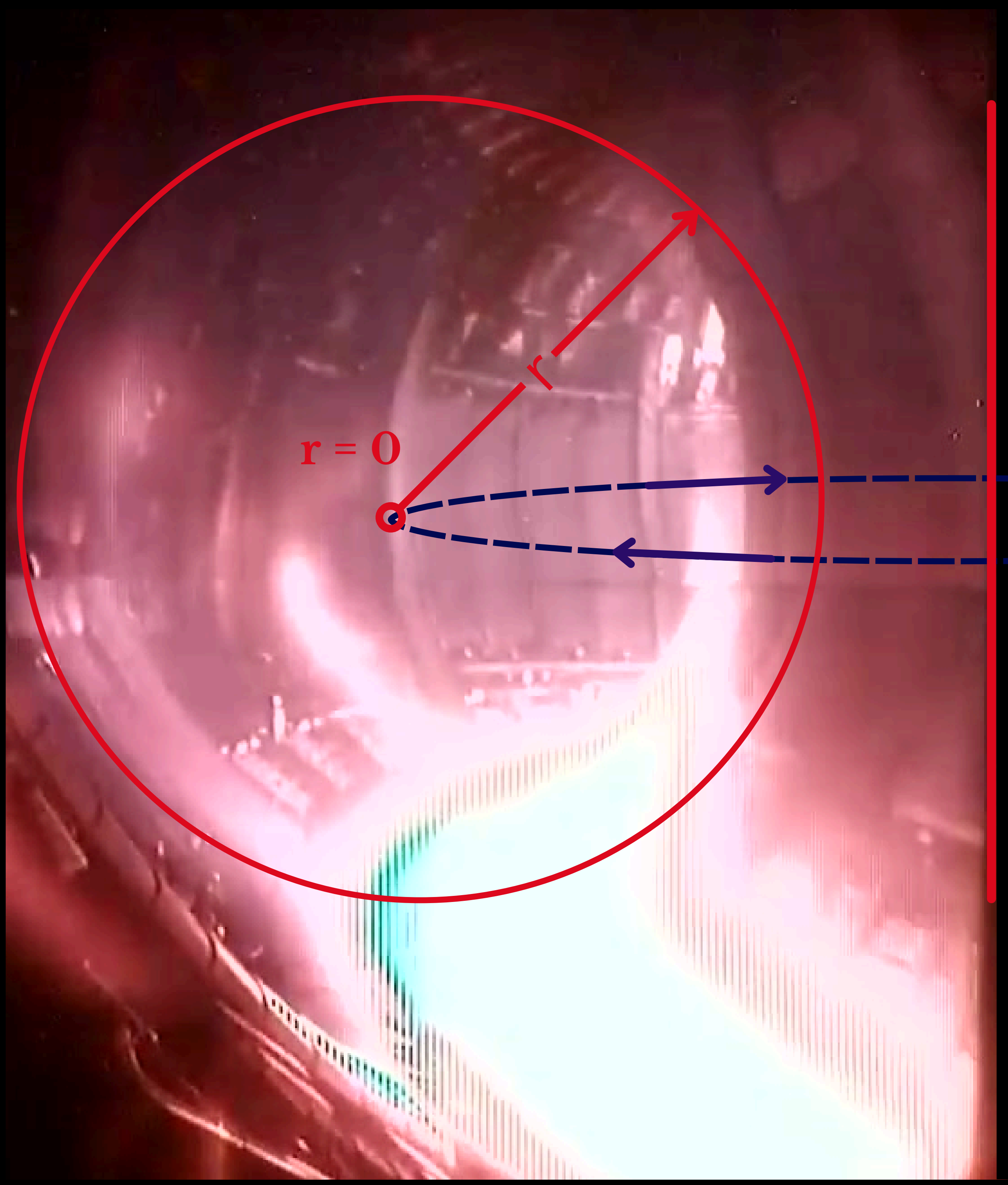


Generally a lot of measurement uncertainties…

Interpretable Fitting of the Data



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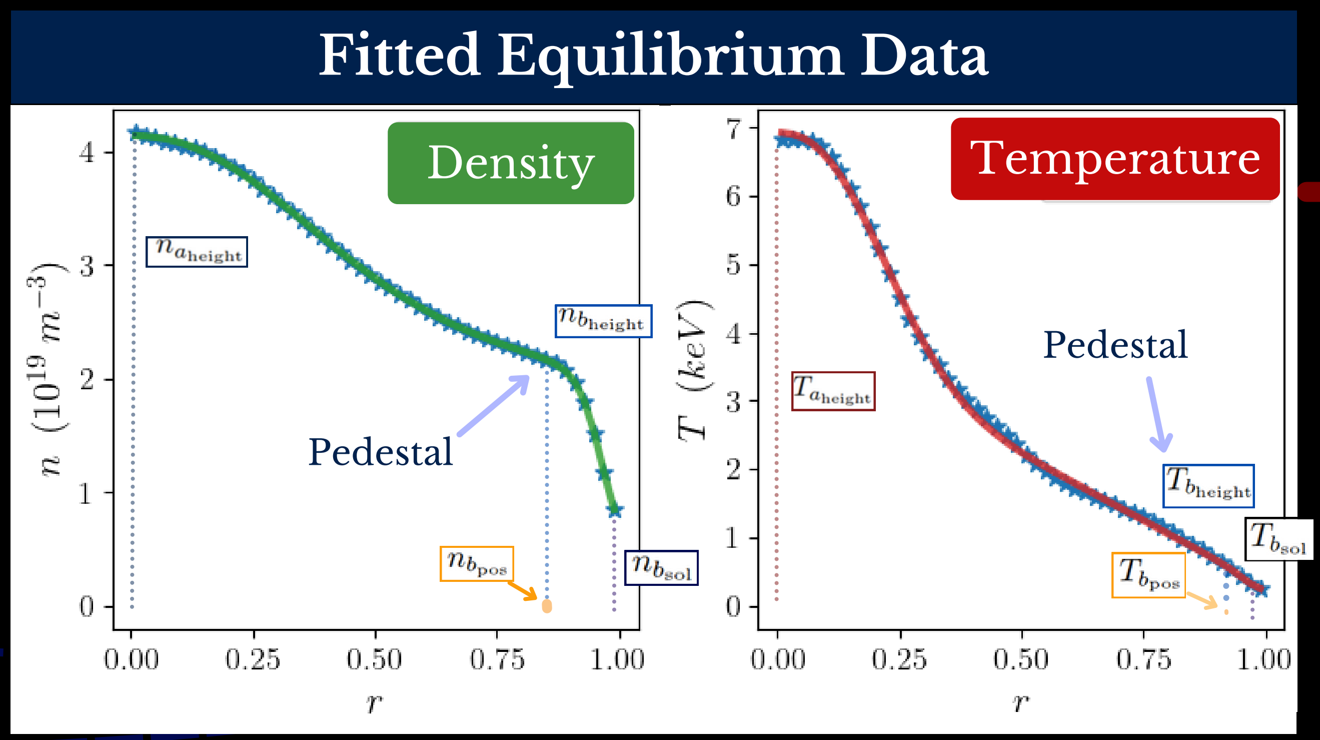
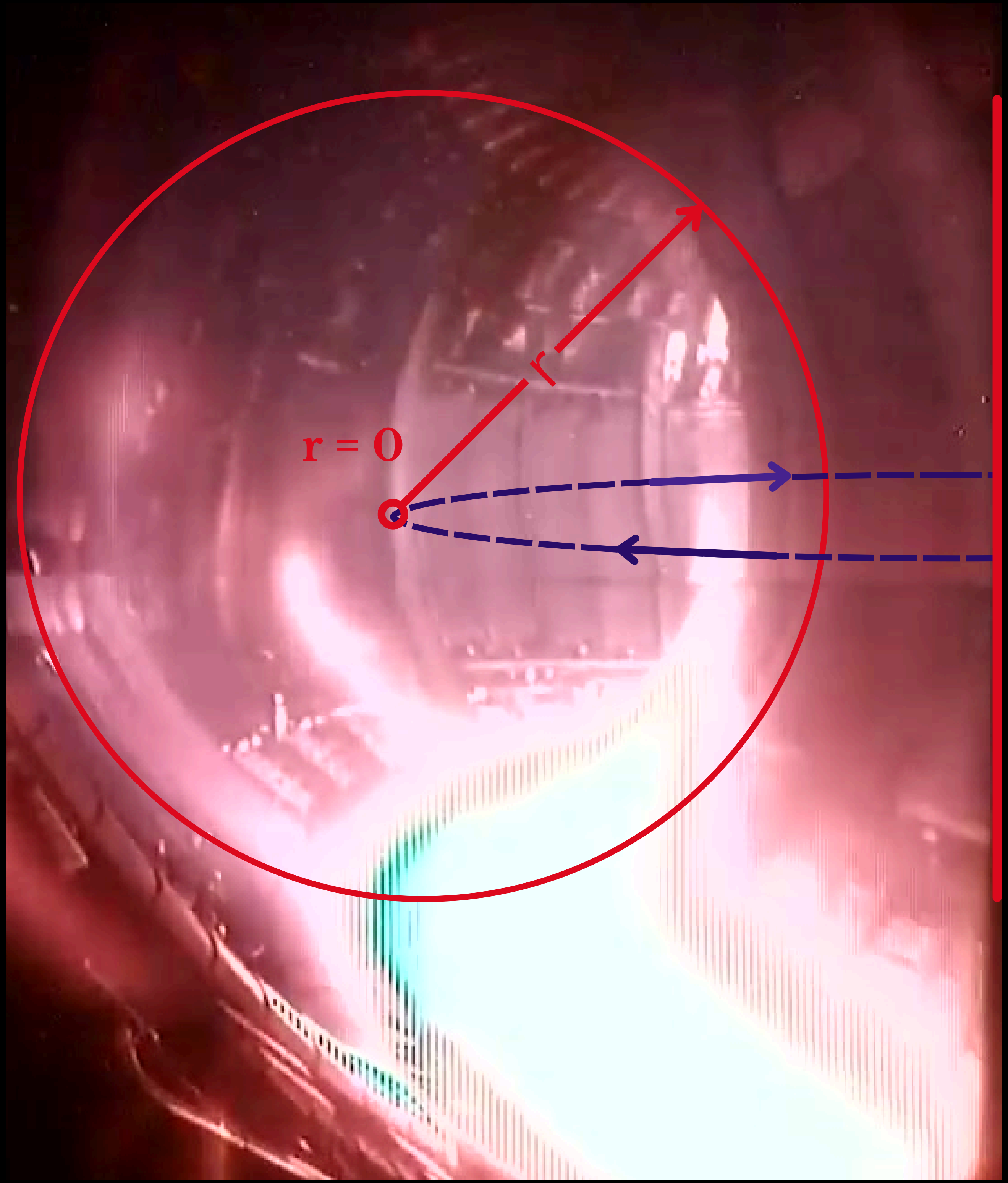


Fit with Interpretable Function F

- $F_{\text{full}}(r) = F_{\text{ped}}(r) + \left[a_{\text{height}} - F_{\text{ped}}(r)\right] \cdot e^{\left(r/a_{\text{width}}\right)^{a_{\text{exp}}}}$ [Stefanikova]
- $F_{\text{ped}}(r) = \left[1 + \text{mtanh}\left(\frac{b_{\text{pos}} - r}{2 \cdot b_{\text{width}}},\ b_{\text{slope}}\right)\right] \cdot \frac{b_{\text{height}} - b_{\text{SOL}}}{2} + b_{\text{SOL}}$
- $\text{mtanh}(x, b_{\text{slope}}) = \frac{(1 + x \cdot b_{\text{slope}})\, e^{x} - e^{-x}}{e^{x} + e^{-x}}$ [Groebner & Carlstrom]

Interpretable Fitting of the Data



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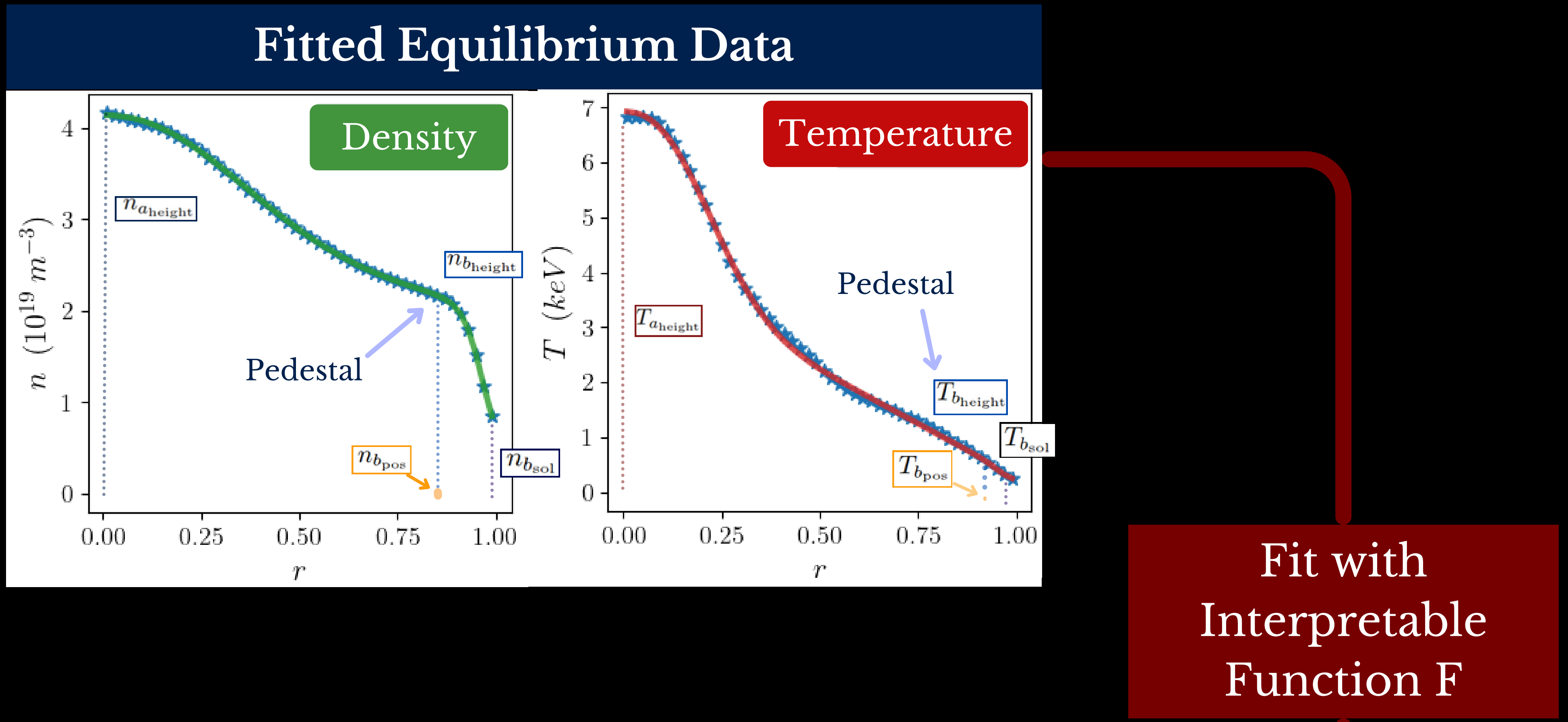

Fitted Parameters

Density	Temperature
$n_{a,\text{height}}$	$T_{a,\text{height}}$
$n_{a,\text{width}}$	$T_{a,\text{width}}$
$n_{a,\text{exp}}$	$T_{a,\text{exp}}$
$n_{b,\text{pos}}$	$T_{b,\text{pos}}$
$n_{b,\text{height}}$	$T_{b,\text{height}}$
$n_{b,\text{SOL}}$	$T_{b,\text{SOL}}$
$n_{b,\text{width}}$	$T_{b,\text{width}}$
$n_{b,\text{slope}}$	$T_{b,\text{slope}}$

