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Optimal Sensor Selection and Ensemble-Based Inversion for Steady State Nuclear Reactor Models

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Acknowledgments

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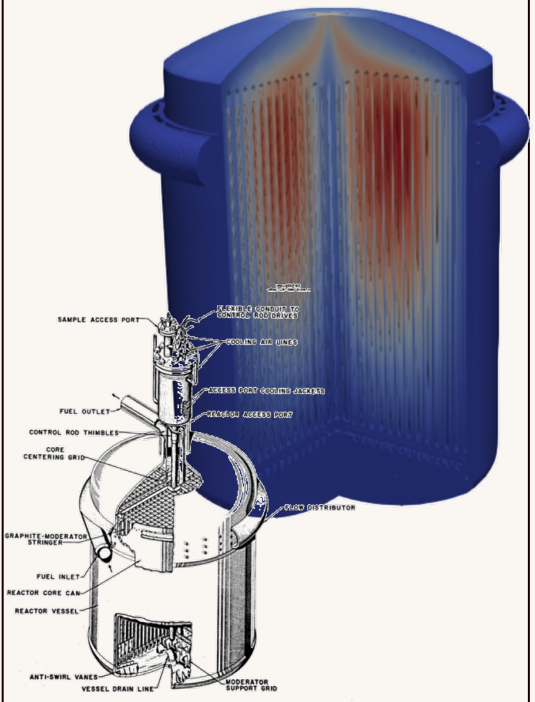
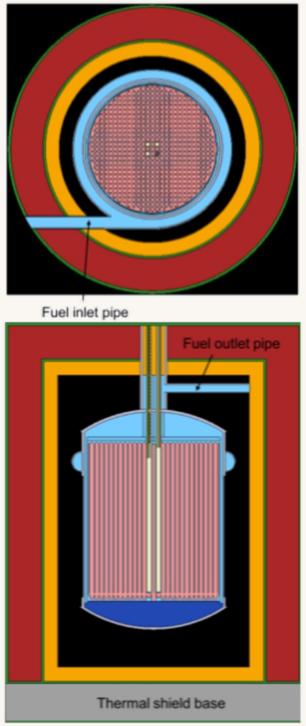
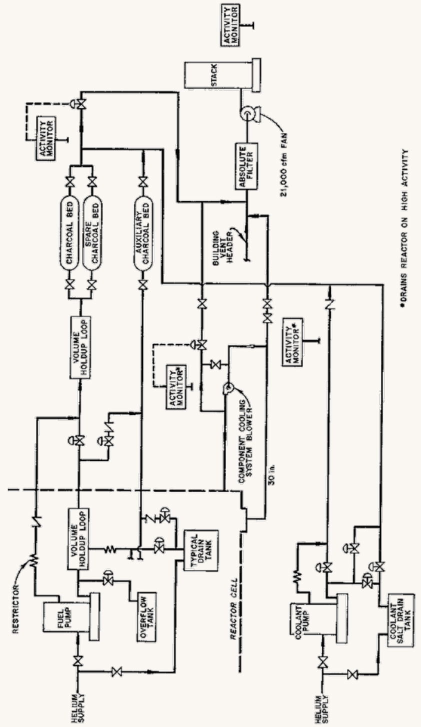
Motivations



