Metamodeling Techniques for Model Validation Applications*

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*Based on work by Dr. Dongli Huang and Mr. Jeongwon Seo

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What is Meta-Modeling?

- A computationally clever way to replace one model by another for a given target application

  - Original model is often **general-purpose**
  - Target application does not need all features of general-purpose model

  - Can you design another (meta) model with minimal complexity to perform same function of original model for intended target application?

Meta-Modeling Philosophy

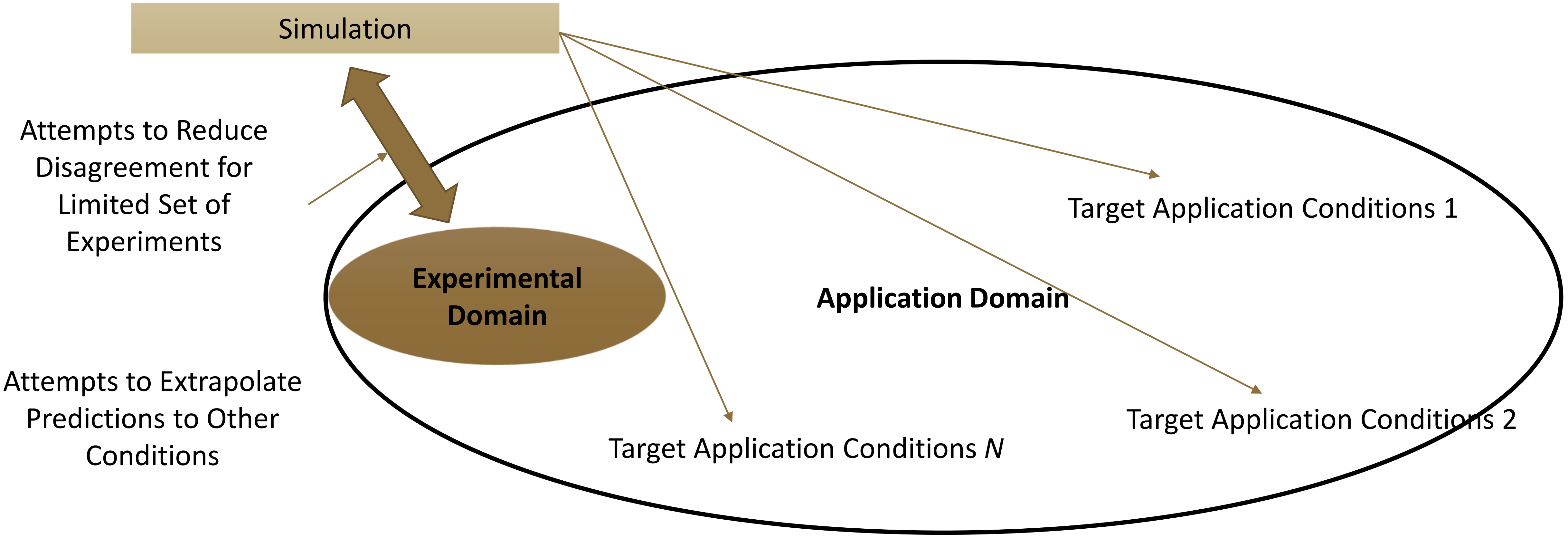
Vapnik's principle

"when solving a problem of interest, do not solve a more general problem as an intermediate step"

Meta-Modeling Context

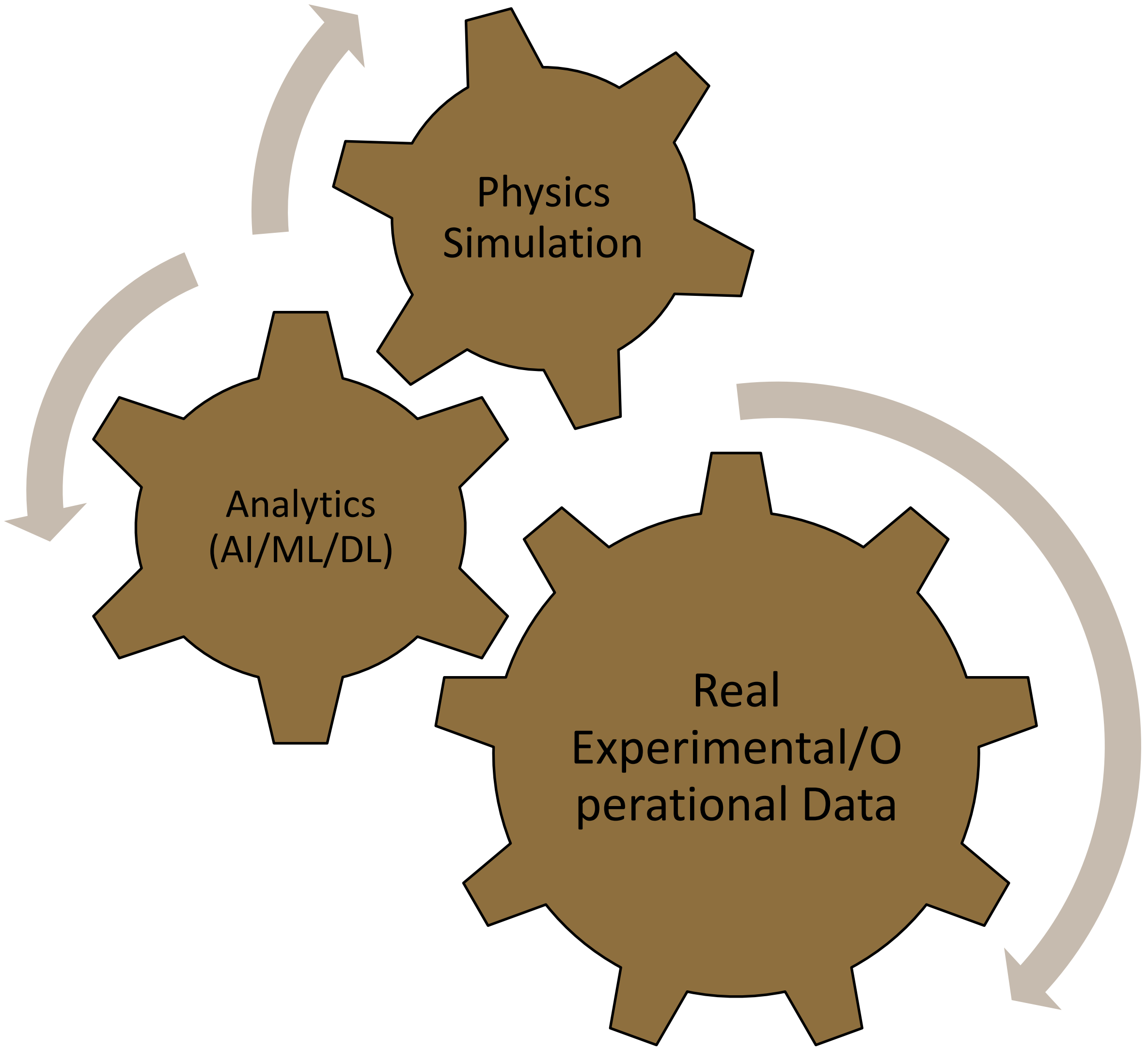
Meta-modeling is entangled with many other topics, e.g., surrogate modeling, reduced order modeling, model order reduction, predictive analytics, data mining, artificial intelligence, machine learning, pattern recognition, feature engineering, statistical inference, etc.