Uncertainty In each Parameter

16 Dimensions

Uncertainty Sources

	Parameter X_i	Units	Marginal pdf f_{X_i}
Ionization Cross-Section	σ_{ion}	10^{-16} cm^2	$\mathcal{N}(1.3745,\ 0.01188)$
	σ_{CX}	10^{-16} cm^2	$\mathcal{N}(0.09978, 0.0004)$
Density	$n_{a_{\text{height}}}$	m^{-3}	$\mathcal{U}(3.636,\ 4.636)$
	$n_{a_{\text{width}}}$	m / a	$\mathcal{U}(0.3197, 0.5197)$
	$n_{a_{\text{exp}}}$	–	$\mathcal{U}(1.089,\ 3.089)$
	$n_{b_{\text{pos}}}$	m / a	$\mathcal{U}(0.9165, 1.0165)$
	$n_{b_{\text{height}}}$	m^{-3}	$\mathcal{U}(1.742,\ 2.342)$
	$n_{b_{\text{sol}}}$	m^{-3}	$\mathcal{U}(0.098,\ 0.698)$
	$n_{b_{\text{width}}}$	m / a	$\mathcal{U}(0.0188, 0.0288)$
	$n_{b_{\text{slope}}}$	–	$\mathcal{U}(0.036,\ 0.076)$
Temperature	$T_{a_{\text{height}}}$	keV	$\mathcal{U}(5.92,\ 7.92)$
	$T_{a_{\text{width}}}$	m / a	$\mathcal{U}(0.201,\ 0.301)$
	$T_{a_{\text{exp}}}$	–	$\mathcal{U}(1.835,\ 2.835)$
	$T_{b_{\text{pos}}}$	m / a	$\mathcal{U}(0.874,\ 1.074)$
	$T_{b_{\text{height}}}$	keV	$\mathcal{U}(0.375,\ 0.395)$
	$T_{b_{\text{sol}}}$	keV	$\mathcal{U}(0.21,\ 0.23)$
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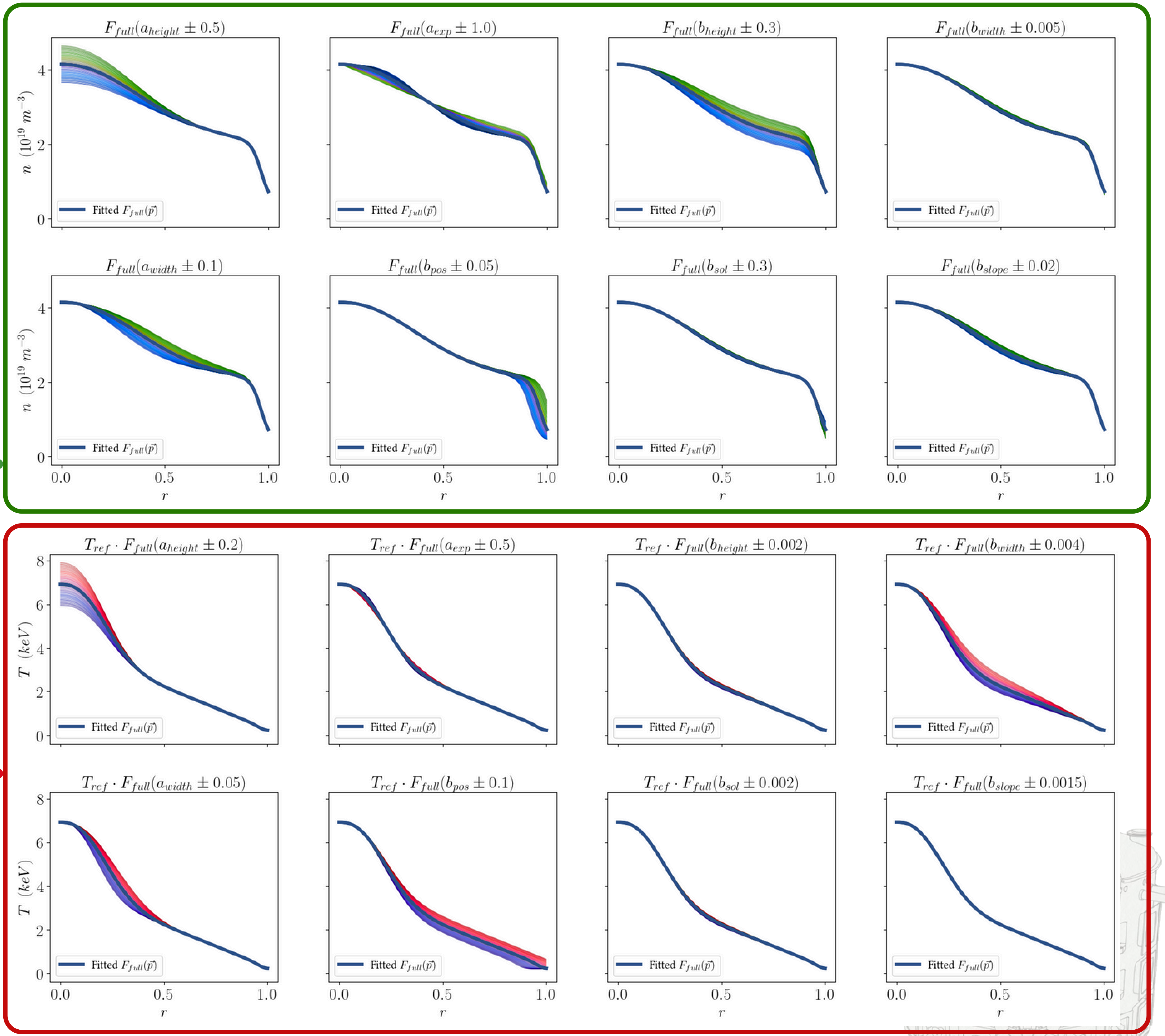

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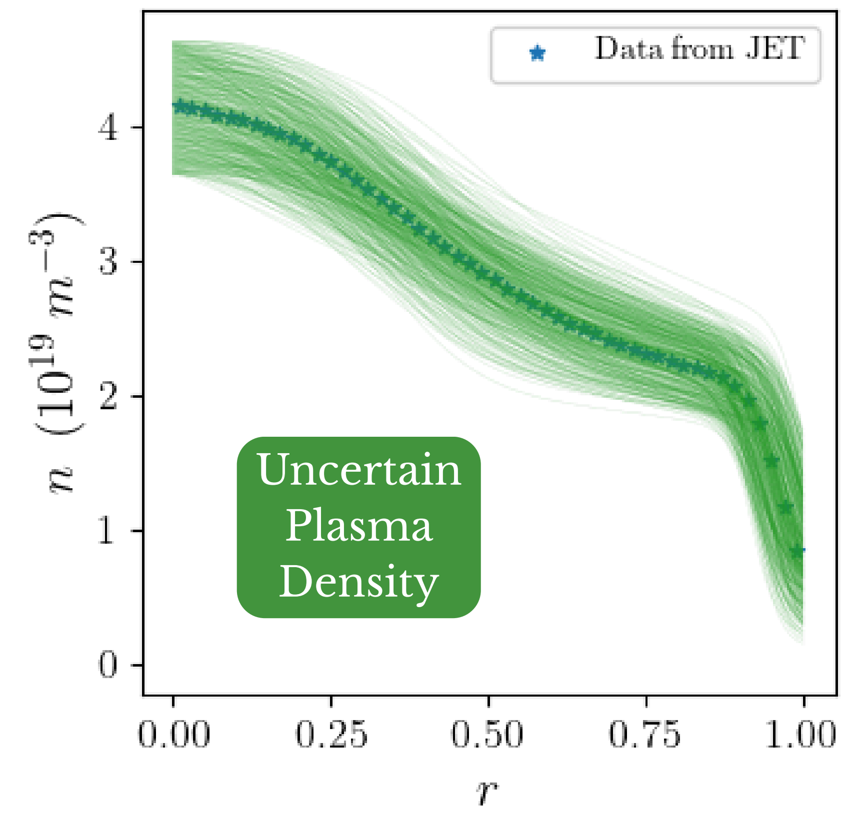
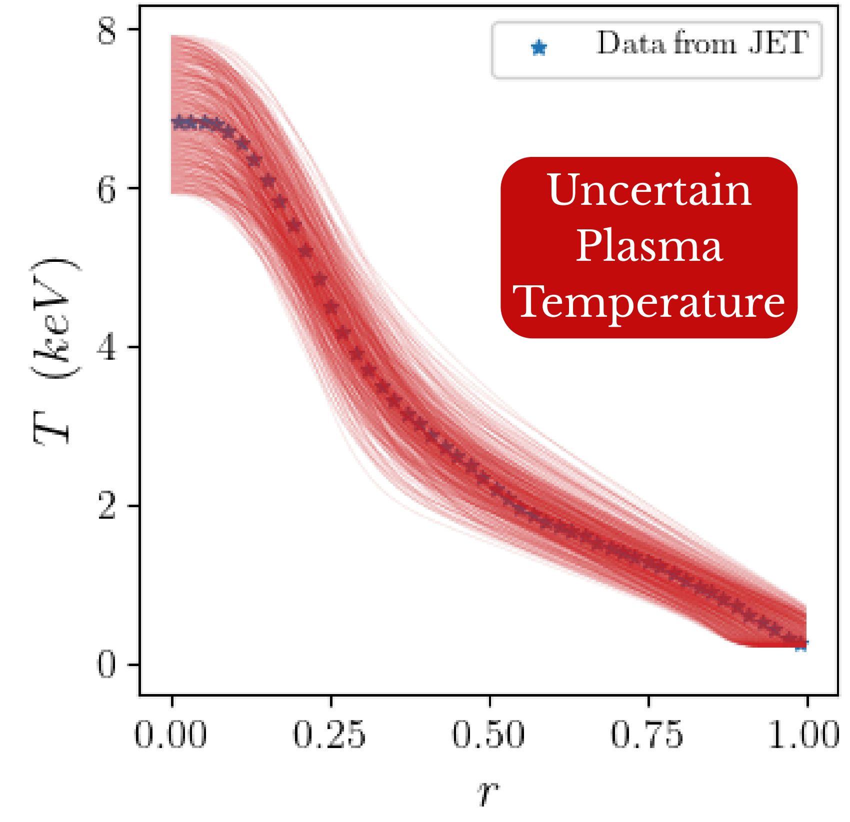
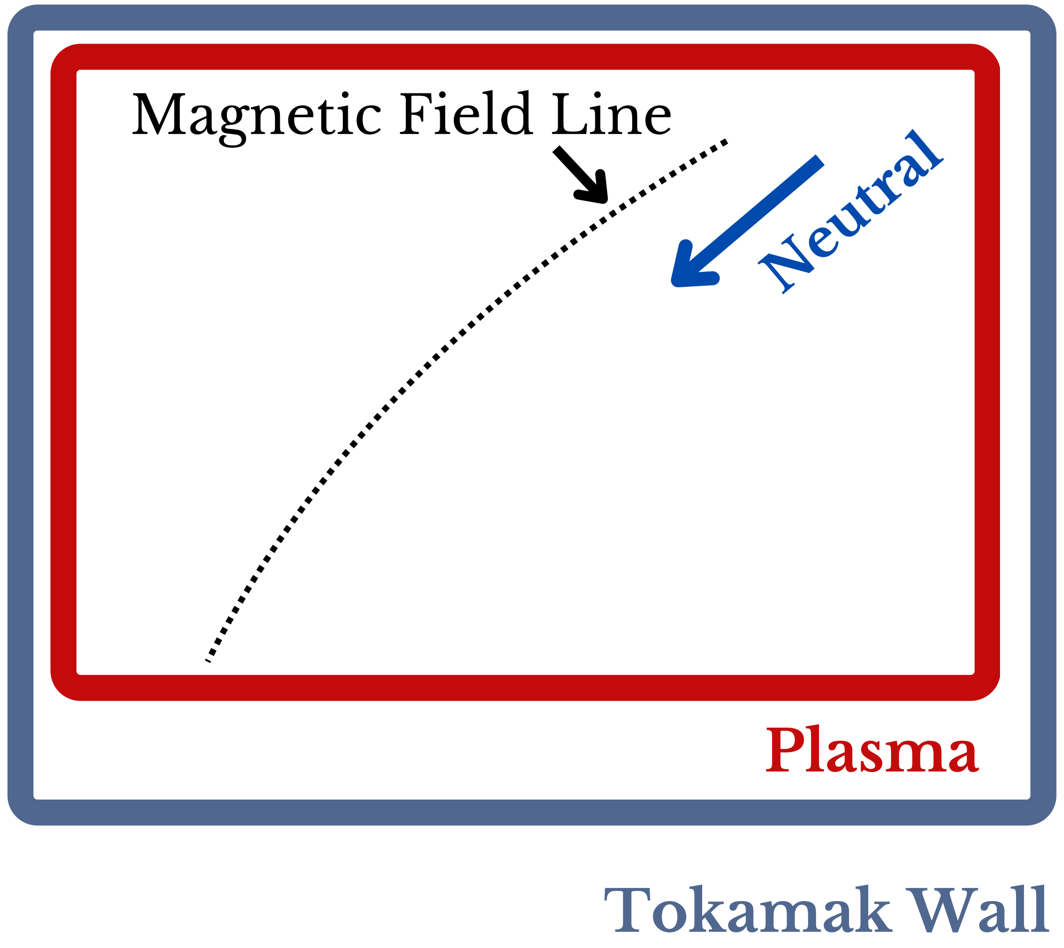


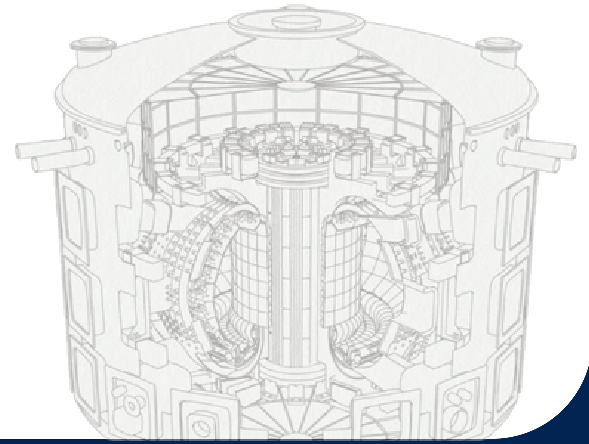
Today we only focus here



Modeling the NBI – Plasma Interaction

Ionization :
A particle gaining Charge





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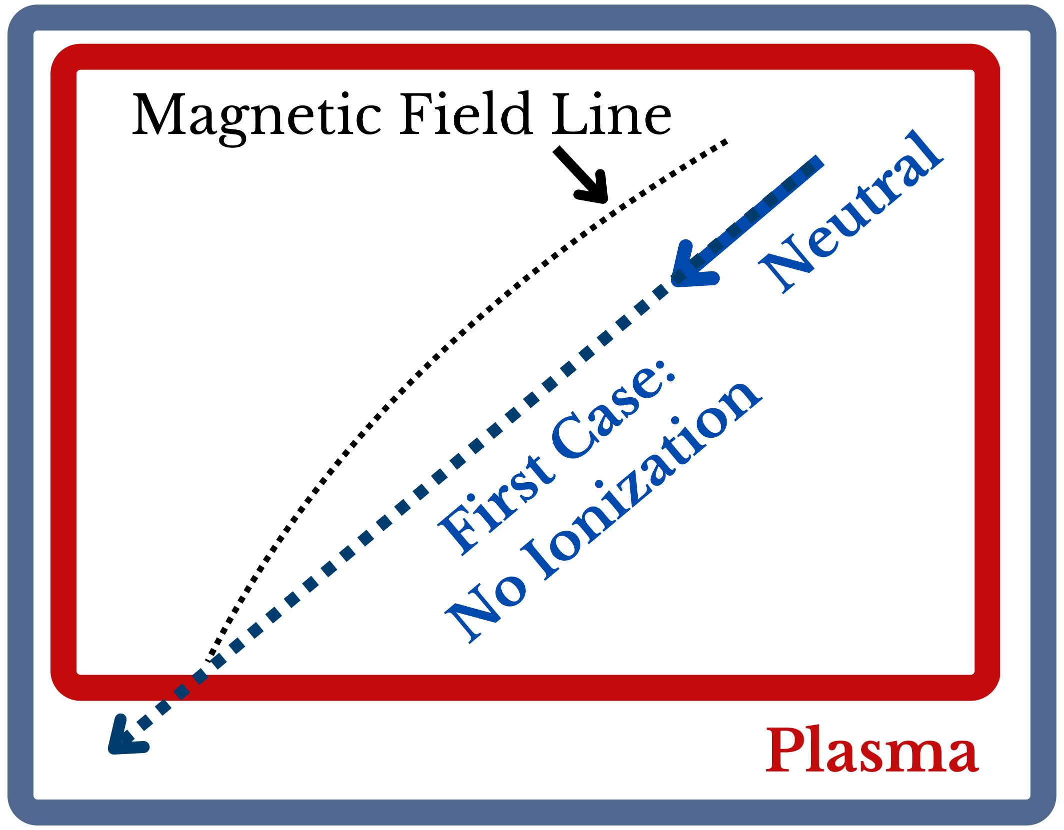
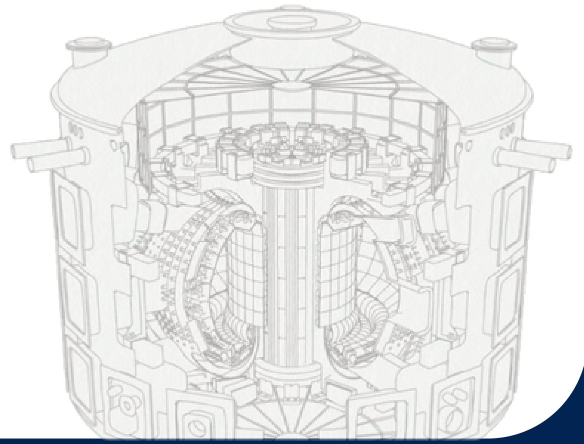