DIGITAL TWINNING



MODEL CALIBRATION



SYESTM CONTROLL

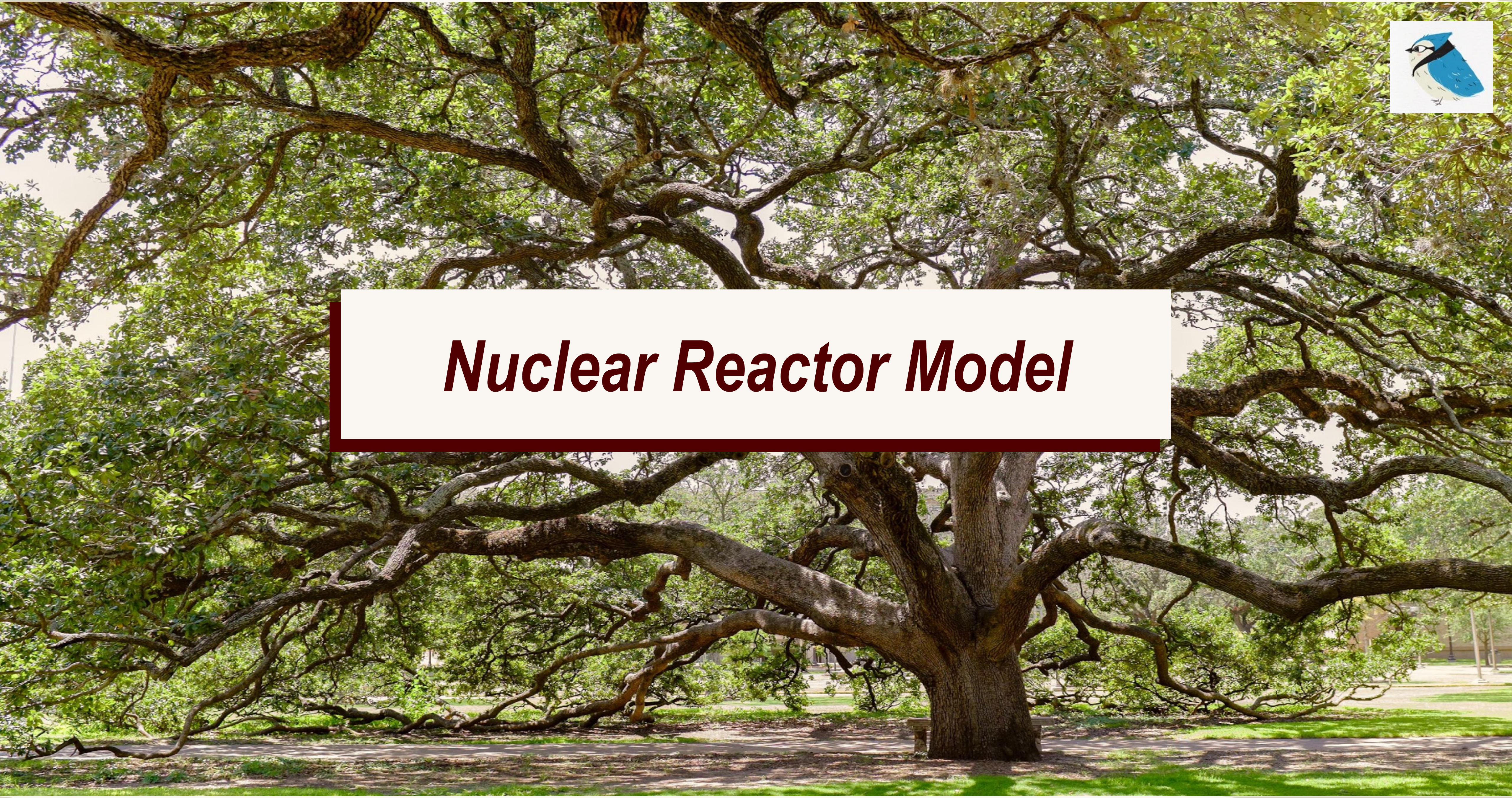
Challenges and Possible Approaches

DATA ASSIMILATION

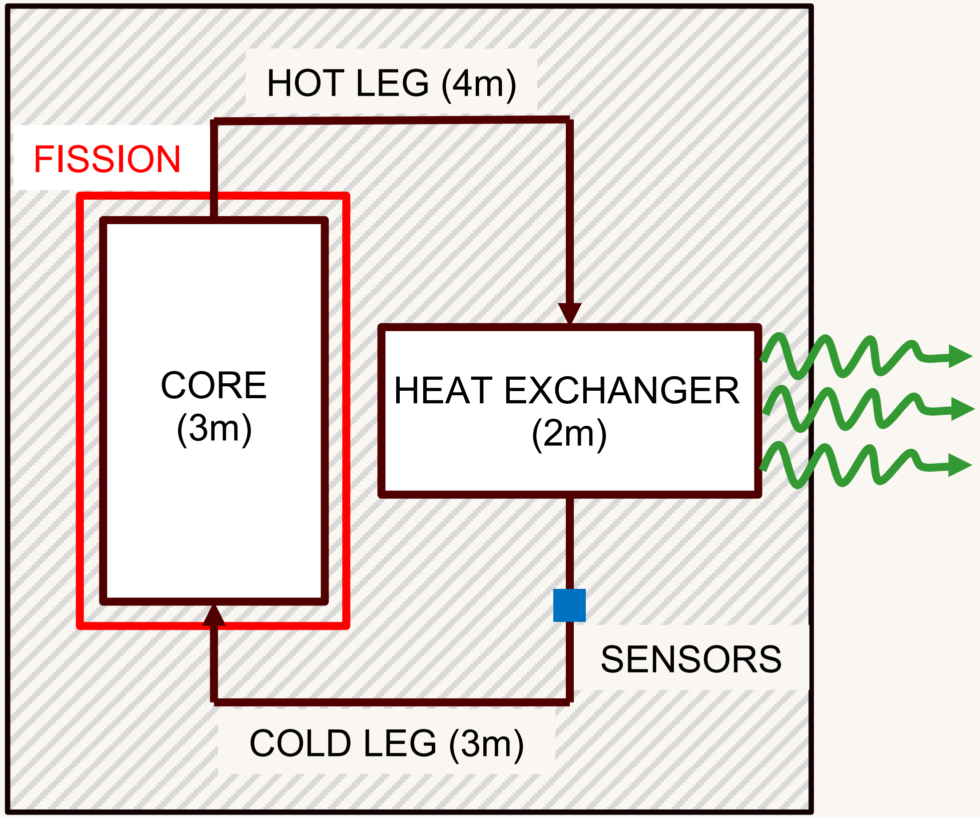
- Bayesian filters
- Kalman(-ized) filters
- Variational methods
- Data interpolation
- Variational data fitting
- Variational parameter inversion (e.g., EnKI, …)

OPTIMAL EXPERIMENTAL DESIGN

- Bayesian OED
- Model-aware sequential OED
- Model-free sequential OED
- “Alphabetical” OED (e.g., A/E/D/…-OED)
- …


Nuclear Reactor Model

A Simplified Model



GEOMETRY

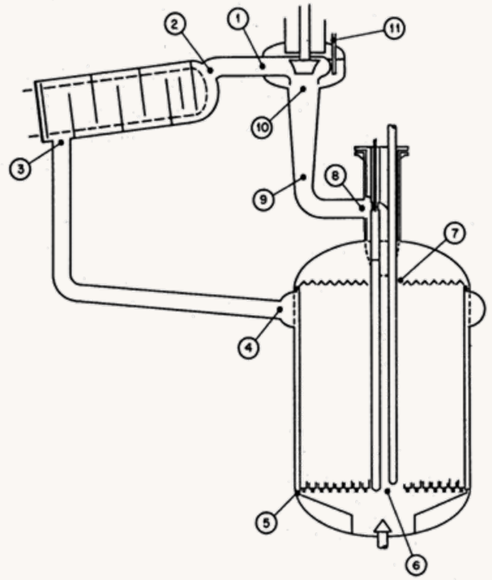
- closed loop geometry
- uniform velocity
- no radial effects