Central Problem in Model Validation



Premise of Analytics for Model Validation

- Optimal integration of experimental and computational branches of science requires
  1. **Efficient/Accurate Simulation**
     - Multi-Fidelity Tools/Reduced Order Modeling
  2. **Designing Relevant Experiments**
     - Quantifying/Optimizing Relevance
  3. **Characterize Confidence**
     - Quantifying uncertainties
     - Consolidate features extracted from simulation with those from experiments
     - Mapping uncertainties
  4. **Enabling Machine Learning Algorithms**



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- Reducing Dimensionality of Interfaces (more efficiency for UQ/SA/DA)
- Impact of Modeling Errors on Validation Domain and supporting Analyses
- Reducing Dimensionality of State Function (more efficient numerical solvers, i.e., born-reduced Models)
- Non-intrusive, forward models only

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Generalized definition of relevance (i.e., similarity) between experiments and application, suitable for

*multi-physics models,
*nonlinear feedback,
*non-Gaussian uncertainties,
*general non-matching responses,
*new/planned experiments, and
*prior knowledge

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- Realistic Measures of Confidence, i.e., go beyond the unrealistically high code-based uncertainties
- Realize value of high-fidelity simulation in capturing responses "correlations" very accurately.
- Assumptions-free approach for extracting, consolidating, and mapping features

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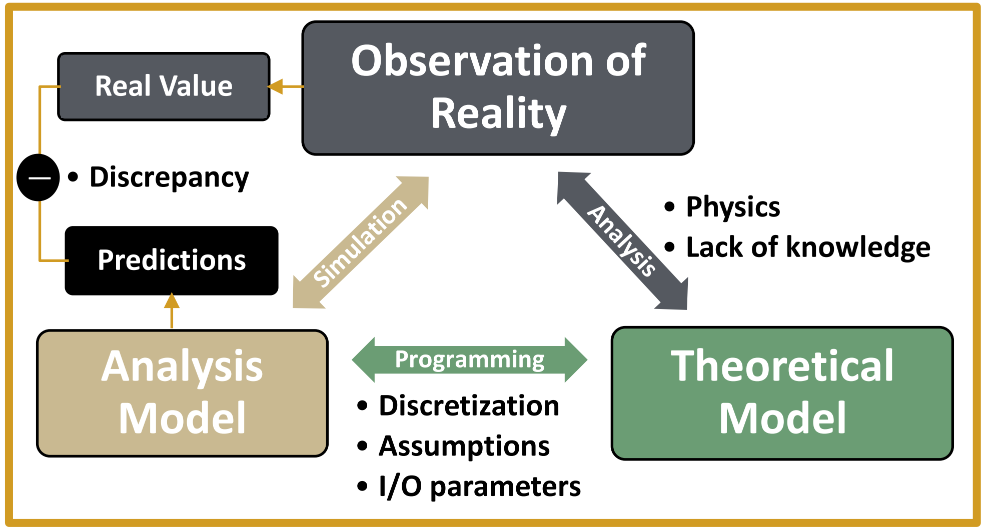
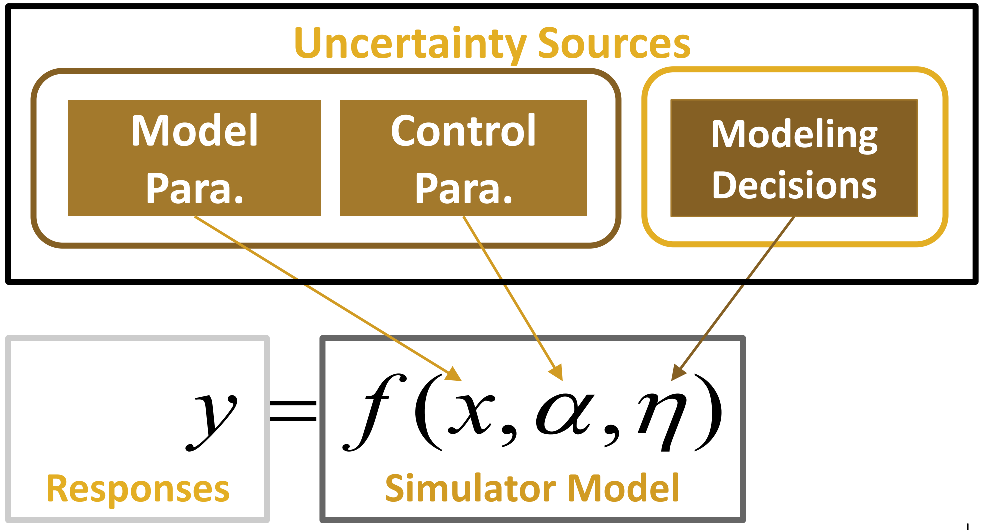
- Minimal Preprocessing
- Generic to Types of Responses
- Insensitivity to Modeling Errors
- Assumption-free Feature Extraction for Inference
- Reliable/Realistic Estimates of Mapped Uncertainties
- Experiment Relevance Optimization