Damage on the Tokamak Wall

(shine-through loss)



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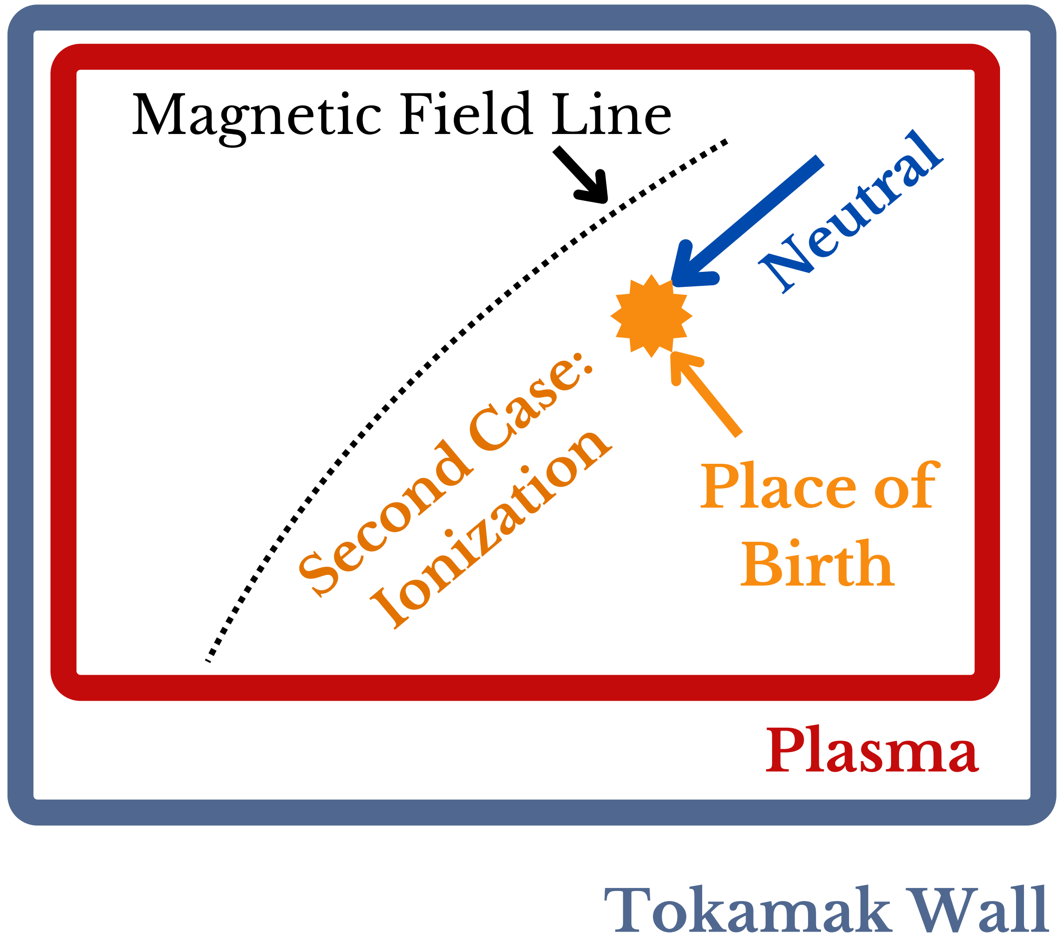

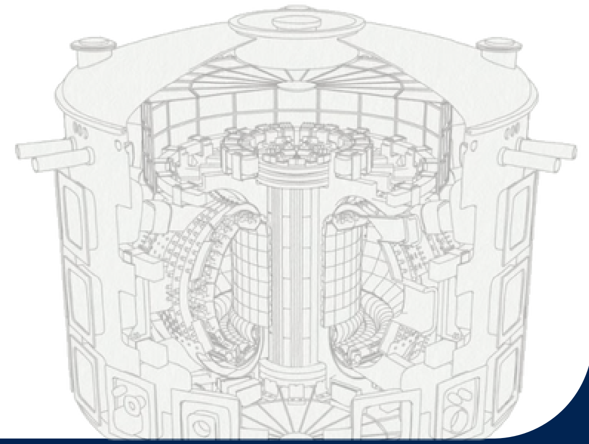

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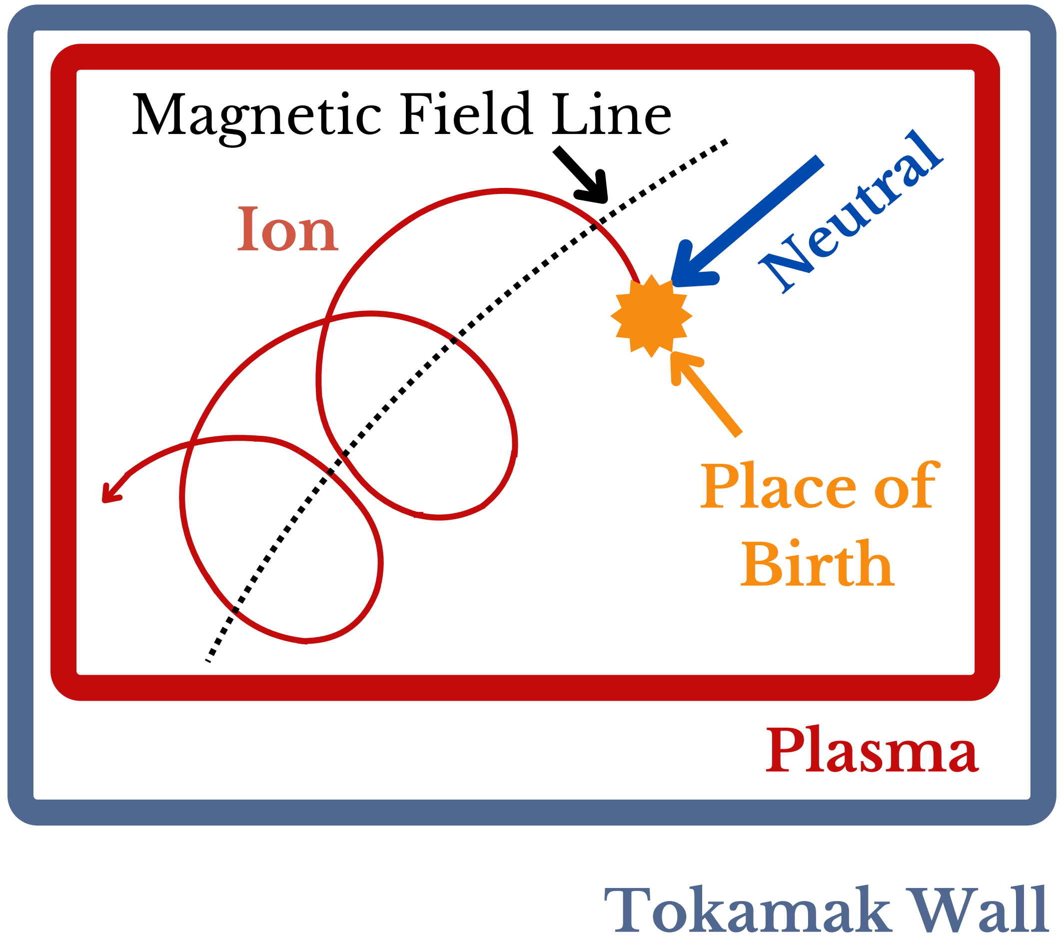

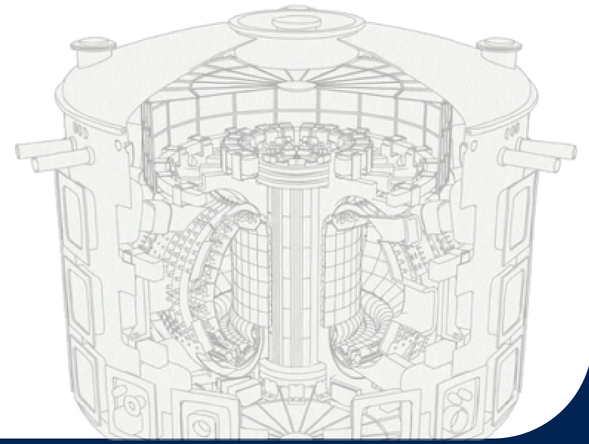

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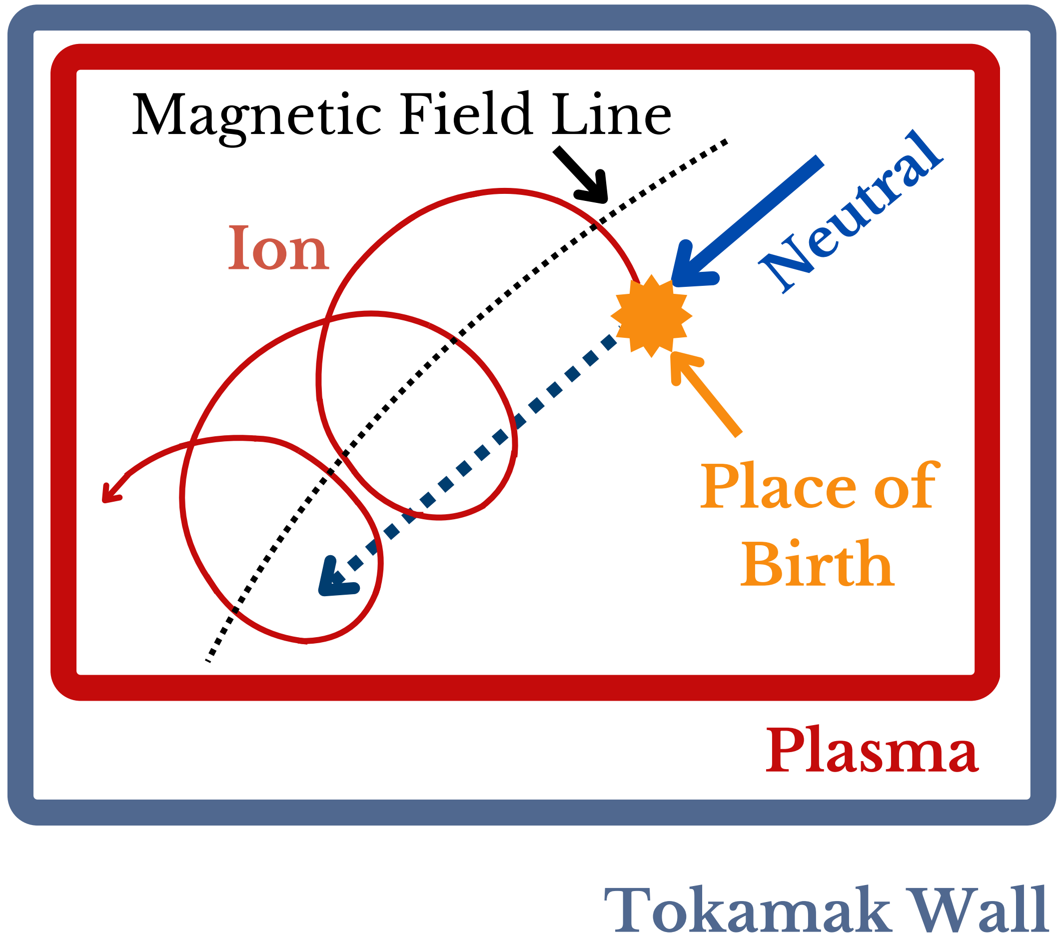
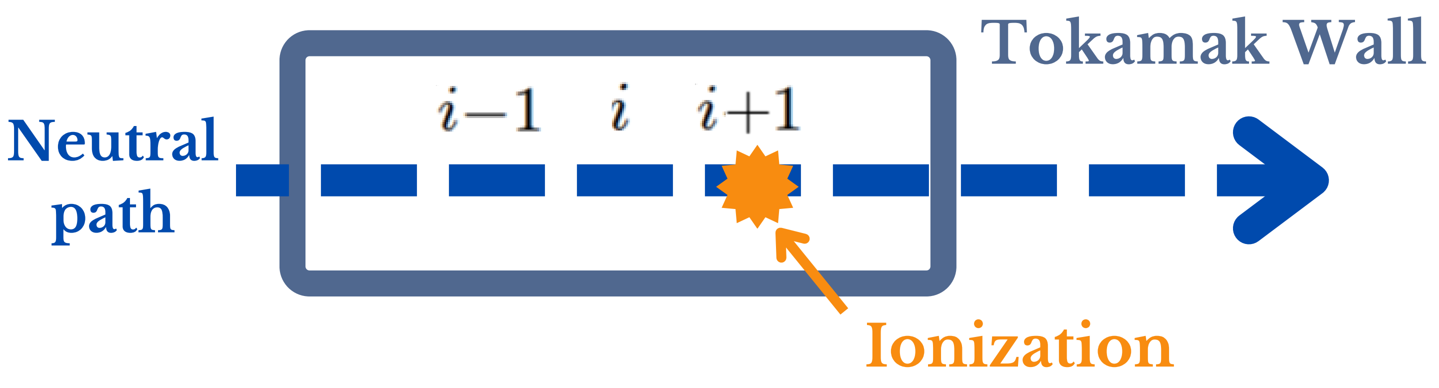


Ionization Scheme : A Stochastic Process

[Hirvijoki]

- Initialize a Neutral Particle (position, velocity)



- Sample $\lambda \sim \mathrm{U}(0,1)$

- For every i-interval :

$$P_i = P_{i-1} \exp\left(\Sigma_i u_n \, \Delta t\right)$$

Based on Quantum Processes
Both analytical fits

[Hill] [Janev, Smith]

$$\Sigma_i = n_{ion}(r_i)\left[\sigma_{\text{ion}}(E_n) + \sigma_{CX}(E_n)\right]$$