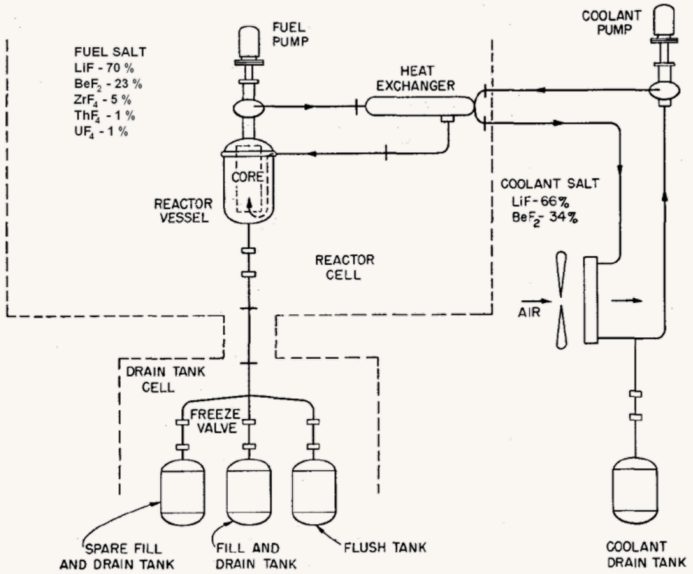
MISSING

- graphite coupling
- pipe cross-sections
- momentum equation

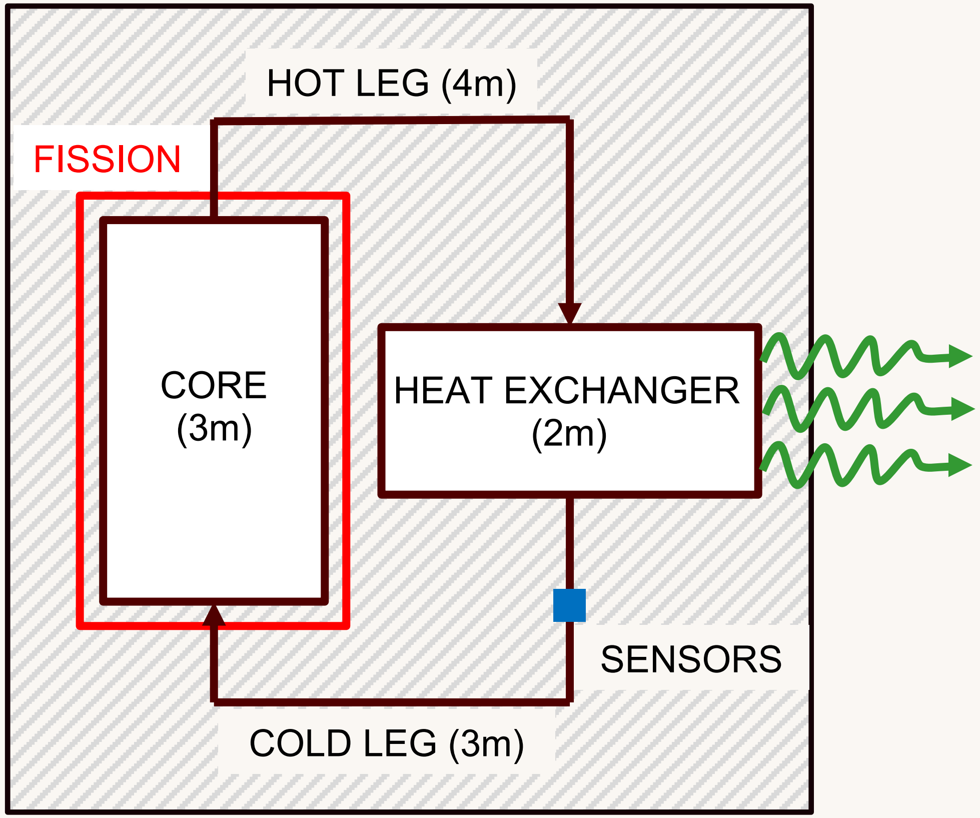
MODEL GOALS

- parameter calibration
- state reconstruction
- sensor collocations





A Simplified Model



NEUTRON DIFFUSION EQUATION

- 6 energy groups
- diffusive transport
- fission only in core

$$-\partial_x D(T)\partial_x \psi^g - \sigma_t^g(T)\psi^g + \sum_{g'=1}^{6}(1-\beta)\chi_p^g \nu_f^{g'}\sigma_f^{g'}(T,x)\psi^{g'}/k_{eff} + \sum_{g'=1}^{6}\sigma_s^{g'\to g}(T)\psi^{g'} - \chi_d^g\sum_{p=1}^{8}\lambda^p c^p = 0$$

PRECURSOR TRANSPORT EQUATION

- 8 precursor groups
- advection at constant speed
- no heating effect

$$-\partial_x v c^p - \lambda^p c^p + \beta^p \sum_{g=1}^{6} \nu_f^g\sigma_f^g(T,x)\psi^g/k_{eff} = 0$$

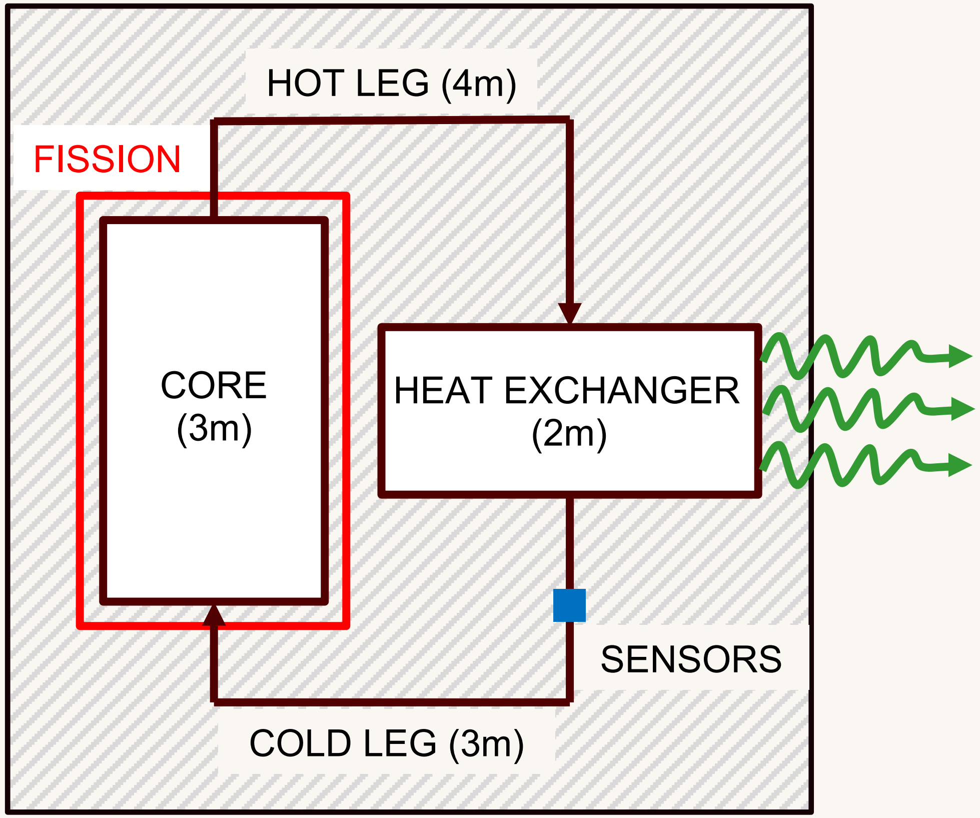
FUEL ENERGY EQUATION

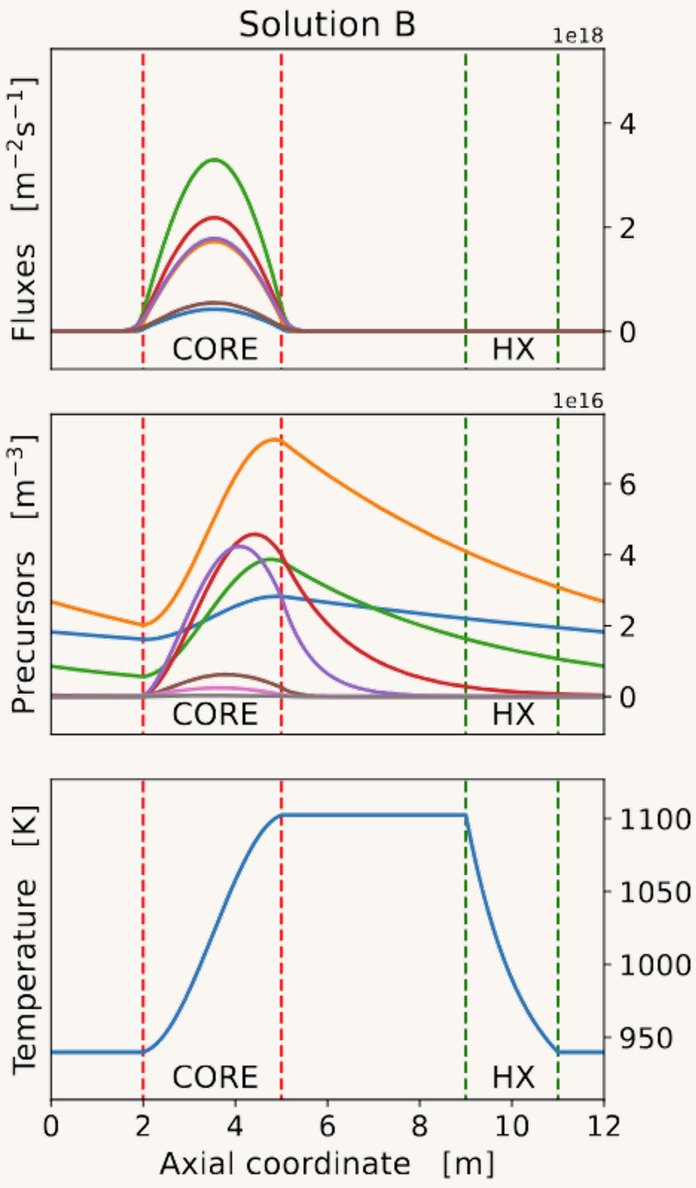
- constant properties
- advection at constant speed
- average value for h, T_∞

$$-\rho c_p \partial_x v T + \partial_x k \partial_x T - h(x)(T-T_\infty) + \sum_{g=1}^{6} E_f\sigma_f^g(T,x)\psi^g/k_{eff} = 0$$

$$\int_{\Omega_{Core}} \sum_{g=1}^{6} E_f \sigma_f^g(T,x)\psi^g dx = P$$

A Simplified Model





FREE PARAMETERS

- $v = 10^{-1} - 10^{1}$ m/s
- $P = 10^{6} - 10^{8}$ W
- $h = 10^{5} - 10^{7}$ W/mK