Efficient/Accurate Simulation

- **Uncertainties in Reactor Physics Calculations**
  - Parameter uncertainties
    - ROM-based few-group cross-section covariance
    - Quantification and prioritization of uncertainty sources
    - Propagation of compressed cross-section library
  - Modeling uncertainties
    - Impact of modeling assumptions and approximations on uncertainty propagation

- **Applications:**
  - Water-cooled Reactors: BWR and CANDU-6 Representative Reactor Core Models





Efficient/Accurate Simulation

Reactor Physics Calculational Sequence

Past 15 years have seen wide adoption of ROM techniques for completing UQ/SA/DA analyses.

Raw Cross-Sections

- Differential cross-section measurement experiments

Point-wise Cross-Sections (ENDF)

- Para.: nuclear reaction model parameters
- Mod.: assumed flux shapes

*Para.: parameter uncertainty
Mod.: modeling uncertainty

Multi-Group Cross-Sections (Multi-Group Generation Codes)

- Para.: 44-group covariance, Sandwich equation
- Mod.: flux weights assumed to collapse cross-sections

Few-Group Cross-Sections (Lattice Calculations)

- Para.: MG uncertainties
- Mod.: boundary conditions, transport/stochastic solver, continuous/MG approx., numerical technique

Core Attributes (Core Simulator)

- Para.: FG uncertainties
- Mod.: diffusion solver, FG approx., numerical technique

ROM Methodology

Dimensionality Reduction Step

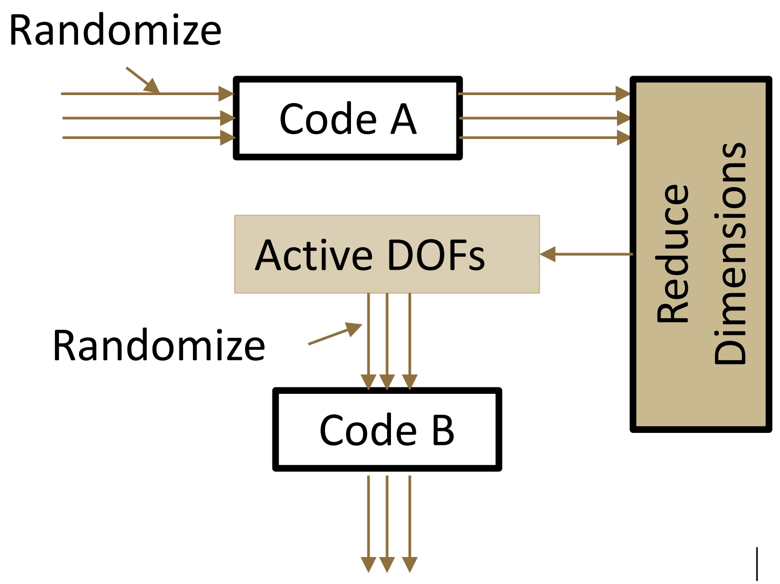
- Recast variables using active DOFs

$$y = f(x, \alpha, \eta) \quad \rightarrow \quad y^{(r)} = f(x^{(r)}, \alpha, \eta)$$

$$\mathbf{Q}_y y = f(\mathbf{Q}_x x, \alpha, \eta) \qquad \left| y - y^{(r)} \right| \le \varepsilon$$

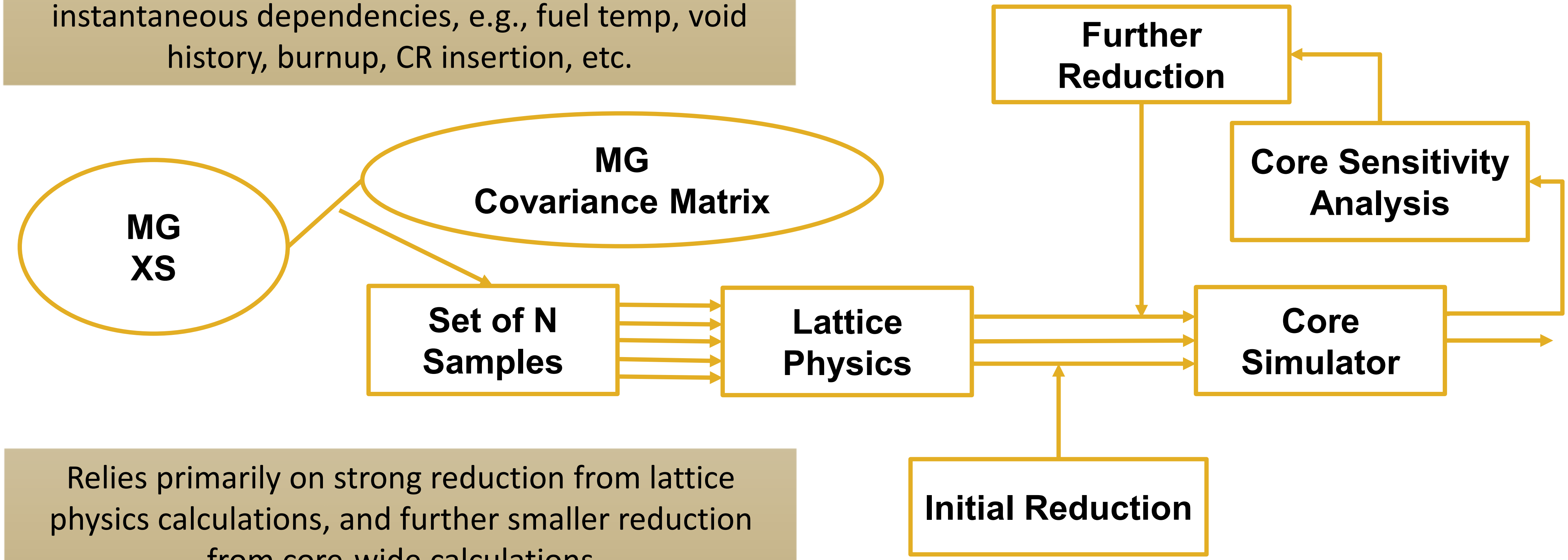
- Active DOFs can be captured using randomized Linear Algebra methods, e.g., Range Finding Algorithm
  - If applied in forward-mode only, it can reduce dimensionality of output code responses.
  - Applied successively at each code-to-code interface, it can reduce dimensionality for loosely-coupled codes
  - Active DOFs preserve nonlinear dependencies