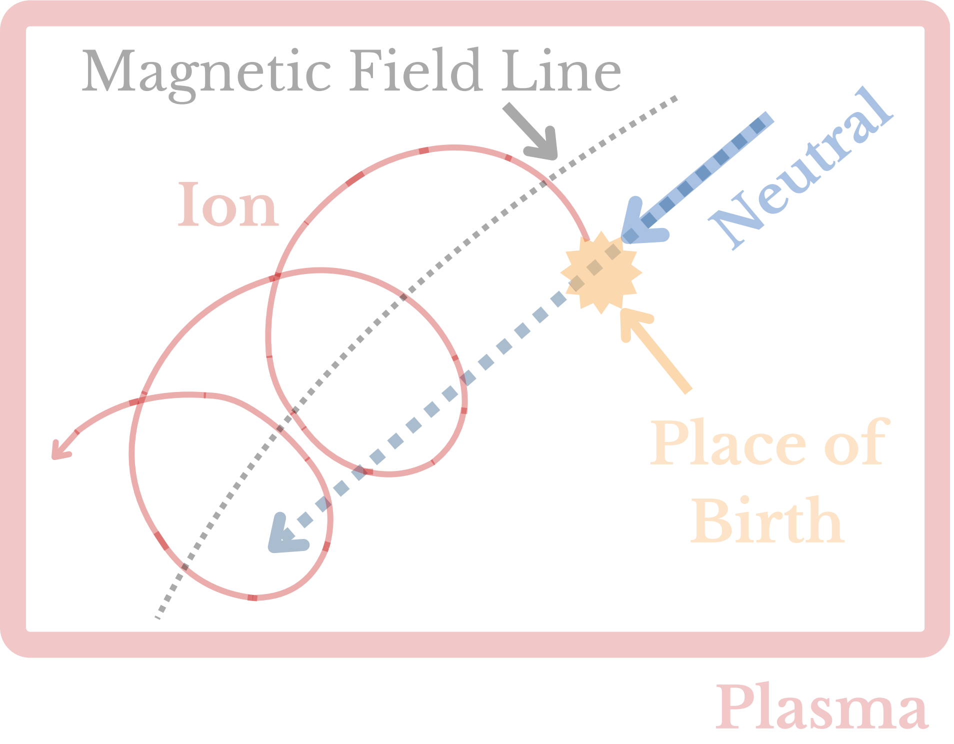
- If $P_i \leq \lambda$: Neutral is **Ionized** & we correct its position.

$$\Delta t_{\text{corr}} = -\frac{1}{u_n \Sigma_i} \ln\left(\frac{\lambda}{P_{i-1}}\right)$$

We only keep Particles that Ionize Inside the Tokamak

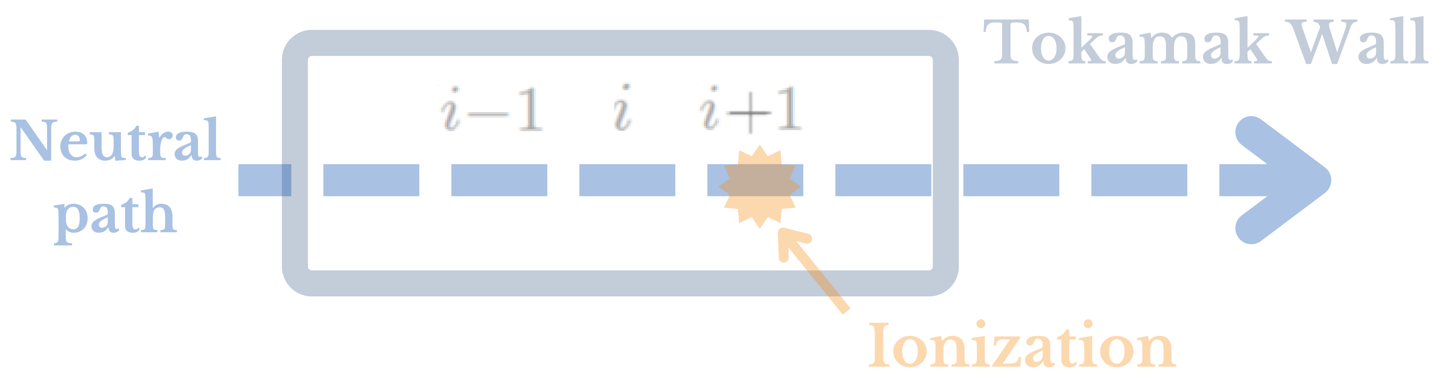
Modeling the NBI – Plasma Interaction

Ionization :
A particle gaining Charge



Ionization Scheme : A Stochastic Process

- Initialize a neutral particle on the wall



$$\Sigma_i = n_{ion}(r_i)\left[\sigma_{\text{ion}}(E_n) + \sigma_{CX}(E_n)\right]$$

[Hill] [Janev, Smith]

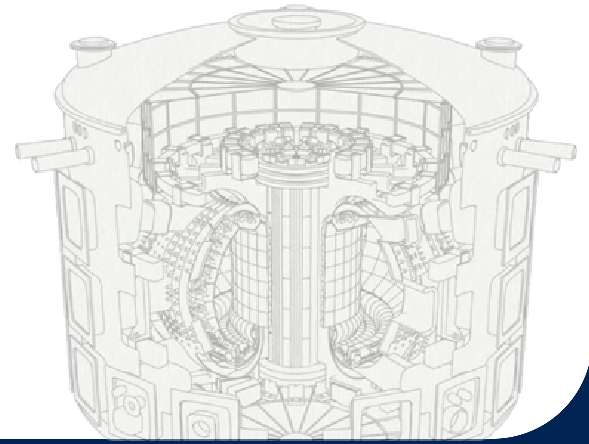
Uncertainty Source 8-Dimensions

- ***Plasma Density*** difficult to measure directly in experiments.

Uncertainty Source 2 Dimensions

- ***Ionization Cross-Sections*** stem from atomic data.
- Theoretical and Experimental results disagree.

10-dimensional Input Space to be Explored



Modeling the NBI – Plasma Interaction

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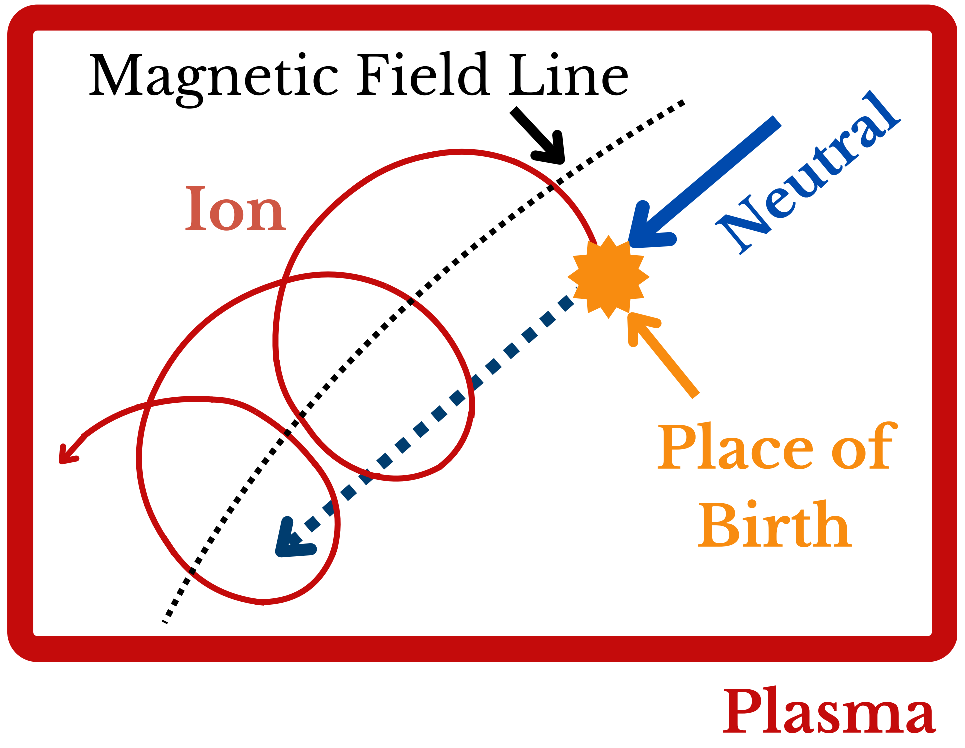
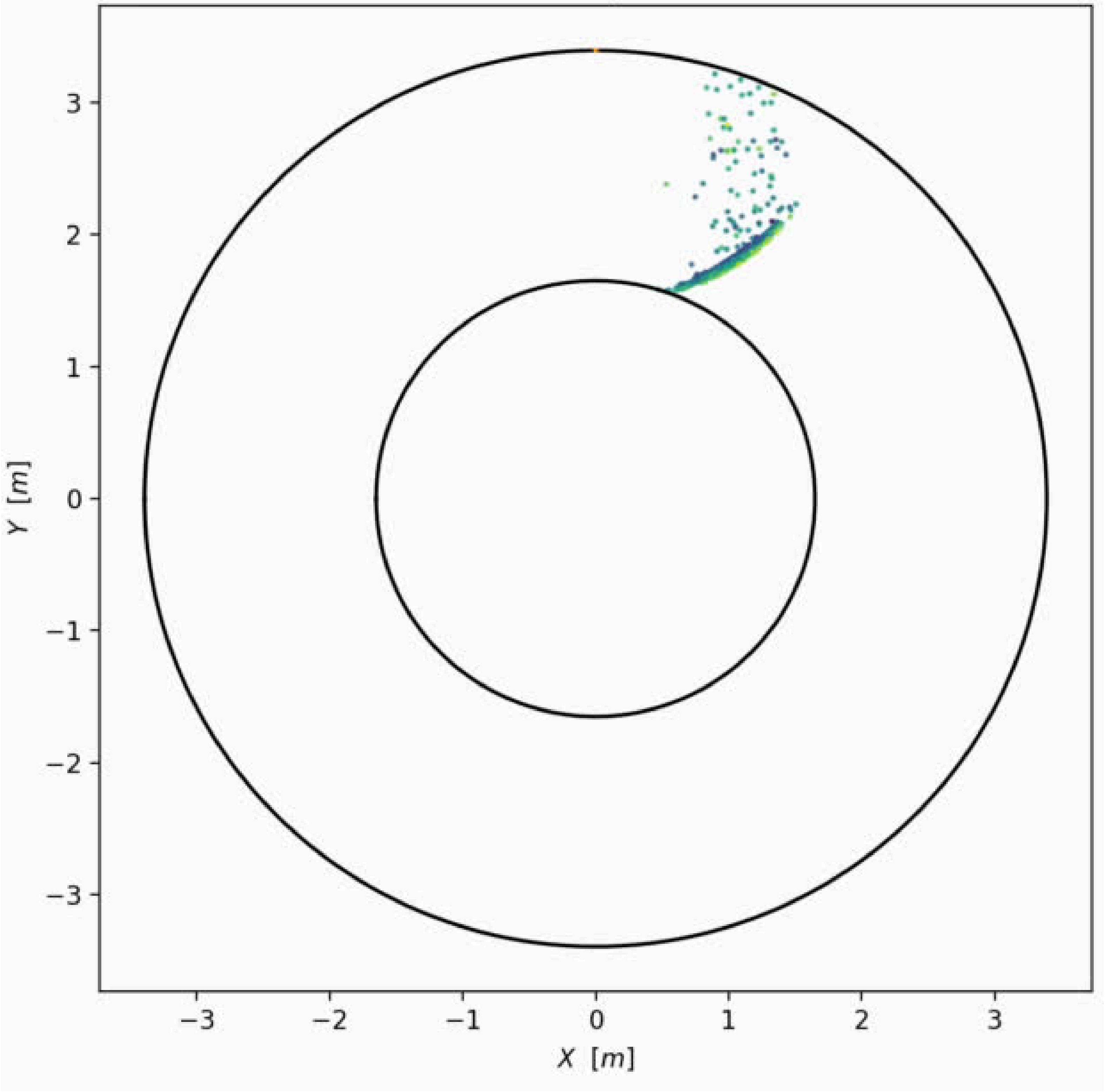
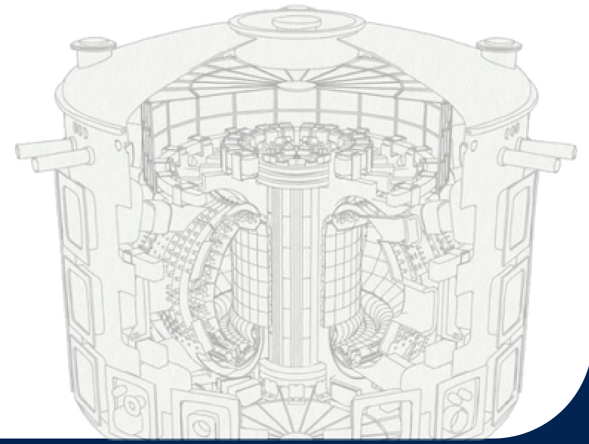


QoI : Shinethrough Losses

Number of NBI Neutrals
that hit the opposite wall.

NBI in TAPAS
(tokamak view from the top)

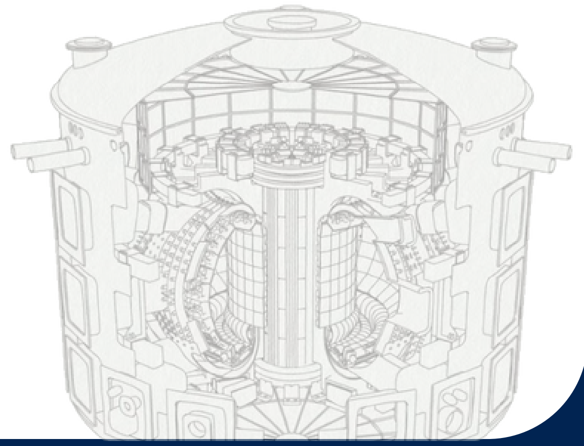




Surrogate Models – Code output Approximation

We want to approximate the output distribution of the response Y, the result of our code's model M acting on the input uncertainties, X.

$$Y = \mathcal{M}(\boldsymbol{X})$$



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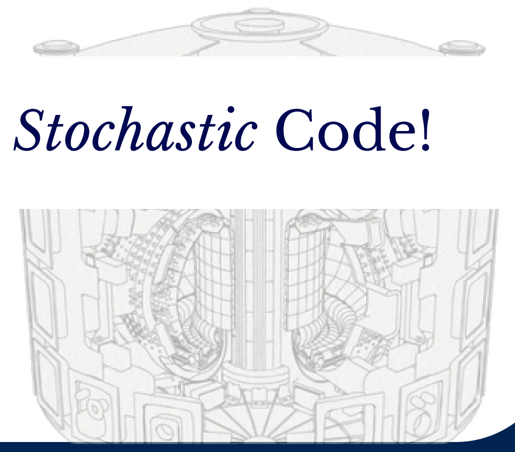
	Brief Description	Description
Gaussian Process (GP)	Assume M(X) follows a Gaussian Process.	Assumes a *Deterministic* Code! (Given that Y is noise-free, interpolation is used)
Polynomial Chaos Expansion (PCE)	Expand M(X) through a Polynomial Basis of X in Hilbert Space.	Assumes a *Deterministic* Code!
Stochastic PCE	Assumes a latent and noise variable to replicate the stochasticity of the model M.	Assumes a *Stochastic* Code!