OBSERVABLE FIELDS

- Thermal flux (ψ_6)
- Temperature (T)

MODEL GOALS:

- Parameter calibration
- State reconstruction
- Sensor collocations

Notation and Assumptions

MODEL PARAMETERS ← **PARAMETER LIKELIHOOD** ← **EXPERIMENTAL DATA**

$$\boldsymbol{\vartheta} = \{\mathrm{v}, \mathrm{P}, \mathrm{h}; \mathrm{D}, \sigma^{\mathrm{g}}_{\mathrm{f},0}, \sigma^{\mathrm{g}}_{\mathrm{s},0}, \sigma^{\mathrm{g}}_{\mathrm{t},0}, \dots\} \sim \Pi_0(\boldsymbol{\Theta})$$

$$\mathcal{L}(\boldsymbol{\vartheta}|\mathbf{d}) \propto \exp\left(-\|\mathbf{d} - \mathcal{G}(\boldsymbol{\vartheta})\|^2_{(\sigma\mathbf{I})^{-1}}\right)$$

$$\mathbf{d} = \mathcal{H}(u(\boldsymbol{\vartheta}^\star)) + \boldsymbol{\varepsilon} = \mathcal{G}(\boldsymbol{\vartheta}^\star) + \boldsymbol{\varepsilon}$$

MULTI-PHYSICAL STATE

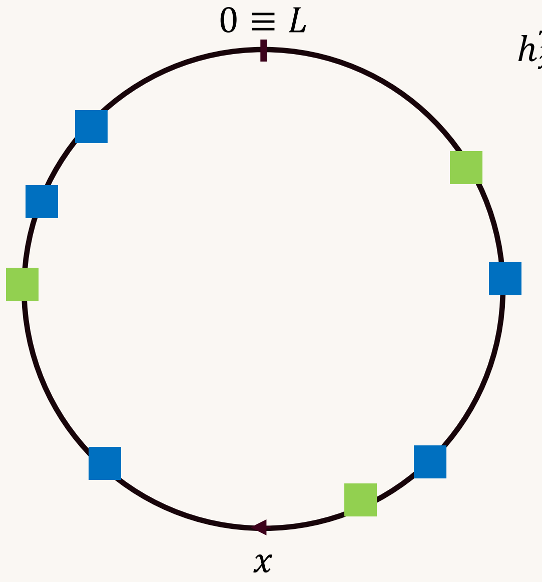
$$u(\boldsymbol{\vartheta}) = \{\psi^1, \dots, \psi^6, \mathrm{c}^1, \dots, \mathrm{c}^8, \mathrm{T}\}$$

SENSOR MODEL

$$\mathcal{H} = \left[h^{\psi^6}_{x_1}, \dots, h^{\psi^6}_{x_N}, h^{\mathrm{T}}_{x_1}, \dots, h^{\mathrm{T}}_{x_M}\right]^\top \subset \mathcal{O}$$

NOISE MODEL

$$\boldsymbol{\varepsilon} = \left[\varepsilon^{\psi^6}_{x_1}, \dots, \varepsilon^{\psi^6}_{x_N}, \varepsilon^{T}_{x_1}, \dots, \varepsilon^{T}_{x_M}\right]^\top \sim \mathcal{N}(0, \sigma\mathbf{I})$$



$$h^{T}_{x_1}(u) = \frac{\int_\Omega (T(x) - T_R) e^{\kappa \cos\left(\frac{2\pi(x - x_1)}{L}\right)} dx}{\int_\Omega \Delta T_R e^{\kappa \cos\left(\frac{2\pi(x - x_1)}{L}\right)} dx}$$

$$h^{\psi^6}_{x_1}(u) = \frac{\int_\Omega \psi^6(x) e^{\kappa \cos\left(\frac{2\pi(x - x_1)}{L}\right)} dx}{\int_\Omega \psi_R e^{\kappa \cos\left(\frac{2\pi(x - x_1)}{L}\right)} dx}$$

$\kappa = 5\times10^4$

$L = 12\mathrm{m}$

$\Delta T_R = 65.041\ \mathrm{K}$

$T_R = 900.000\ \mathrm{K}$

$\psi_R = 4.234\times10^{17}\ \mathrm{pm^{-2}s^{-1}}$

Optimal Sensor Selection

Average D-optimal Experimental Design

SENSOR DICTIONARY

$\mathcal{O} = \{h_1, h_2, \dots, h_{N_s}\}$. (accessible fields + locations)

BUDGET ALLOCATION

$\boldsymbol{\omega} = \{\omega_1, \omega_2, \dots, \omega_{N_s}\}, \qquad \sum_{k=1}^{N_s} \omega_k = 1, \qquad \omega_k > 0.$

LOCAL FISHER INFORMATION MATRIX

$$\mathrm{M}(\boldsymbol{\omega}; \boldsymbol{\vartheta}^\star) = \sum_{k=1}^{N_s} \omega_k \left. \frac{\partial h_k(u(\boldsymbol{\vartheta}))}{\partial \boldsymbol{\vartheta}} \right|_{\boldsymbol{\vartheta}^\star} \left. \frac{\partial h_k(u(\boldsymbol{\vartheta}))}{\partial \boldsymbol{\vartheta}} \right|_{\boldsymbol{\vartheta}^\star}^\top .$$

OPTIMAL EXPERIMENTAL DESIGN

$$\begin{aligned} \boldsymbol{\omega}_{\mathrm{opt}} &= \underset{\substack{\sum_{k=1}^{N_s} \omega_k = 1 \\ \omega_k > 0}}{\arg\min} \; - \int_{\mathcal{P}} \log\big(\det\big(M(\boldsymbol{\omega}; \boldsymbol{\vartheta})\big)\big)\, \Pi_0(d\boldsymbol{\vartheta}) \\ &\approx \underset{\substack{\sum_{k=1}^{N_s} \omega_k = 1 \\ \omega_k > 0}}{\arg\min} \; - \frac{1}{N_\Xi} \sum_{n=1}^{N_\Xi} \log\big(\det\big(M(\boldsymbol{\omega}; \boldsymbol{\vartheta}_n)\big)\big) := \bar{\Psi}(\boldsymbol{\omega}) \end{aligned}$$

employing the training set $\{u(\boldsymbol{\vartheta}_n),\ \boldsymbol{\vartheta}_n \sim \Pi_0(\boldsymbol{\Theta})\}_{n=1}^{N_\Xi}$, and (quasi-)Montecarlo integration

Optimization Algorithm

[Ucinski]

0. INITIALIZE $\boldsymbol{\omega}_0 = \{\omega_{0,1}, \omega_{0,2}, \dots, \omega_{0,N_s}\},\ \sum_{k=1}^{N_s} \omega_{0,k} = 1,\ \omega_{0,k} > 0$