$\mathbf{Q}_x$	Projector onto an active subspace
r	# Active Degrees of Freedom (DOFs)
ε	User-defined tolerance



Forward-based (Adjoint-Free) ROM Methods

ROM reconstructs all FG XS historical and instantaneous dependencies, e.g., fuel temp, void history, burnup, CR insertion, etc.



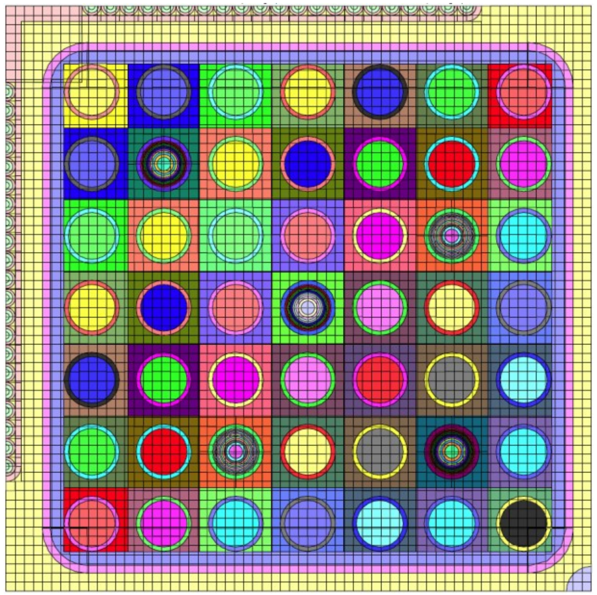
Relies primarily on strong reduction from lattice physics calculations, and further smaller reduction from core-wide calculations

DOFs very small (~ few tens) and weakly sensitive to lattice types and core loading pattern

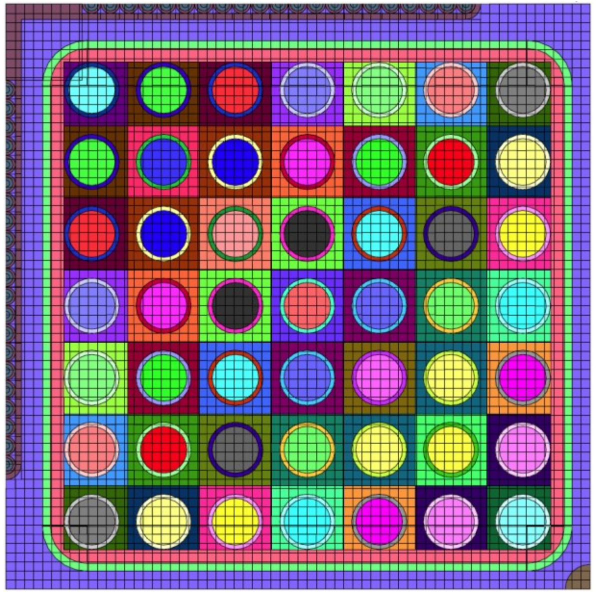
Efficient/Accurate Simulation: ROM Application to BWR Example

BWR Lattice and Core Models

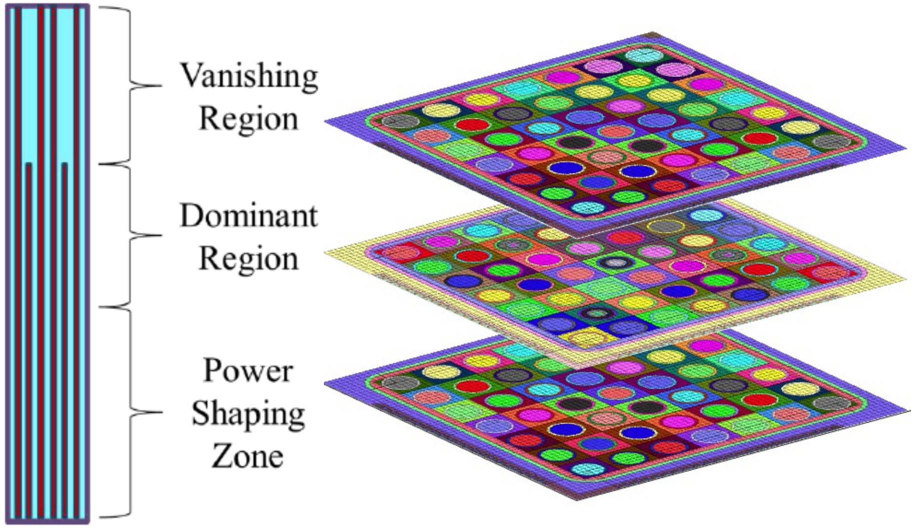
- 7x7 BWR lattice model by TRITON-NEWT through 32 depletion steps
- Quarter core model (11x11) along 30 axial nodes by NESTLE