Surrogate Models – Code output Approximation

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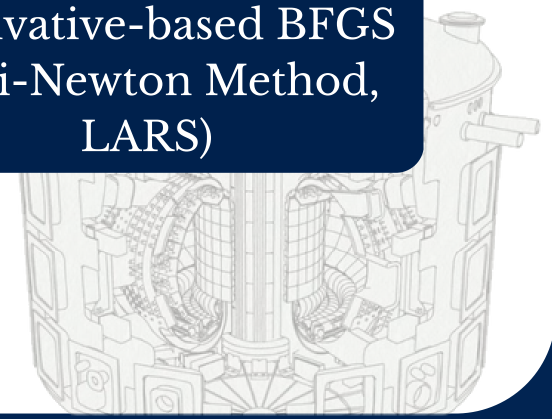
	Brief Formulation	Coefficient Estimation
Gaussian Process (GP)	$Y \approx M_{GP}(\boldsymbol{X};\ \boldsymbol{\theta}, \boldsymbol{\beta}, \sigma^2)$	Genetic Algorithm, Least Squares Estimation, Cross-Validation
Polynomial Chaos Expansion (PCE)	$Y \approx M_{PCE}(\boldsymbol{X};\ c_{\boldsymbol{\alpha}}, \mathcal{A} \ni \boldsymbol{\alpha})$	Sparse Regression (LARS)
Stochastic PCE	$Y \stackrel{d}{=} Y \vert \boldsymbol{X} = \boldsymbol{x} \approx M_{SPCE}(\boldsymbol{X};\ c_{\boldsymbol{\alpha}}, \mathcal{A} \ni \boldsymbol{\alpha}, \sigma^2, \epsilon)$	Maximum Likelihood (Derivative-based BFGS quasi-Newton Method, LARS)

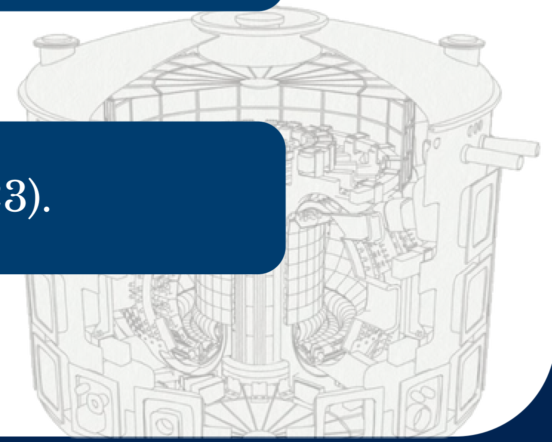


Surrogate Models – Code output Approximation

We want to approximate the output distribution of the response Y, the result of our code's model M acting on the input uncertainties, X.

$$Y = \mathcal{M}(\boldsymbol{X})$$

	Researcher's Choice	Key References
Gaussian Process (GP)	• Prediction : Interpolation • Ordinary Trend • Matern 5/2 Correlation Function • Anisotropic, Ellipsoidal Family of Correlation Function • Optimization Method : Genetic Algorithm	• Santer *et al.* 2003 • Bachoc, 2013 • Dubourg, 2011 • Rasmussen and Williams, 2006 • Goldberg, 1989
Polynomial Chaos Expansion (PCE)	• LARS Regression estimation • Adaptive Polynomial Degree up to 5 • q Norm for truncation set = 1	• Xiu and Karniadakis, 2002 • Sudret, 2007 • Blatmand and Sudret, 2011 • Blatman, 2009
Stochastic PCE	• LARS Regression • Latent Variable follows Normal(0, 1) • Adaptive Polynomial Degree up to 2 • q Norm for truncation set = 1	• Zhu, X. and Sudret, B. (2023).



Sensitivity Analysis - Sobol' Indices

First Sobol' Index

- Individual contribution of each x_i .
- Allows for *Factor Prioritization*.
- If $\sum_i S_i = 1$ no higher-order interactions are present.
- If $\sum_i S_i < 1$ higher-order interactions are present.

- $S_i = \dfrac{V_{x_i}\left(E_{\boldsymbol{x}_{\sim i}}[Y|x_i]\right)}{V(Y)}$, with

$$\boldsymbol{x}_{\sim i} = \{x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N\}$$

Total Sobol' Index

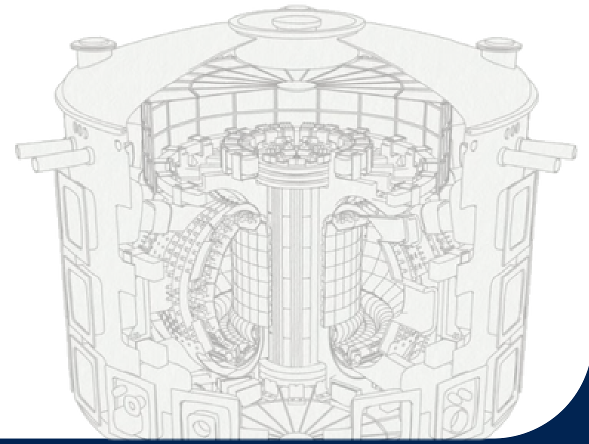
- Total contribution from all x_i .
- Allows for *Factor Filtering*:
  - If $S_i^T \equiv 0$ then x_i can be ommitted.
- If interactions are present, $\sum_i S_i^T > 1$

- $S_i^T = \dfrac{E_{\boldsymbol{x}_{\sim i}}\left(V_{x_i}[Y|\boldsymbol{x}_{\sim i}]\right)}{V(Y)} = 1 - \dfrac{V_{\boldsymbol{x}_{\sim i}}\left(E_{x_i}[Y|\boldsymbol{x}_{\sim i}]\right)}{V(Y)}$

Total Interactions

- Only contributions from $\boldsymbol{x}_{\sim i}$.

- $S_i^T - S_i$



Accuracy of Surrogate Models

Nash-Sutcliffe model efficiency coefficient

$$Q^2 = 1 - \frac{\sum_{i=1}^{n_{\text{test}}} \left(M_{\text{TAPAS}}(\boldsymbol{x}_i) - M_{\text{Surrogate}}(\boldsymbol{x}_i)\right)^2}{\sum_{i=1}^{n_{\text{test}}} \left(M_{\text{TAPAS}}(\boldsymbol{x}_i) - \bar{M}(\boldsymbol{x})\right)^2}$$

$$\bar{M}(\boldsymbol{x}) = \frac{1}{n_{\text{test}}} \sum_{i=1}^{n_{\text{test}}} M_{\text{TAPAS}}(\boldsymbol{x}_i)$$

If $Q^2 = 1$:
Surrogate Predicts Exactly
the Model on the Test Set

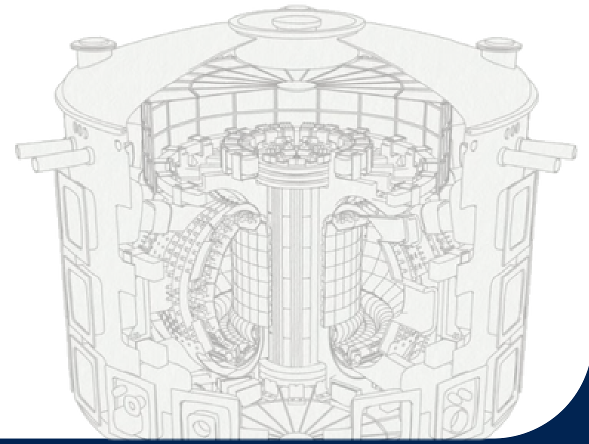
Test and Train Sets to be Compared

$$n_{\text{test}} = 500$$

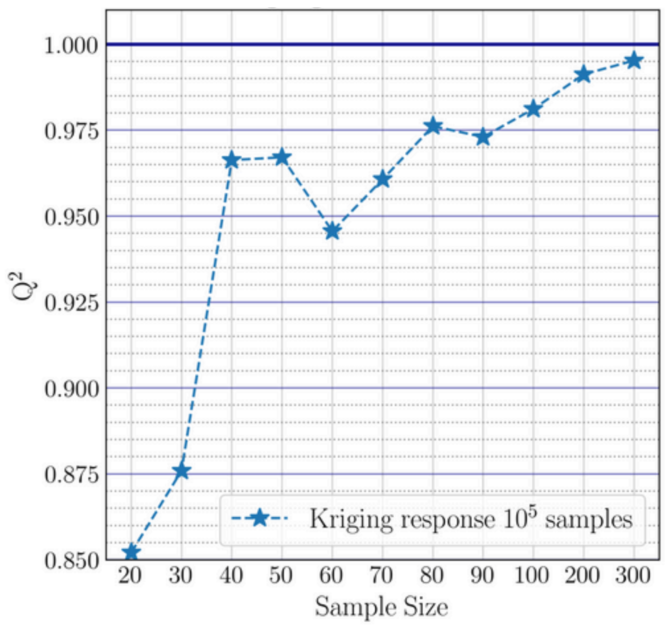
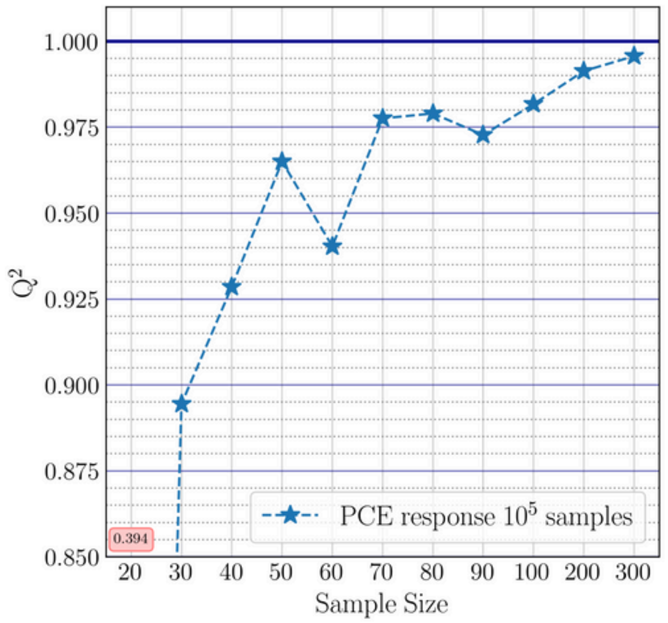
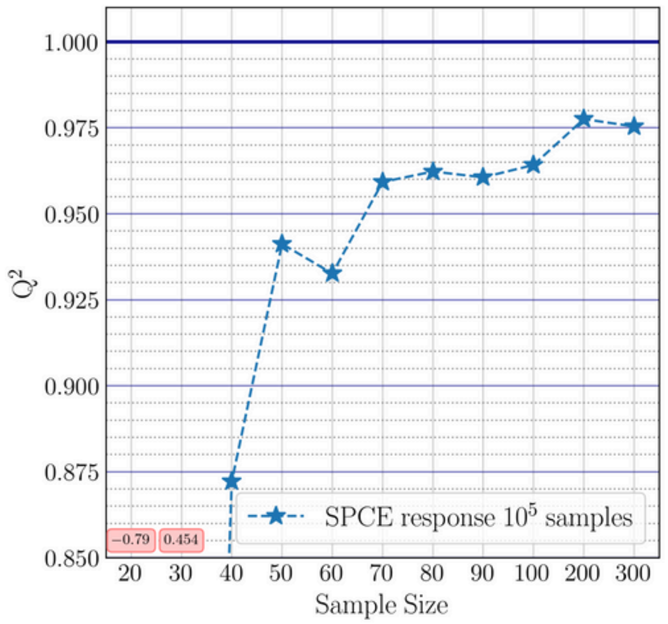
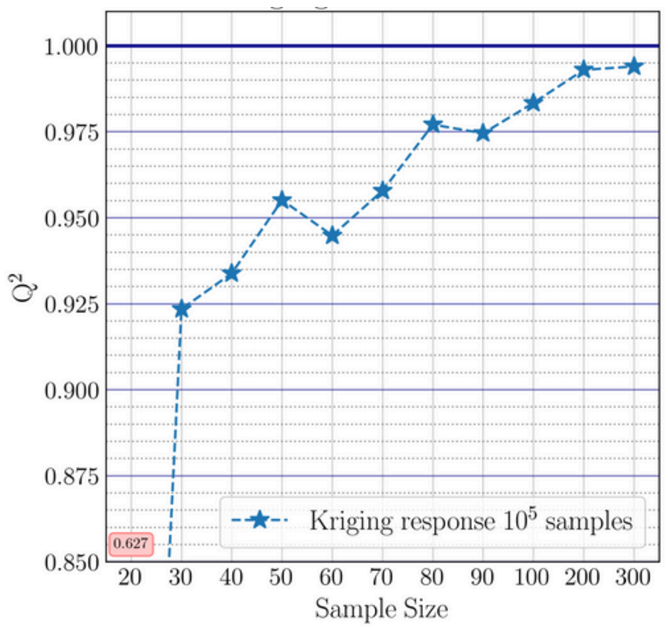
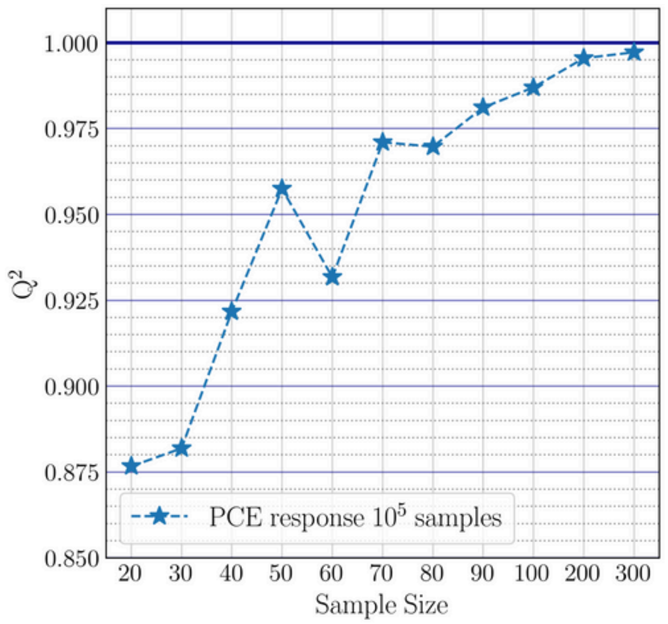
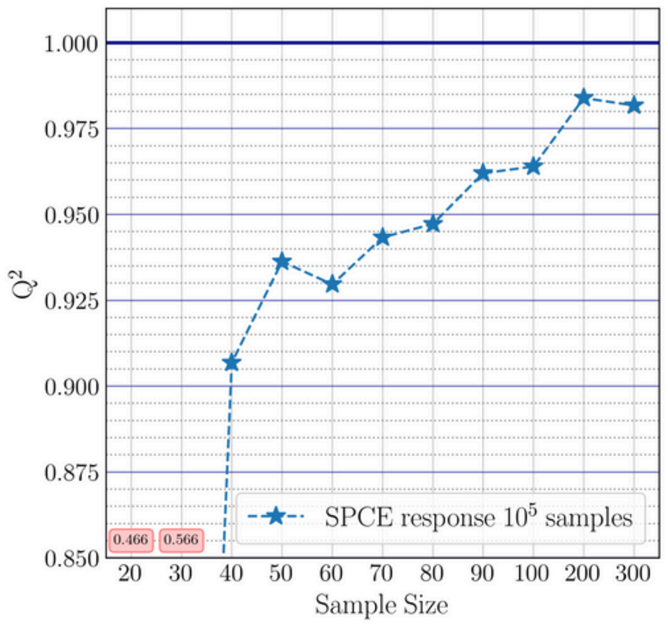
$$n_{\text{train}} = 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300$$

For every n_{train} , we build the metamodel, and compute its output on n_{test}

- Gratiet *et al.* 2016
- Nash, Sutcliffe, 1970



Surrogate Model Accuracy

	Gaussian Process	Polynomial Chaos Expansion	Stochastic PCE
Latin Hypercube Sampling			
Random Sampling			