FOR $s = 0, 1, 2, \dots$

1. **DIFFERENCIATE** $$\boldsymbol{\xi}_k(\boldsymbol{\omega}_s) = \frac{1}{N_\Xi} \sum_{n=1}^{N_\Xi} \left. \frac{\partial h_k\big(u(\boldsymbol{\vartheta})\big)}{\partial \boldsymbol{\vartheta}} \right|_{\boldsymbol{\vartheta}^\star}^{\top} \mathrm{M}^{-1}(\boldsymbol{\omega}_s; \boldsymbol{\vartheta}_n) \left. \frac{\partial h_k\big(u(\boldsymbol{\vartheta})\big)}{\partial \boldsymbol{\vartheta}} \right|_{\boldsymbol{\vartheta}^\star}^{\top} = \frac{\partial \bar{\Psi}(\boldsymbol{\omega})}{\partial \omega_k}$$

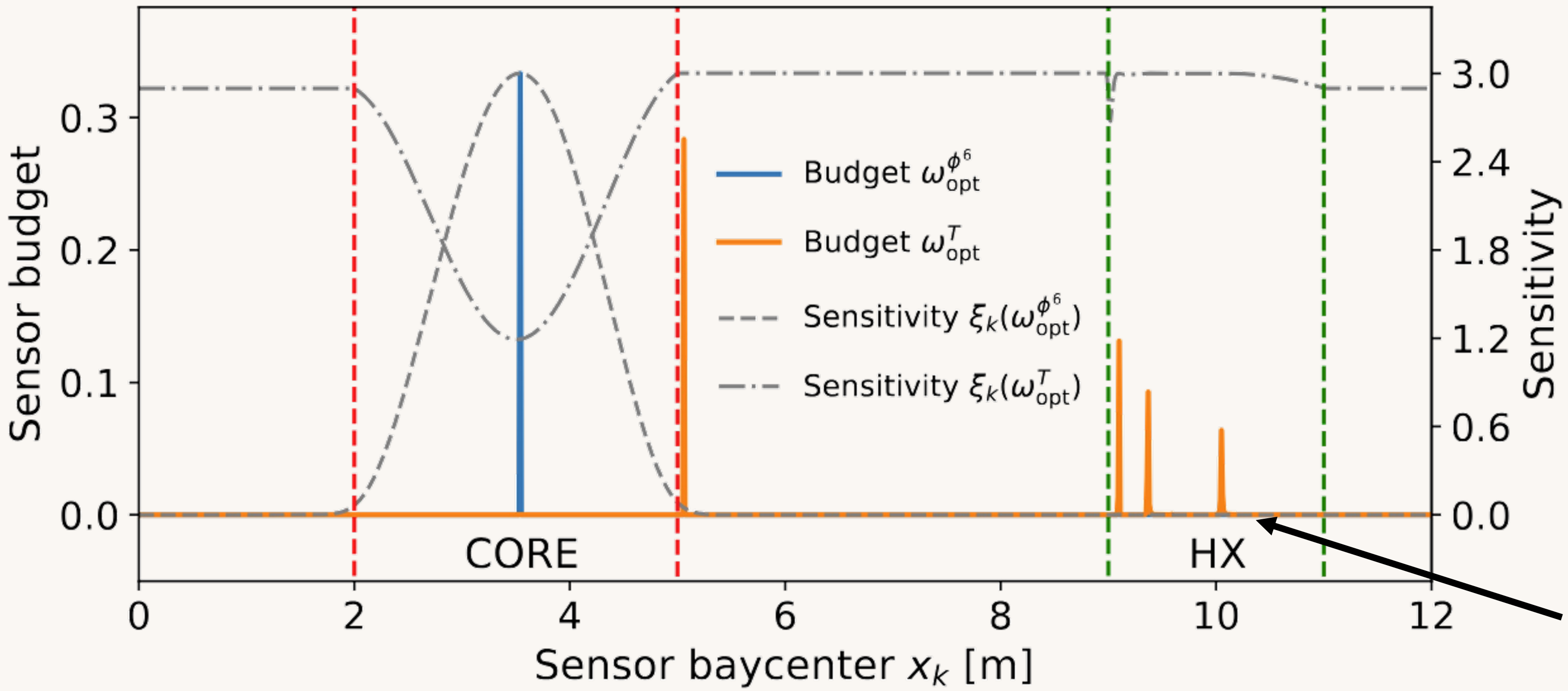
2. **MAXIMIZE** $$k_s^\star = \underset{k=1,\dots,N_\Xi}{\arg\min}\, \boldsymbol{\xi}_k(\boldsymbol{\omega}_s)$$

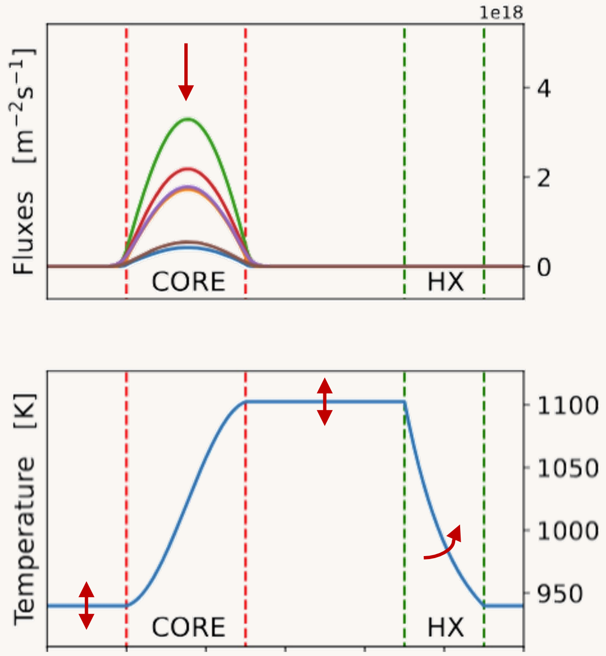
3. **LINE SEARCH** $$\gamma_s = \underset{0<\gamma<1}{\arg\min} -\frac{1}{N_\Xi} \sum_{n=1}^{N_\Xi} \log\Big(\det\big((1-\gamma) M(\boldsymbol{\omega}_s; \boldsymbol{\vartheta}_n)\big) + \gamma M(\boldsymbol{\delta}_{k,k_s^\star}; \boldsymbol{\vartheta}_n)\Big)$$

4. **UPDATE** $$\boldsymbol{\omega}_{s+1} = (1-\gamma_s)\boldsymbol{\omega}_s + \gamma_s \boldsymbol{\delta}_{k,k_s^\star}$$

⋆. **BREAK IF** $\xi_k(\boldsymbol{\omega}_s) - N_p < \mathrm{tol}$

Average D-optimal Experimental Design





The support of $\boldsymbol{\omega}_{opt}$ identifies the sensor in $\mathcal{H}$, and therefore $\mathcal{G}$

Ensemble Based Inversion

Maximum Likelihood Estimation

[Iglesias]

$$\boldsymbol{\vartheta}_{\mathrm{opt}} = \underset{\boldsymbol{\vartheta}\in\mathcal{D}}{\arg\max} \, \|\mathbf{d} - \mathcal{G}(\boldsymbol{\vartheta})\|^2_{(\sigma\mathbf{I})^{-1}}$$

0. SAMPLE $\{\boldsymbol{\vartheta}_0^s \sim \Pi_0(\boldsymbol{\Theta})\}_{s=1}^{N_E}$

FOR $s = 0, 1, 2, \ldots$

1. **EXACT PARAMETER-TO-MEASUREMENTS**

$$\{\mathcal{G}(\boldsymbol{\vartheta}_n^s) = \mathcal{H}u(\boldsymbol{\vartheta}_n^s)\}_{s=1}^{N_E}$$