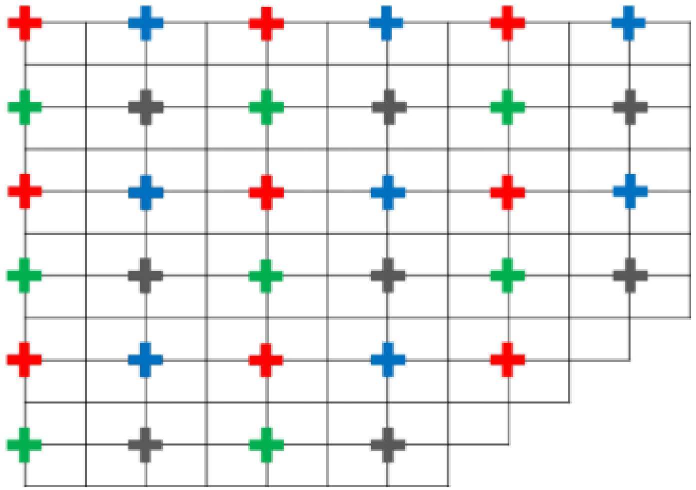


Type 3c lattice w/ Gd_2O_3



Type 1 lattice w/o Gd_2O_3

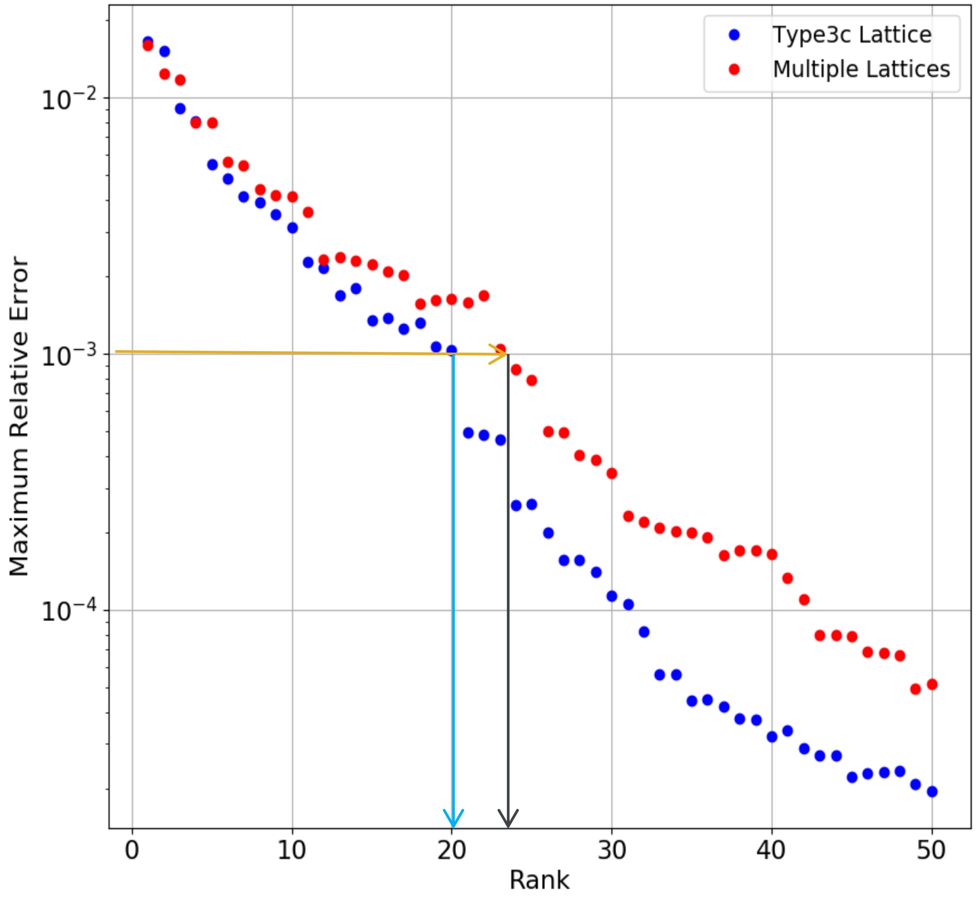




Efficient/Accurate Simulation: ROM Application to BWR Example

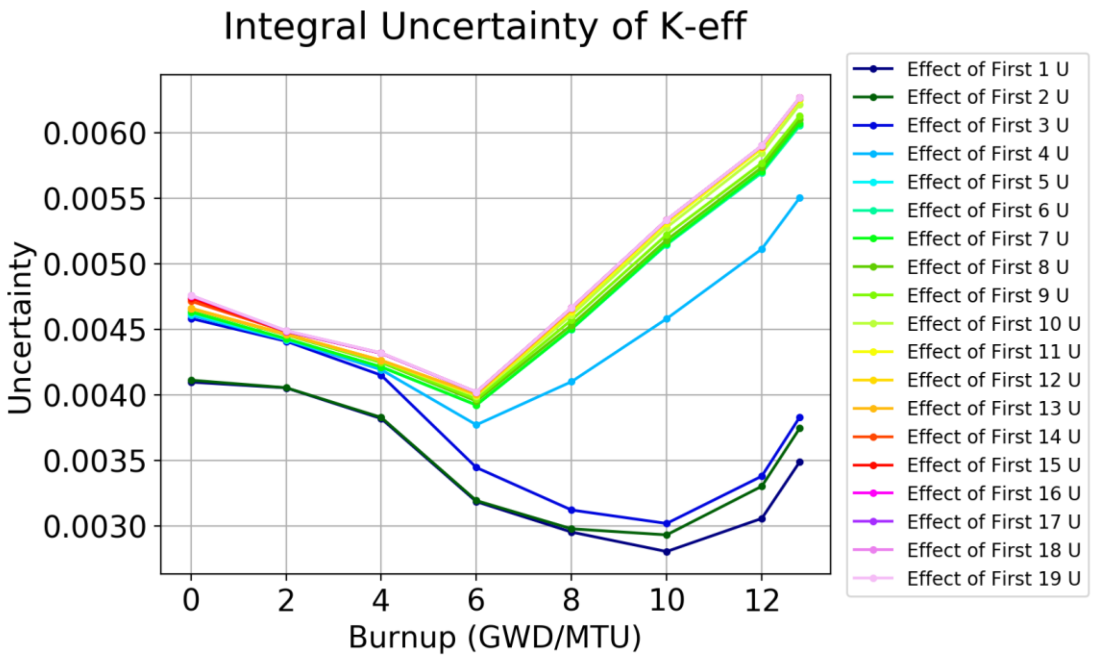
Active DOFs for single/multiple lattices