Fastest Convergence : GP

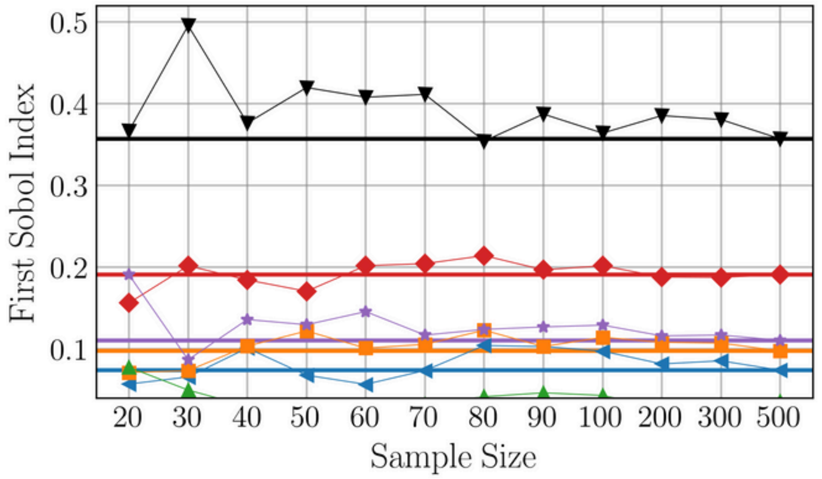
LHS aids only GP at small n_{train}

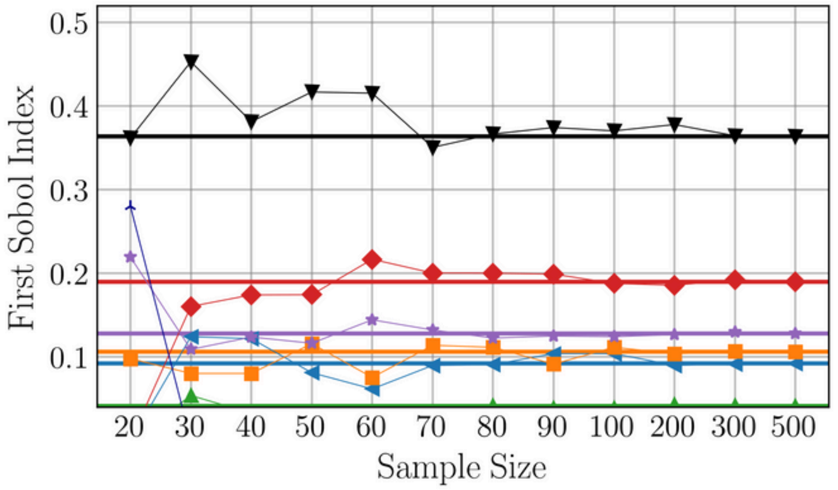
We compare against the Test TAPAS output

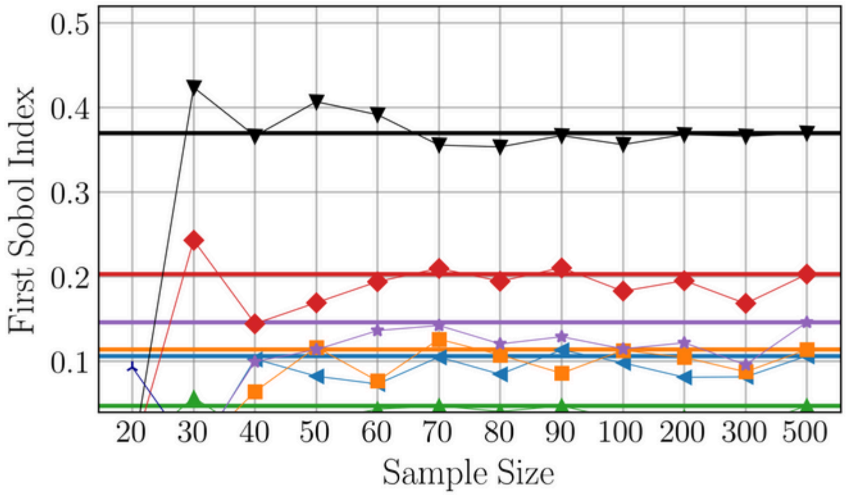
Results – First Sobol' Indices

Gaussian Process | Polynomial Chaos Expansion | Stochastic PCE

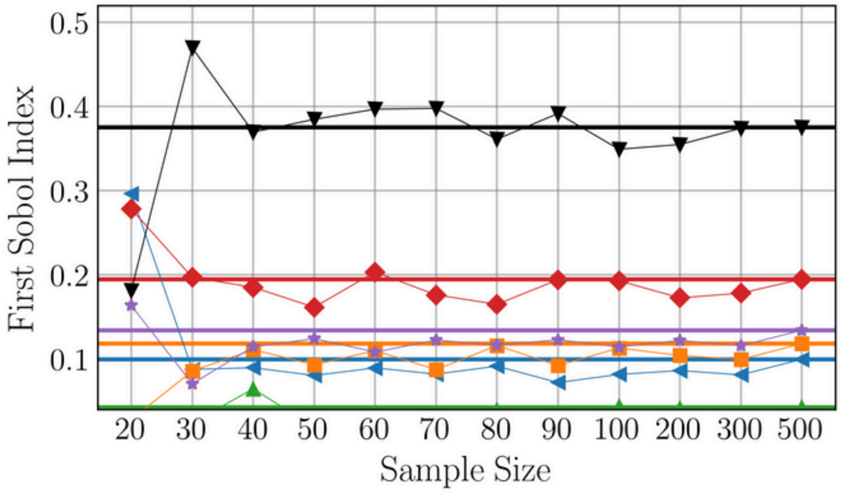
Latin Hypercube Sampling

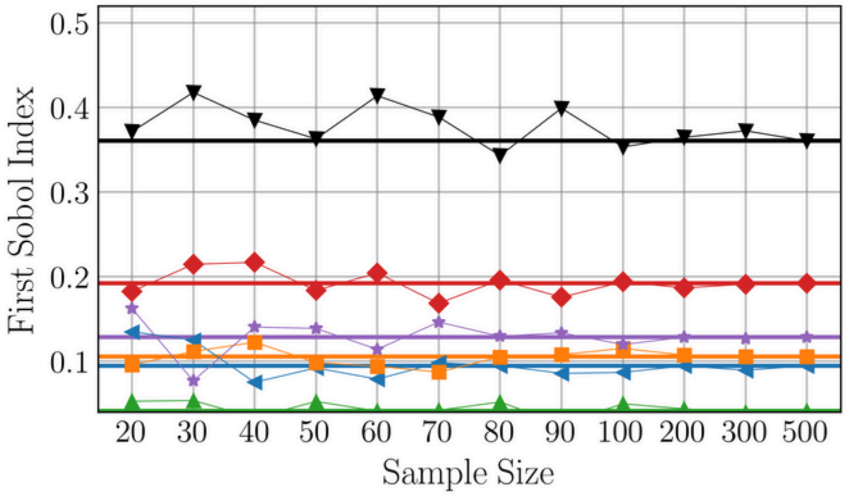


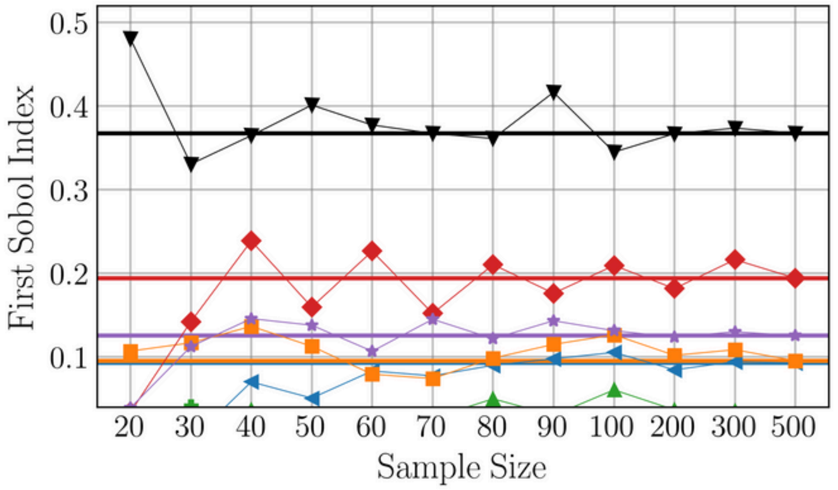




Random Sampling

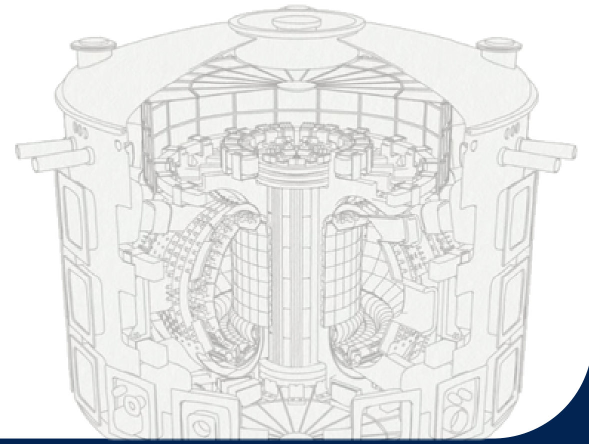




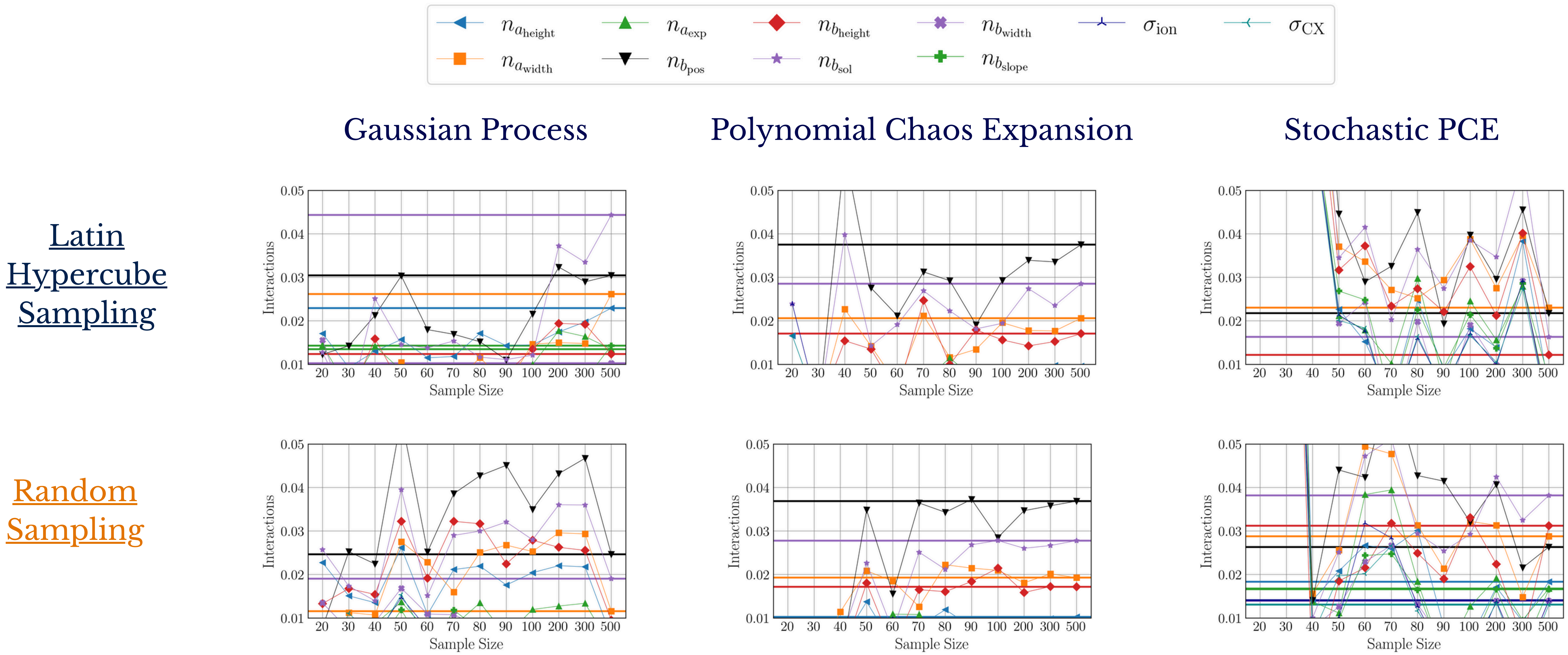


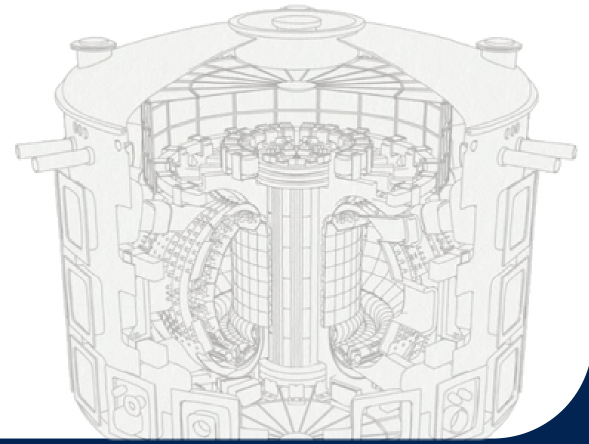
Summary

- LHS has faster convergence for all methods.
- MC increases volatility.
- PCE has fastest convergence
- GP oscillates for top parameter
- SPCE ranks poorly parameters 3-5 at n=300



Results - Interactions Between Parameters





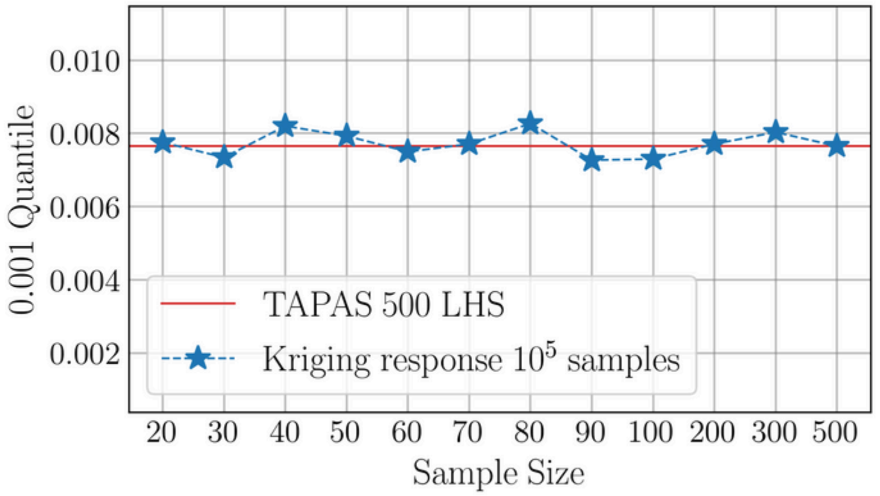
Summary

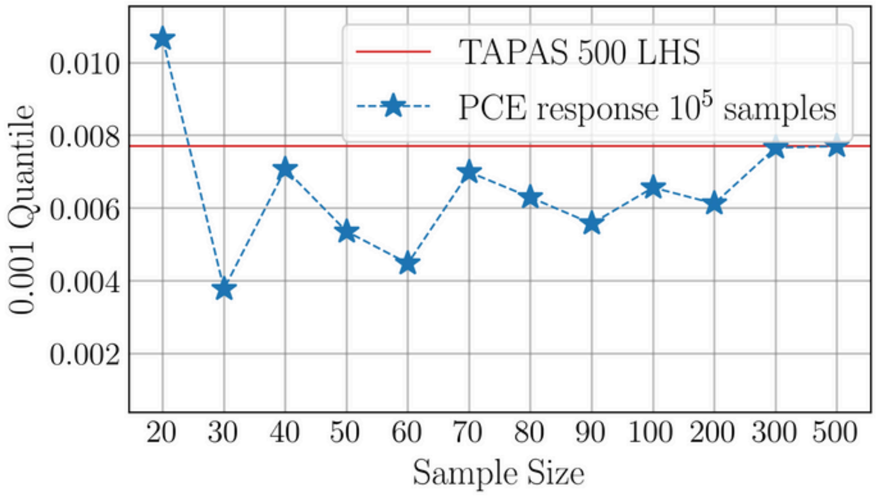
- Unclear Ranking of Influential Parameters
- PCE has the most uniform convergence over n_{train}
- SPCE has the poorest performance