2. **CORRELATION MATRICES**

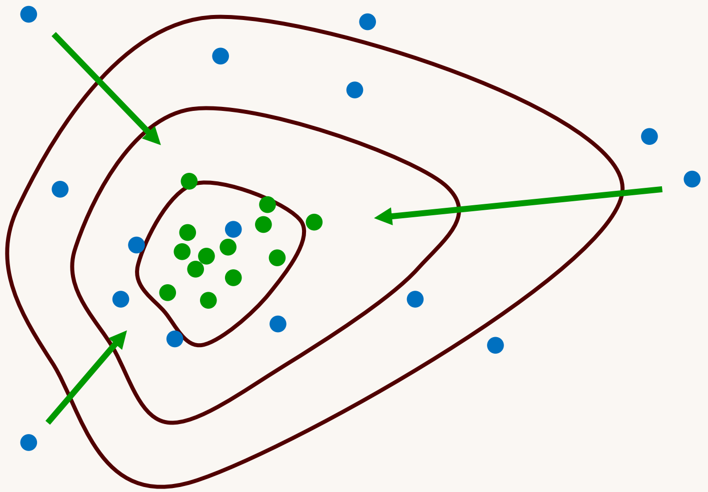
$$\boldsymbol{P}^s = \mathrm{cov}\big(\mathcal{G}(\boldsymbol{\vartheta}_n^s), \mathcal{G}(\boldsymbol{\vartheta}_n^s)\big), \quad \boldsymbol{Q}^s = \mathrm{cov}\big(\boldsymbol{\vartheta}_n^s, \mathcal{G}(\boldsymbol{\vartheta}_n^s)\big).$$

3. **ENSEMBLE KALMAN UPDATE**

$$\boldsymbol{\vartheta}_{n+1}^s = \boldsymbol{\vartheta}_n^s + \boldsymbol{Q}^s(\boldsymbol{P}^s + \sigma\mathbf{I})^{-1}(\mathbf{d} - \mathcal{G}(\boldsymbol{\vartheta}_n^s))$$

$$\boldsymbol{\vartheta}_0^s \sim \Pi_0(\boldsymbol{\Theta})$$

$$\boldsymbol{\vartheta}_n^s \sim \pi_0 \cdot f^s(\boldsymbol{\vartheta}|\mathbf{d})$$

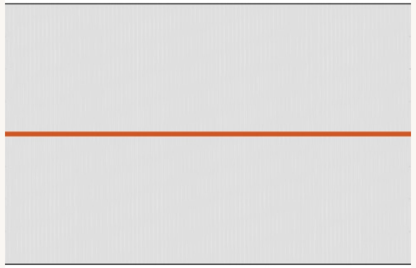


Surrogate Modeling

GPR IS USED TO SURROGATE THE PARAMETER-TO-OBSERVABLE MAP

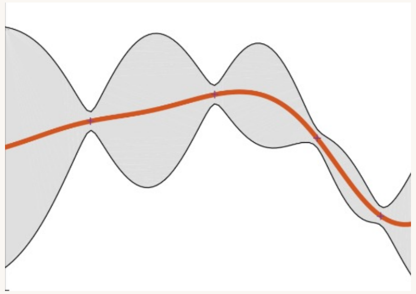
$\mathcal{G}(\boldsymbol{\vartheta}) \approx \mathcal{GP}(\boldsymbol{\vartheta}) \sim \mathcal{N}(\mu(\boldsymbol{\vartheta}), K_{\mathcal{GP}}(\boldsymbol{\vartheta}, \boldsymbol{\vartheta}'))$ ⟵ $\mathcal{N}(0, k^{\mathrm{pr}}(\boldsymbol{\vartheta}, \boldsymbol{\vartheta}'; \boldsymbol{\Lambda}))$: Bayesian Prior

$\boldsymbol{\Lambda}$: Optimized Hyper-parameters



- **COMPUTE THE TRAINING SET**

$$\Xi_{\mathcal{G}} := \{\mathcal{G}(\boldsymbol{\vartheta}_n) = \mathcal{H}u(\boldsymbol{\vartheta}_n),\ \boldsymbol{\vartheta}_n \in \boldsymbol{\Xi}_{\boldsymbol{\vartheta}}\}, \qquad \Xi_{\boldsymbol{\vartheta}} := \{\boldsymbol{\vartheta}_n \sim \Pi_0(\boldsymbol{\Theta})\}_{n=1}^{N_\Xi}$$



- **DEFINE THE TRAINING MEAN AND COVARIANCE**

$$(\boldsymbol{d}_{\mathrm{tr}})_i = \mathcal{G}(\boldsymbol{\vartheta}_i), \qquad (\mathbf{K}_{\mathrm{tr}})_{ij} = k^{\mathrm{pr}}\left(\boldsymbol{\vartheta}_i, \boldsymbol{\vartheta}_j; \boldsymbol{\Lambda}\right)$$

- **UPDATE MEAN AND COVARIANCE**

$$\mu(\boldsymbol{\vartheta}) = \boldsymbol{d}_{\mathrm{tr}}^{\top}\mathbf{K}_{\mathrm{tr}}^{-1} k^{\mathrm{pr}}(\boldsymbol{\vartheta}, \Xi_{\boldsymbol{\vartheta}}; \boldsymbol{\Lambda})$$

$$K_{\mathcal{GP}}(\boldsymbol{\vartheta}, \boldsymbol{\vartheta}') = k^{\mathrm{pr}}(\boldsymbol{\vartheta}, \boldsymbol{\vartheta}'; \boldsymbol{\Lambda}) - k^{\mathrm{pr}}(\boldsymbol{\vartheta}, \Xi_{\boldsymbol{\vartheta}}; \boldsymbol{\Lambda})^{\top}\, \mathbf{K}_{\mathrm{tr}}^{-1}\, k^{\mathrm{pr}}(\boldsymbol{\vartheta}', \Xi_{\boldsymbol{\vartheta}}; \boldsymbol{\Lambda}) \longrightarrow$$

We replace $\mathcal{G}(\boldsymbol{\vartheta})$ with surrogate random variable $\mathcal{GP}(\boldsymbol{\vartheta})$ and use the predictive variance $\mathrm{K}_{\mathcal{GP}}(\boldsymbol{\vartheta}, \boldsymbol{\vartheta})$ to inflate the measurement likelihood

Maximum Likelihood Estimation

$$\boldsymbol{\vartheta}_{\text{opt}} \approx \underset{\boldsymbol{\vartheta}\in\mathcal{D}}{\arg\max} \left\|\mathbf{d} - \mathcal{GP}(\boldsymbol{\vartheta})\right\|^2_{\left(\sigma\mathbf{I}+\mathrm{K}_{\mathcal{GP}}(\boldsymbol{\vartheta},\boldsymbol{\vartheta})\right)^{-1}}$$