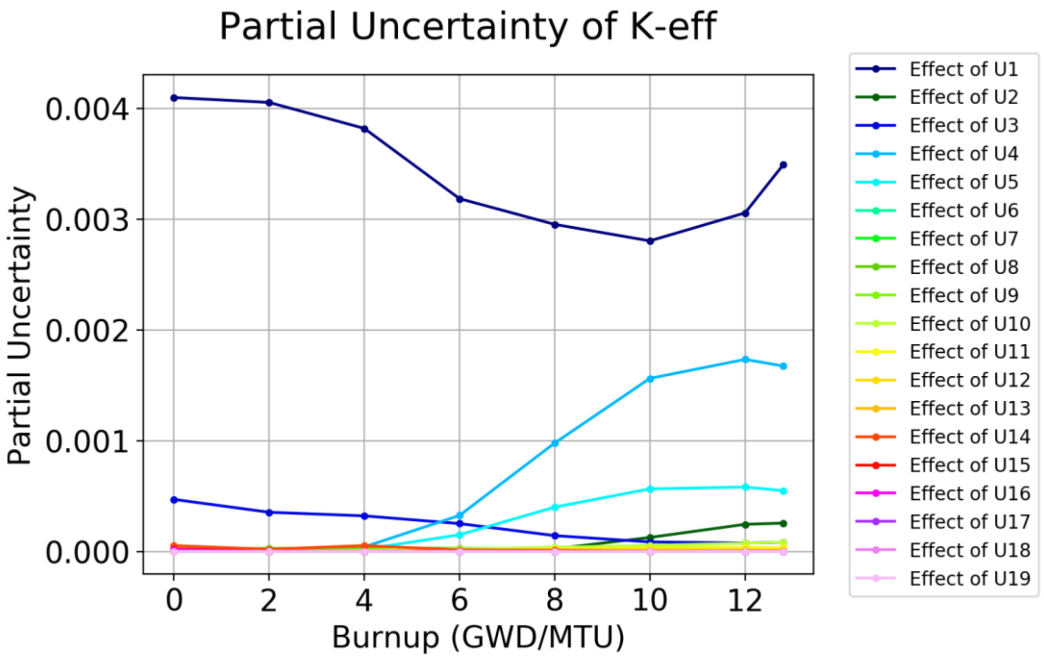
Single Lattice	Multiple Lattices
0.1% accuracy	0.1% accuracy
20 active DOFs	23 active DOFs



Efficient/Accurate Simulation: ROM Application to BWR Example

Core k-eff UQ and SA





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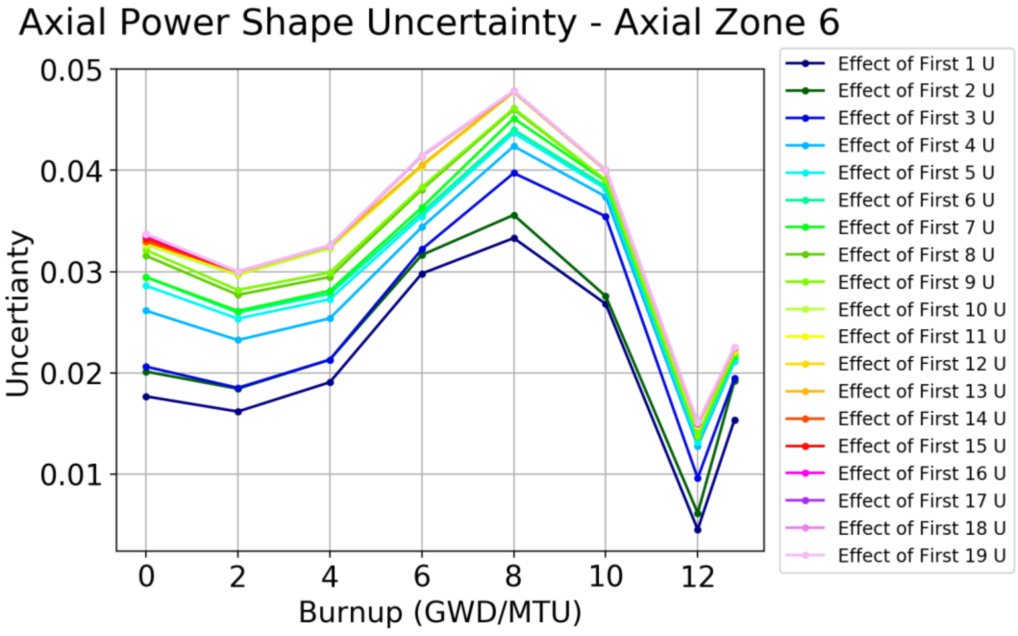
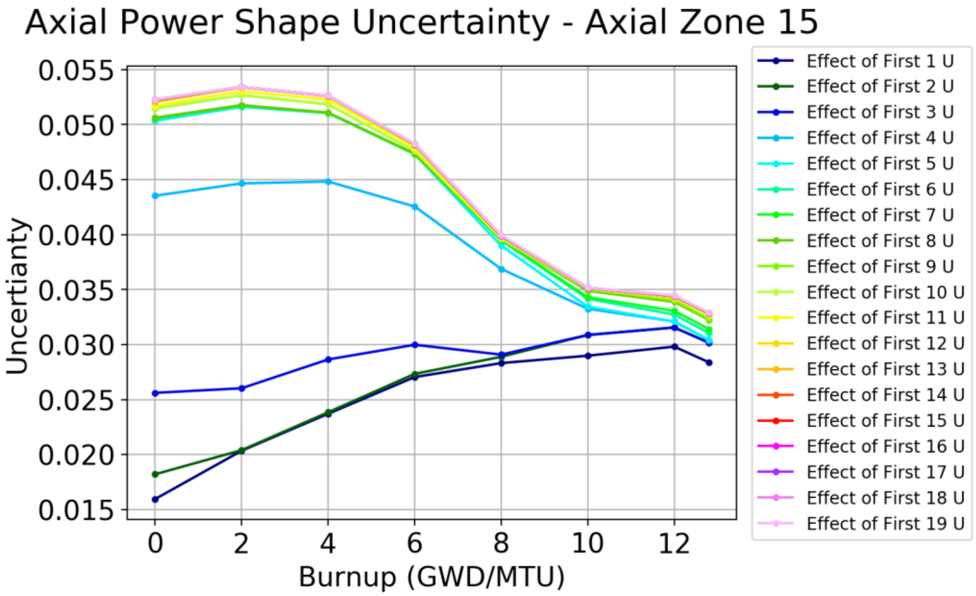
U vectors form a basis for FG XS variations