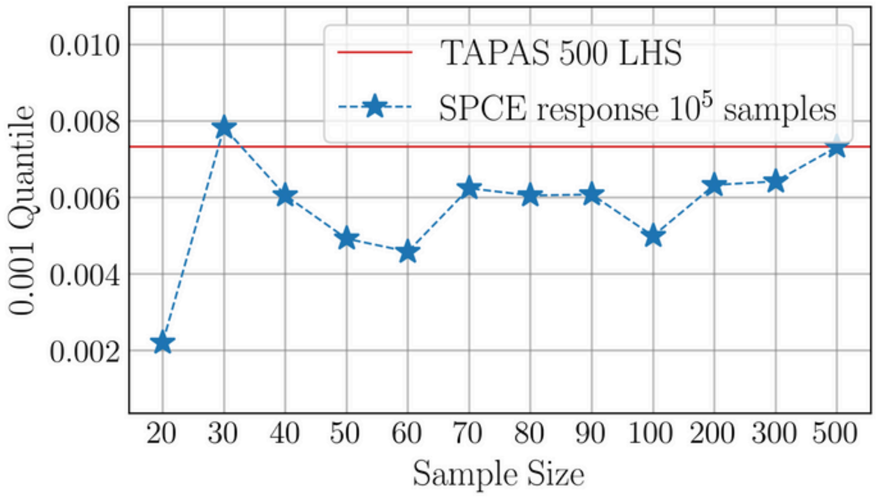
Results – 0.001 Quantile of Surrogate Model

Gaussian Process | Polynomial Chaos Expansion | Stochastic PCE

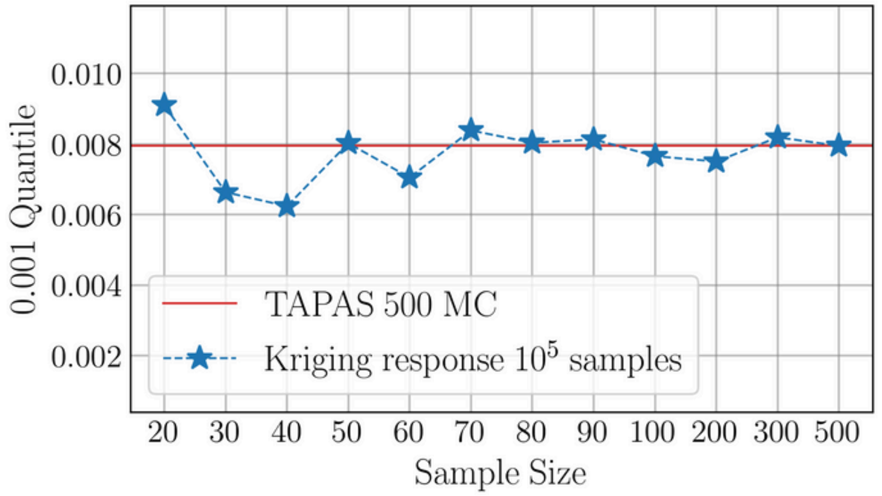
Latin Hypercube Sampling

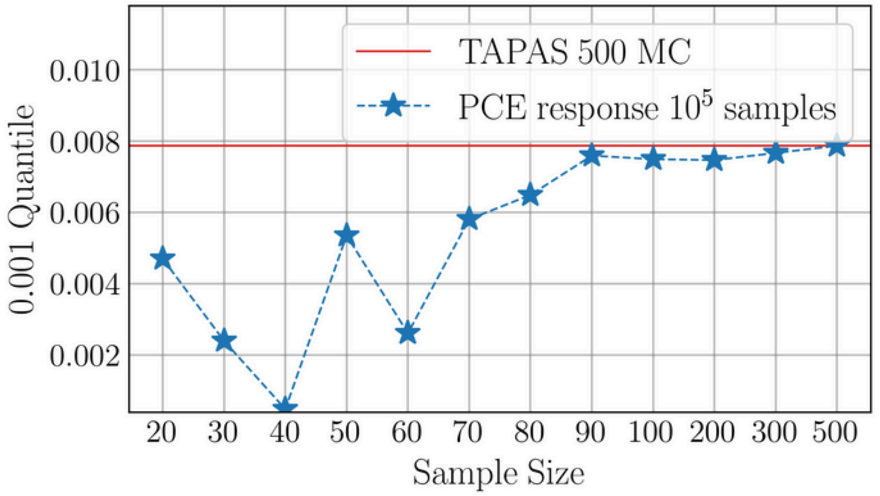


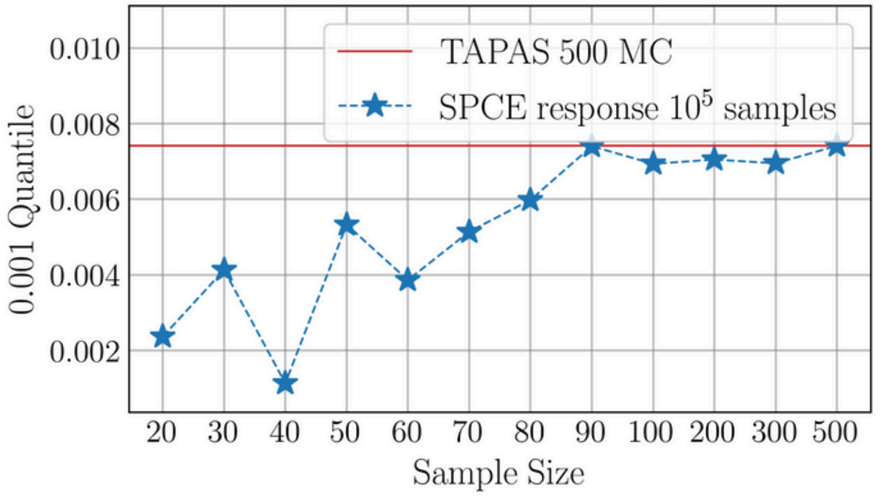




Random Sampling

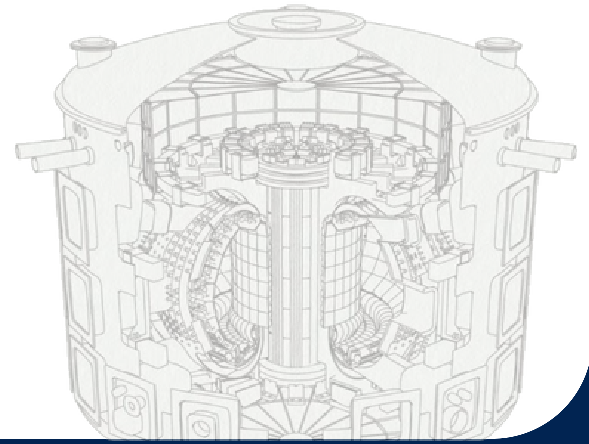






Summary

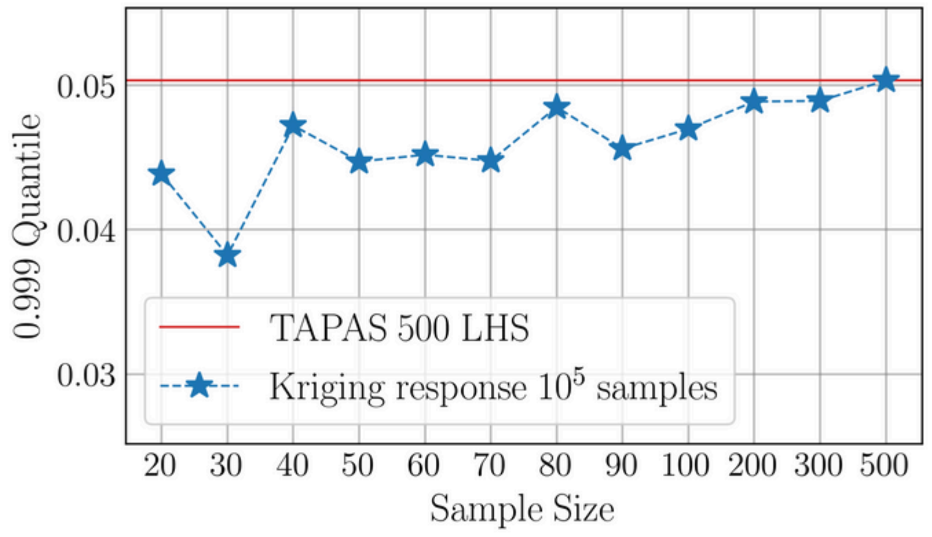
- Best overall convergence : GP with LHS, for few samples.
- PCE, SPCE converge faster with LHS

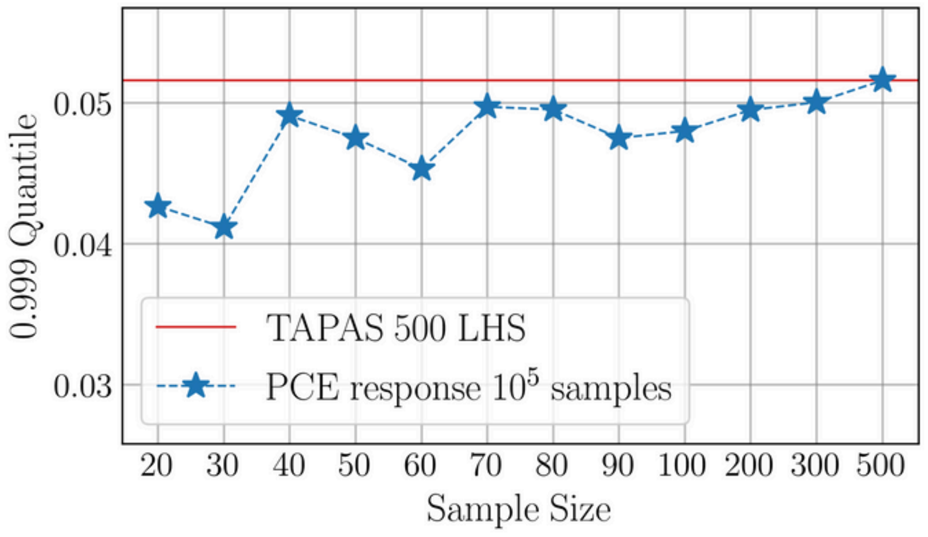


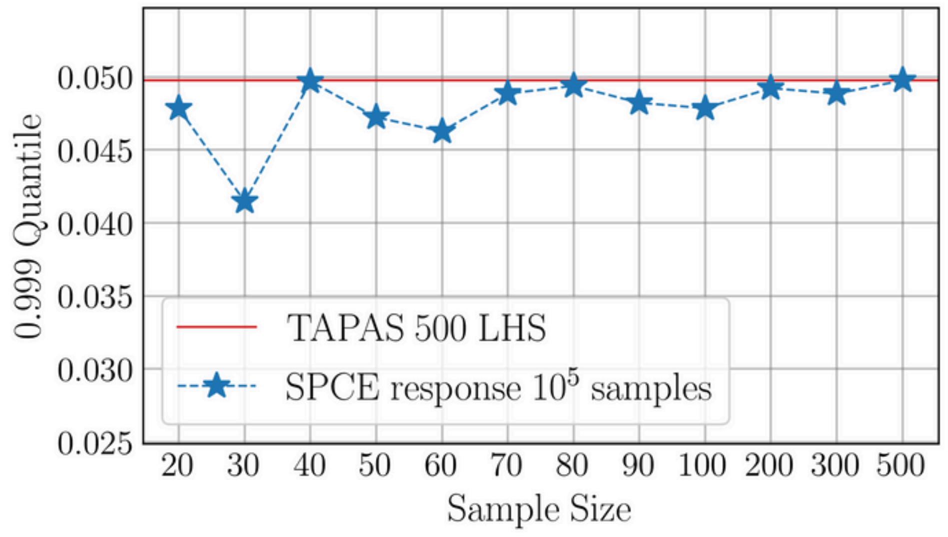
Results – 0.999 Quantile of Surrogate Model