0. SAMPLE $\{\boldsymbol{\vartheta}_0^s \sim \Pi_0(\boldsymbol{\Theta})\}_{s=1}^{N_E}$

FOR $s = 0, 1, 2, \ldots$

1. **SURROGATE PARAMETER-TO-MEASUREMENTS**

$$\{\mathcal{GP}(\boldsymbol{\vartheta}_n^s)\}_{s=1}^{N_E}$$

2. **CORRELATION MATRICES**

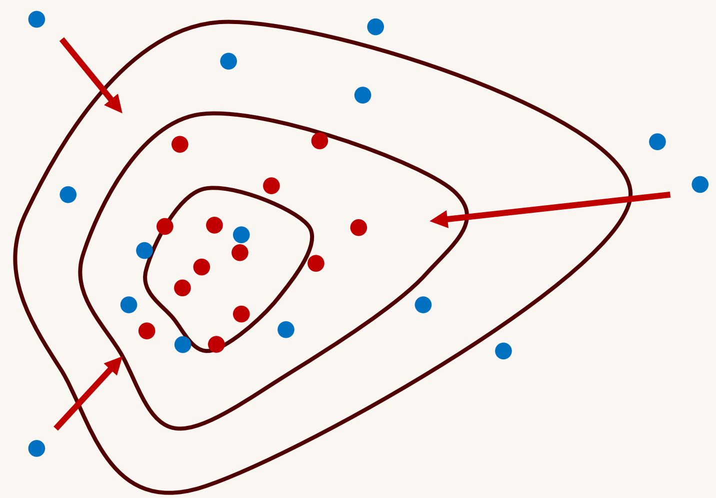
$$\boldsymbol{P}^s = \mathrm{cov}\left(\mathcal{GP}(\boldsymbol{\vartheta}_n^s), \mathcal{GP}(\boldsymbol{\vartheta}_n^s)\right), \qquad \boldsymbol{Q}^s = \mathrm{cov}\left(\boldsymbol{\vartheta}_n^s, \mathcal{GP}(\boldsymbol{\vartheta}_n^s)\right)$$

3. **INFLATED ENSEMBLE KALMAN UPDATE**

$$\boldsymbol{\vartheta}_n^{s+1} = \boldsymbol{\vartheta}_n^s + \boldsymbol{Q}^s\left(\boldsymbol{P}^s + \sigma\mathbf{I} + \mathrm{K}_{\mathcal{GP}}(\bar{\boldsymbol{\vartheta}}^s, \bar{\boldsymbol{\vartheta}}^s)\right)^{-1}(\mathbf{d} - \mathcal{GP}(\boldsymbol{\vartheta}_n^s))$$

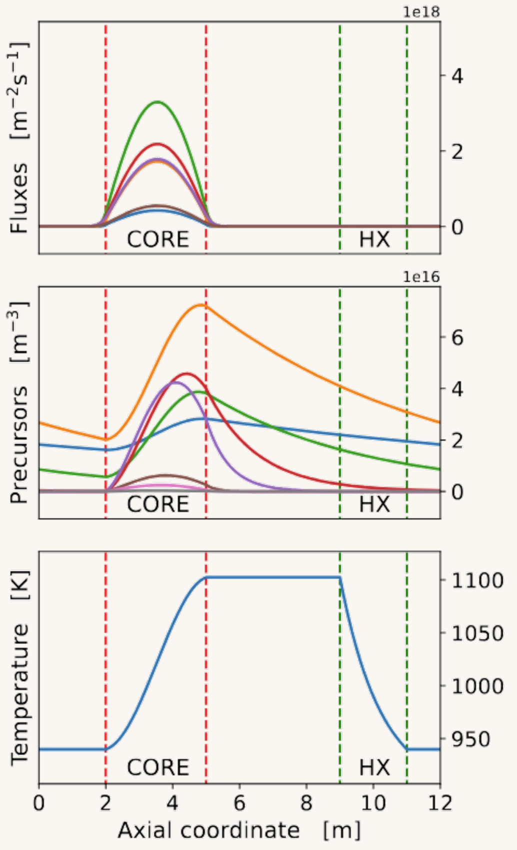
$\boldsymbol{\vartheta}_0^s \sim \Pi_0(\boldsymbol{\Theta})$

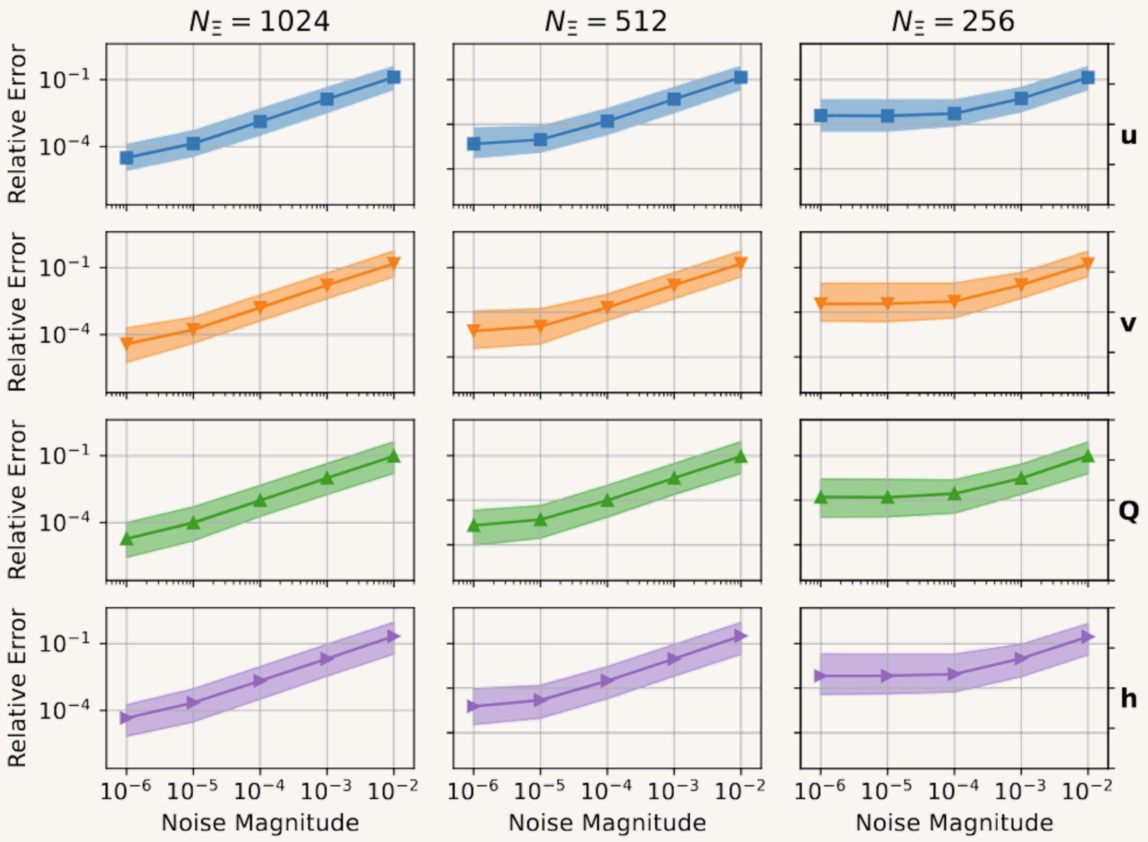
$\boldsymbol{\vartheta}_n^s \sim \pi_0 \cdot f^s(\boldsymbol{\vartheta}|\mathbf{d})$