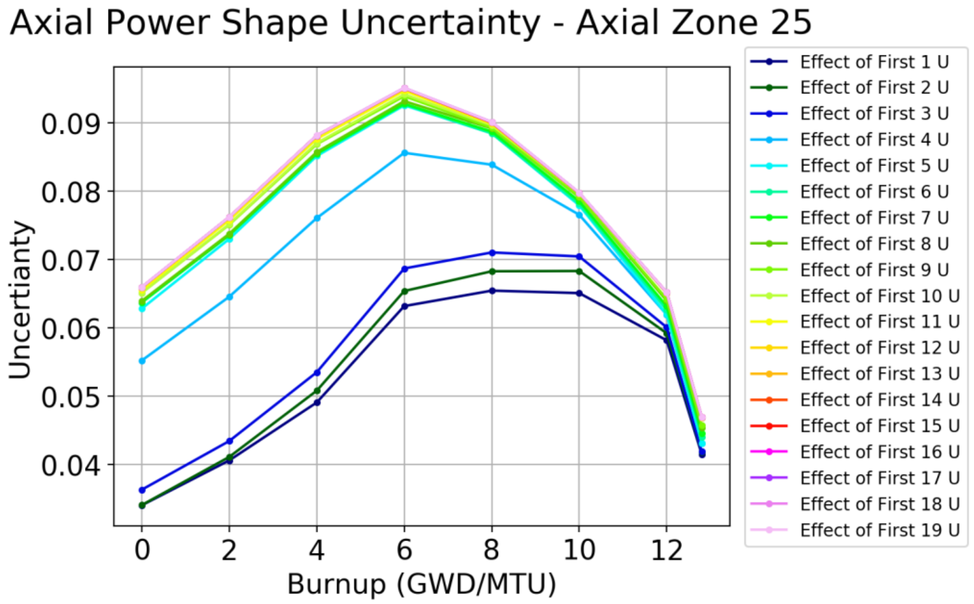
Nominal FG XS Dimensions ~ 10^4.