Gaussian Process | Polynomial Chaos Expansion | Stochastic PCE

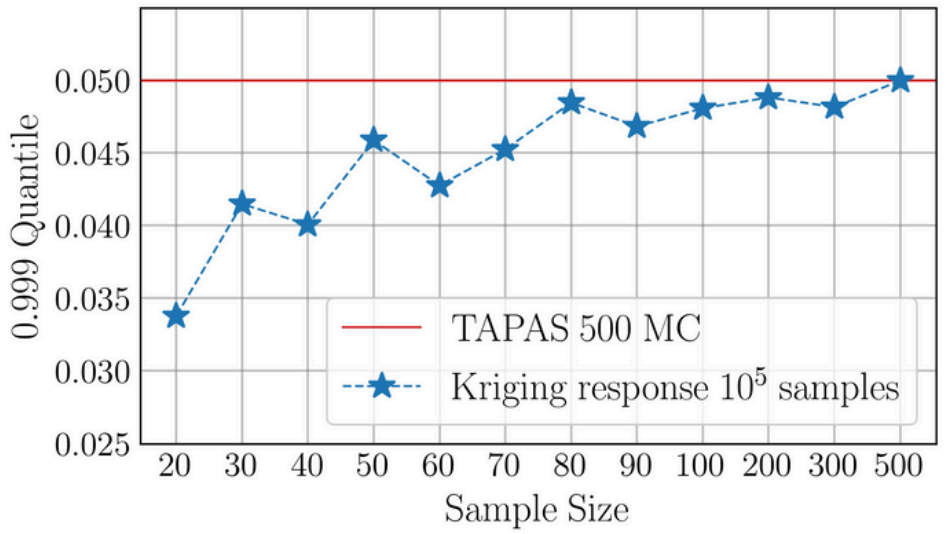
Latin Hypercube Sampling

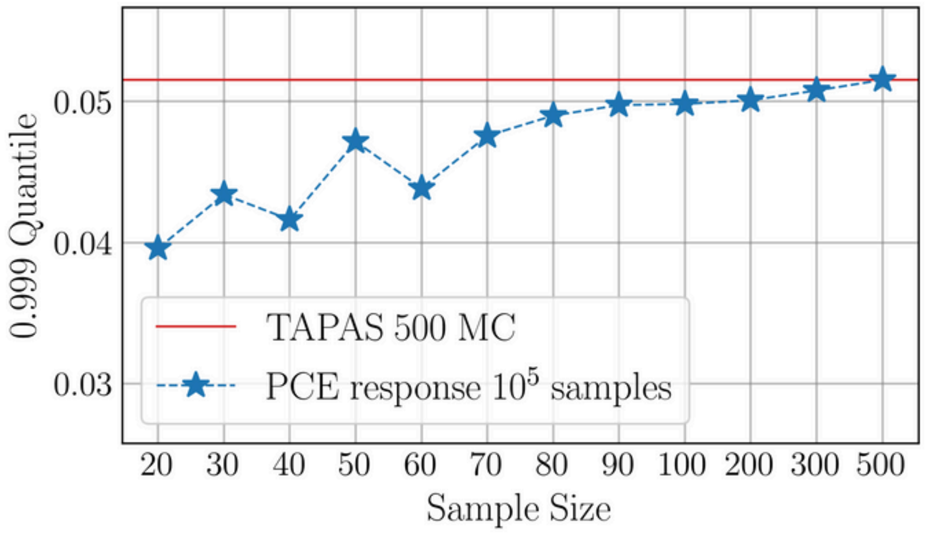


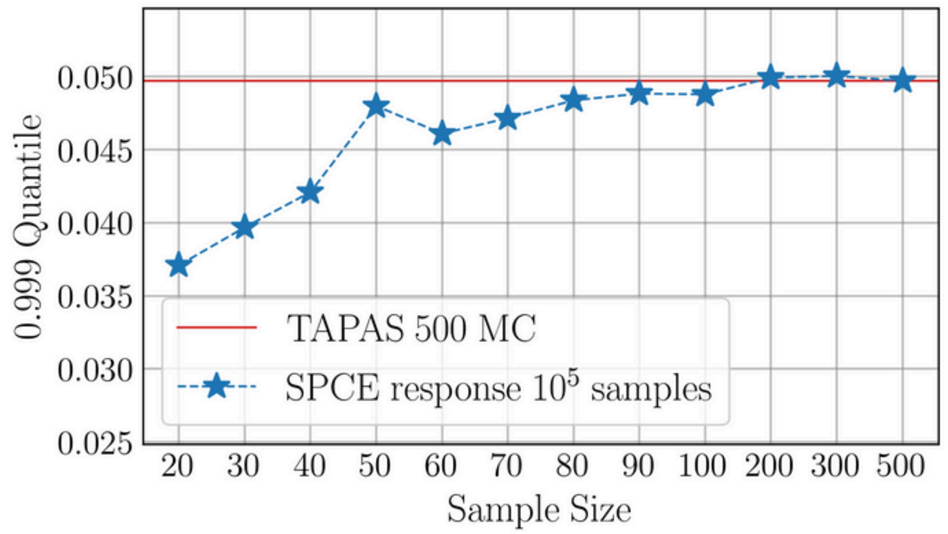




Random Sampling

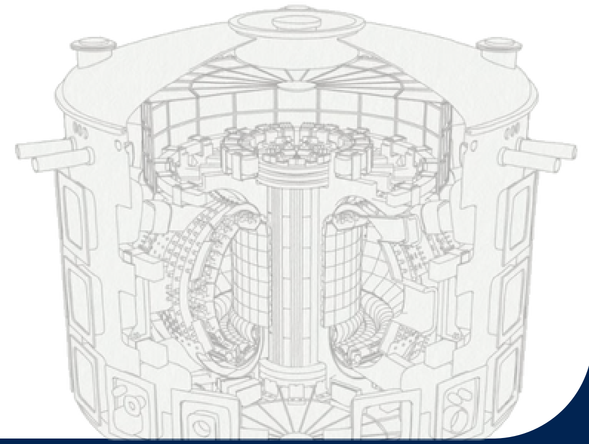






Summary

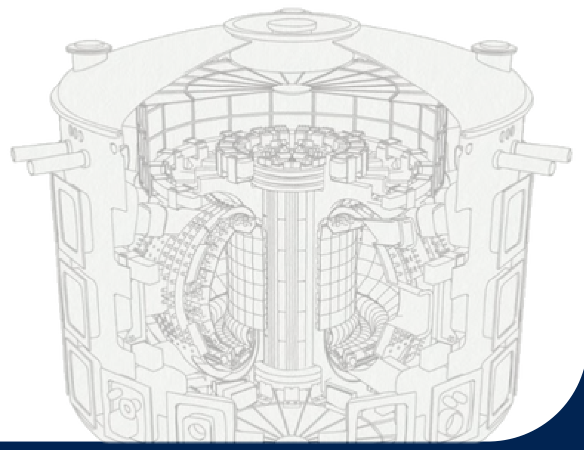
- **Fastest** overall convergence : SPCE
- LHS aids smaller n_{train}



Conclusion

- LHS offers a small advantage over MC for this QoI, especially over smaller n_{train} .
- Rapid convergence for GP and PCE, slowest for SPCE.
- PCE offers greater stability in the computation of the Sobol' Indices and the total Interactions.
- GP rapidly approximates the 0.001 Quantile of the output distribution Y.
- SPCE rapidly approximates the 0.999 Quantile of the output distribution Y.

Thank you for your attention!

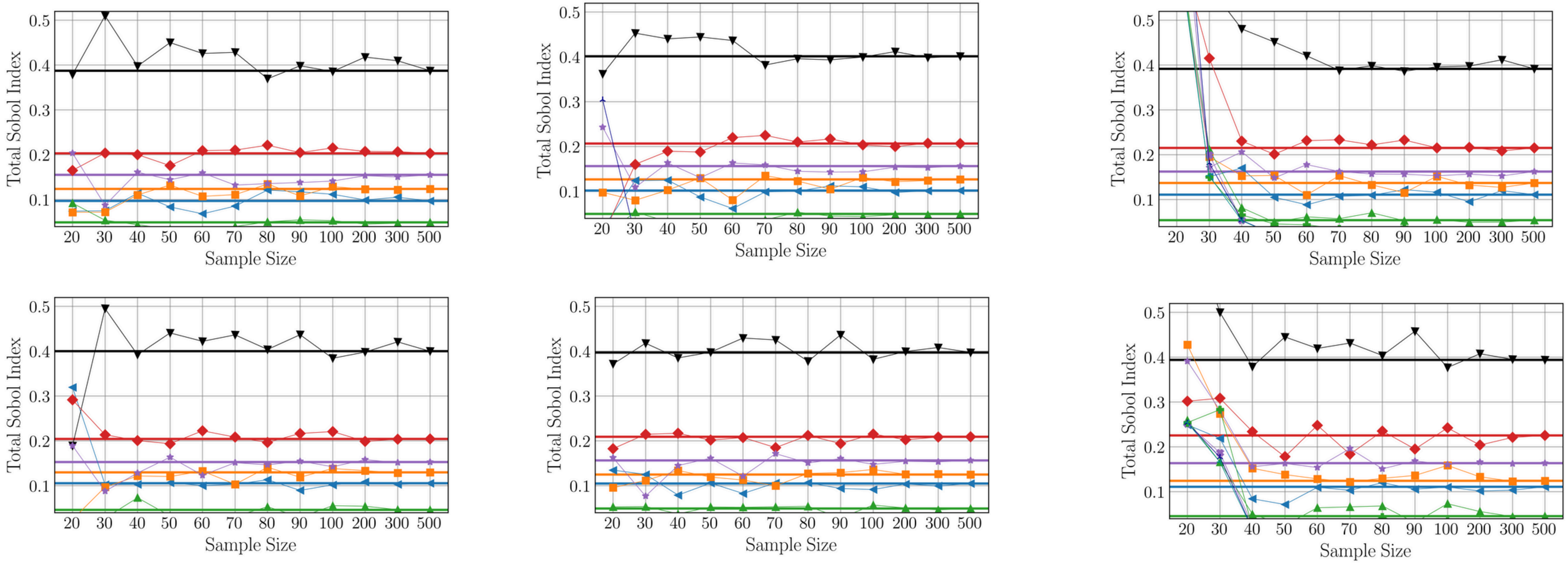


Appendix 1 – Total Sobol Indices

Gaussian Process | Polynomial Chaos Expansion | Stochastic PCE

Latin Hypercube Sampling

Random Sampling

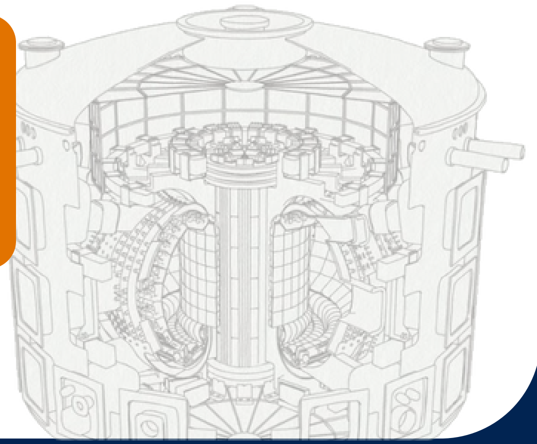


Latin Hypercube Sampling

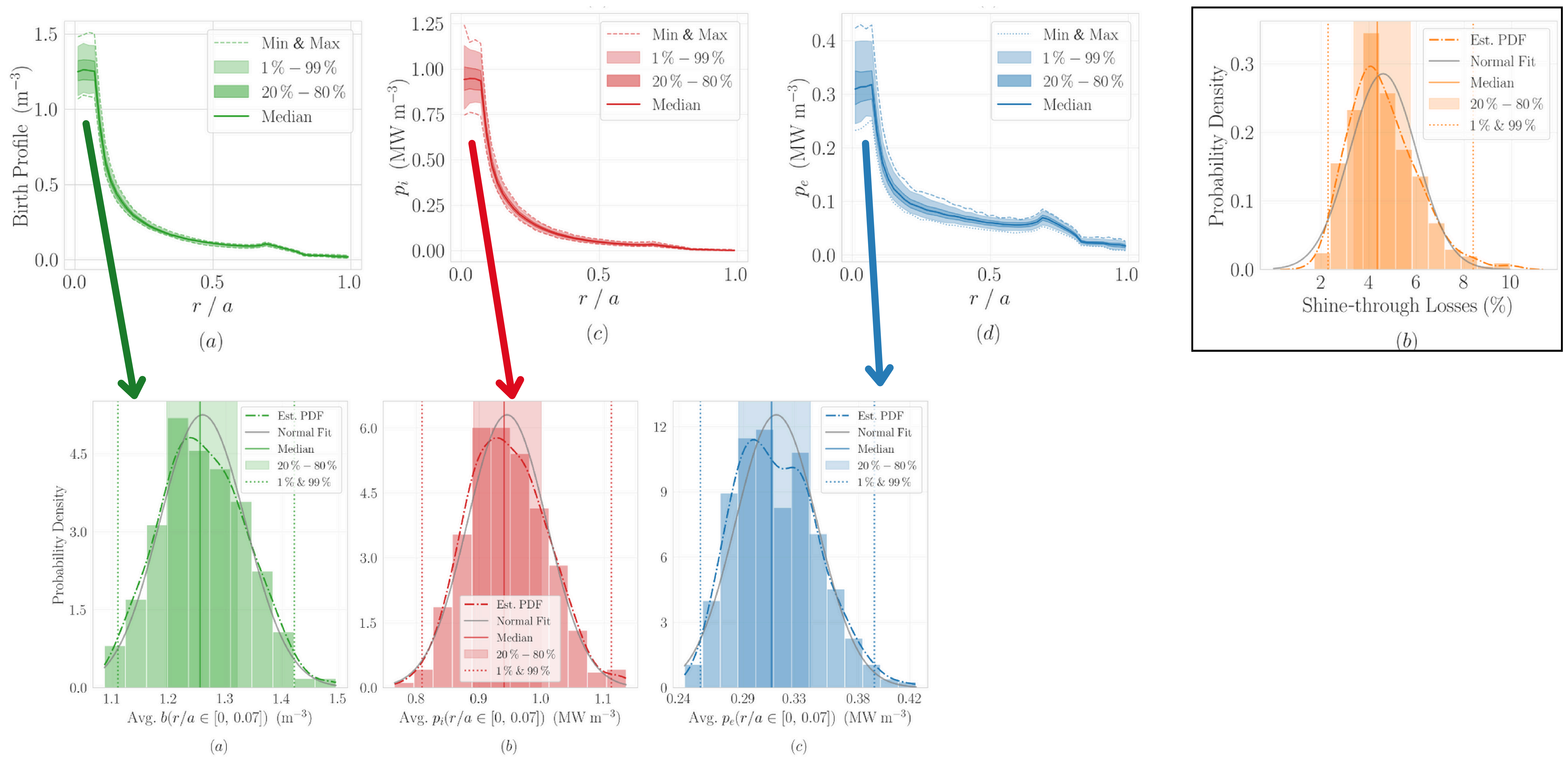
- Faster convergence for all methods
- GP oscillates for top parameter
- PCE faster convergence
- SPCE ranks poorly parameters 3-5 at n=300

Random Sampling

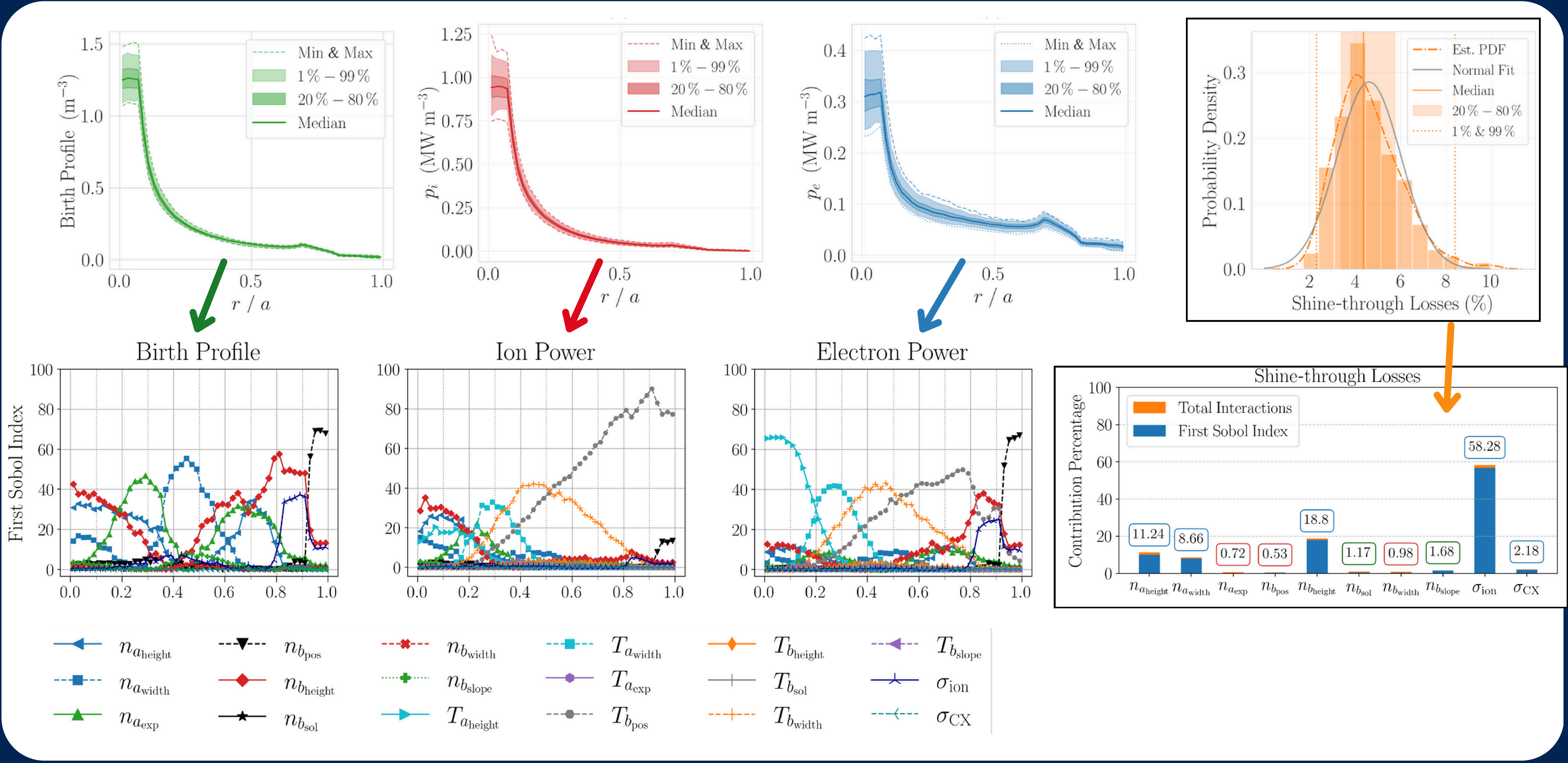
- PCE faster convergence
-



Appendix 2
1D Quantities of Interest



Appendix 4
1D Sensitivity Analysis



Appendix 5

1D Weighted Average – Sensitivity Analysis