Numerical Results

Noise and Accuracy Convergence

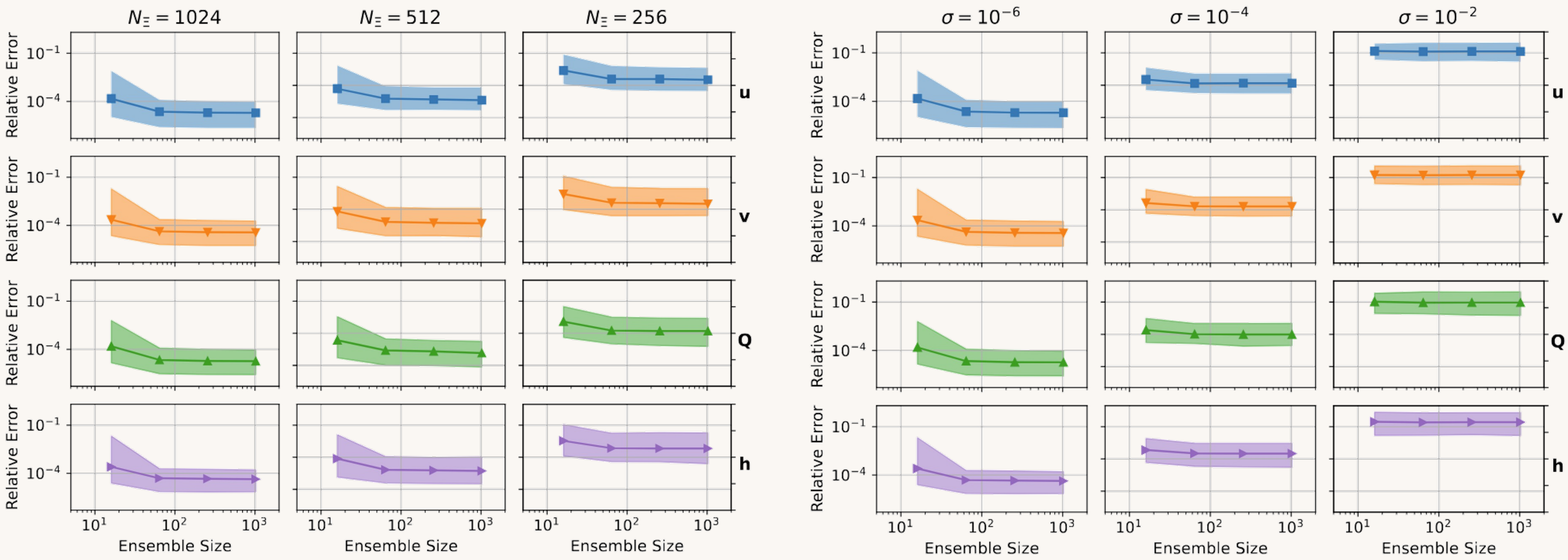




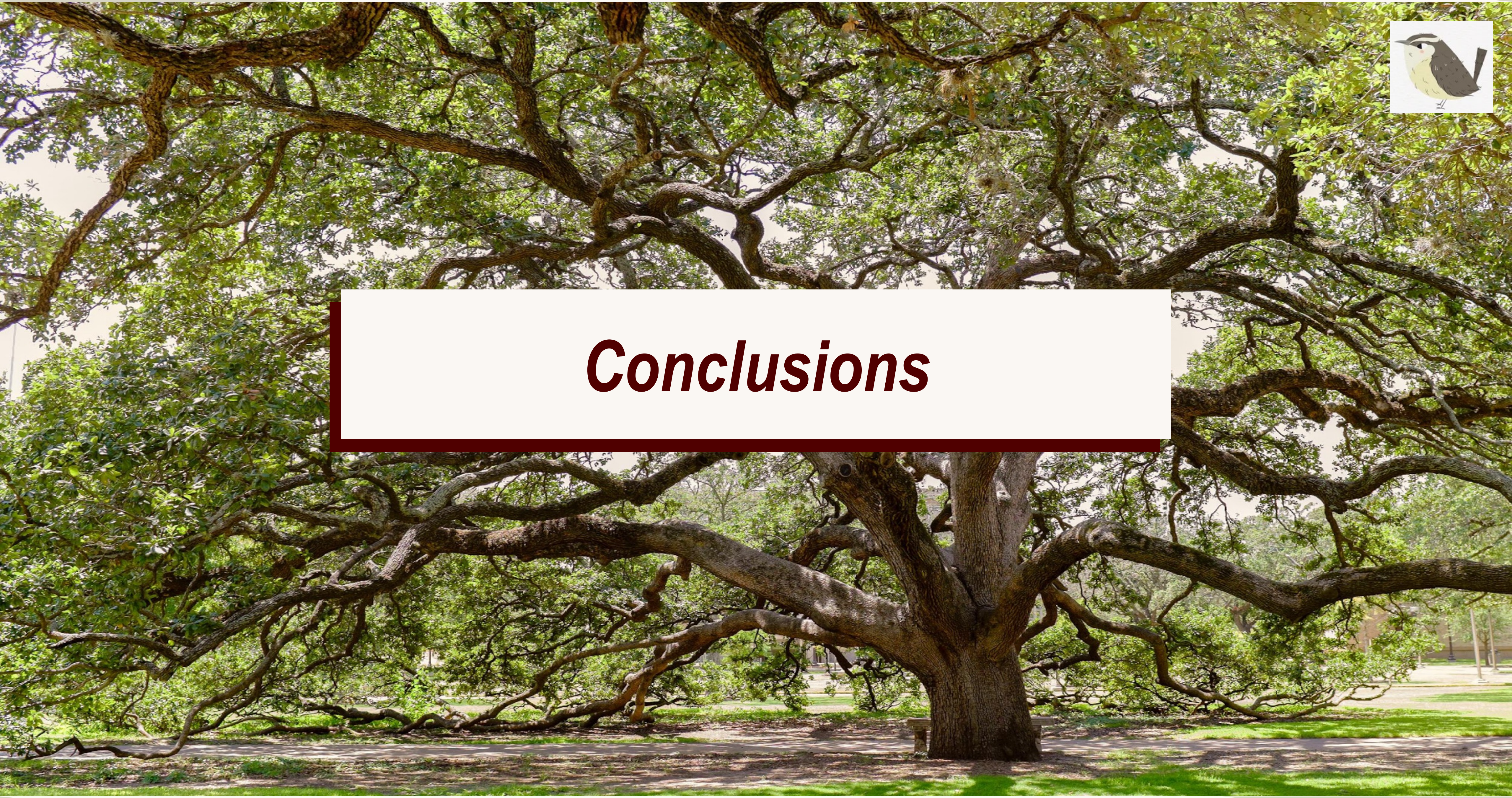
STATE RECONSTRUCTION ERROR

PARAMETER EXTIMATION ERROR

Large-ensemble Convergence



Conclusions



Summary and Developments

SUMMARY

- Computational framework for **parameter estimation** and **state reconstruction** in multi-physics nuclear systems
- Combination of **optimal Experimental Design** and **Ensemble Kalman Inversion**
- **Gaussian Process surrogates** accelerate inference while retaining accuracy
- Method successfully reconstructs reactor states from **sparse, noisy sensor data**

DEVELOPMENTS

- Explore advanced surrogate models **beyond** Gaussian Process Regression
- Incorporate **time-dependent** dynamics for transient analysis
- Extend framework to **higher-dimensional** nuclear reactor models

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THANK YOU

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