Efficient/Accurate Simulation: ROM Application to BWR Example

Axial Power Shape UQ

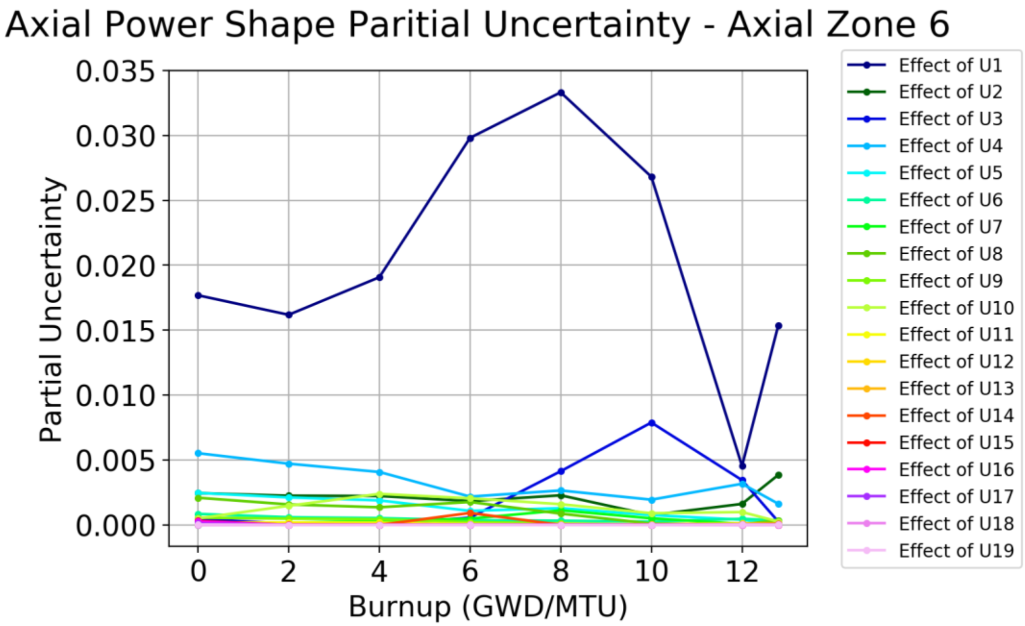


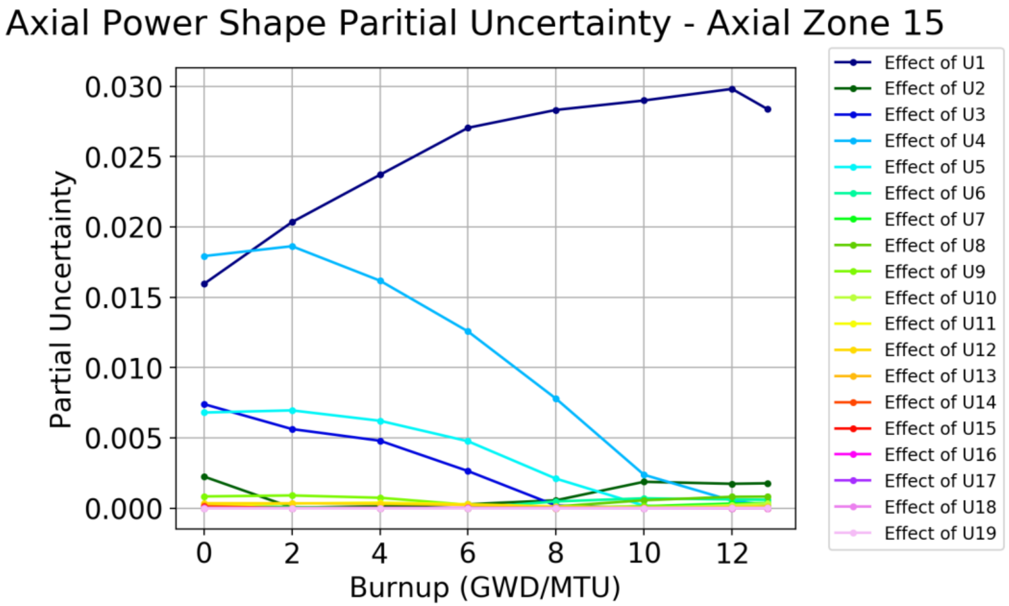


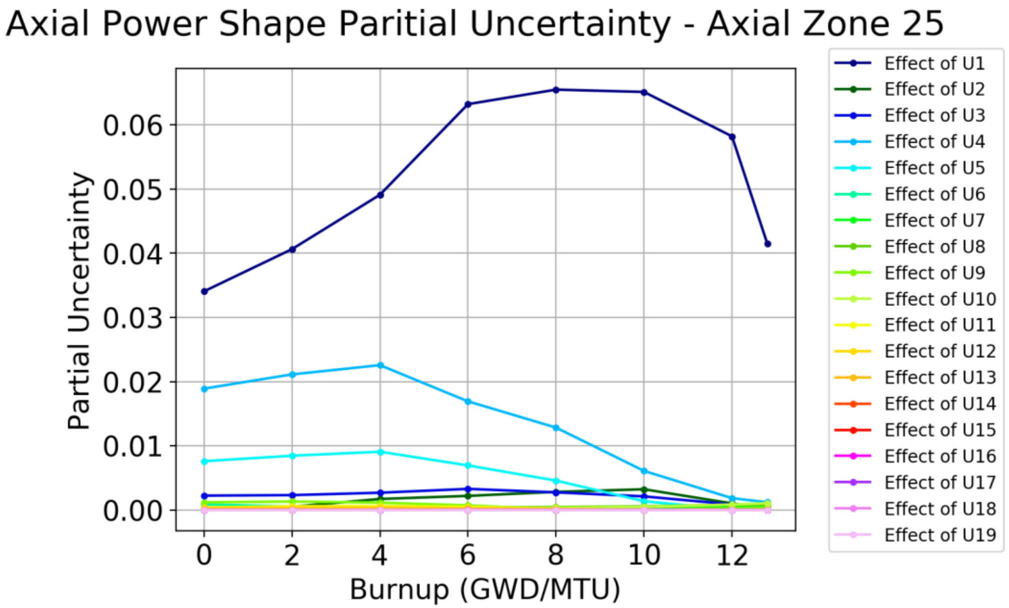


Efficient/Accurate Simulation: ROM Application to BWR Example

Axial Power Shape SA







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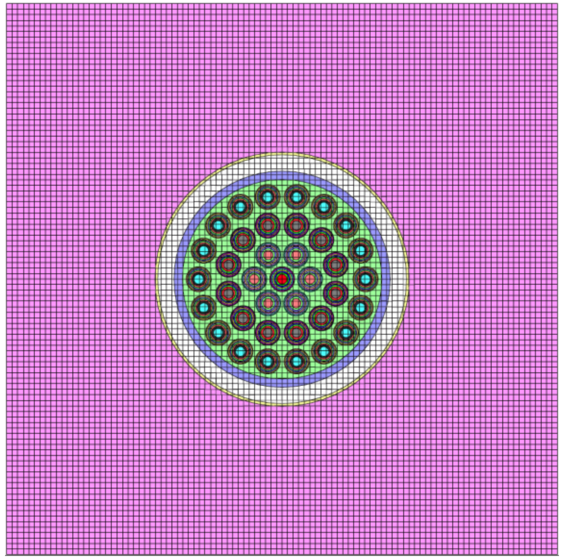
Importance Ranking for Active DOFs 1-19

	k_eff	Node 4	Node 6	Node 8	Node 10	Node 12	Node 14	Node 16	Node 18	Node 20	Node 22	Node 24	Node 26
Effect of U1	1	1	1	1	1	1	1	1	1	1	1	1	1
Effect of U2	5	2	3	3	4	5	5	5	3	5	5	5	5
Effect of U3	4	4	4	6	8	4	4	4	4	4	4	4	4
Effect of U4	2	3	2	2	2	2	2	2	2	2	2	2	2
Effect of U5	3	5	6	4	3	3	3	3	5	3	3	3	3
Effect of U6	15	8	8	8	5	7	7	8	12	8	8	7	8
Effect of U7	12	9	9	10	11	12	12	11	8	12	12	12	12
Effect of U8	7	6	7	7	9	9	8	6	7	9	9	8	7
Effect of U9	8	10	10	9	6	6	6	7	13	7	6	6	6
Effect of U10	6	7	5	5	7	8	10	12	6	6	7	9	9
Effect of U11	10	12	12	11	10	10	11	10	11	11	11	10	10
Effect of U12	11	13	13	12	12	11	9	9	10	10	10	11	11
Effect of U13	19	16	17	18	14	13	14	15	17	16	14	14	14
Effect of U14	9	11	11	13	13	14	13	13	9	13	13	13	13
Effect of U15	13	14	14	16	17	17	18	18	15	17	17	17	17
Effect of U16	14	15	15	14	15	16	17	14	14	14	15	15	15
Effect of U17	17	17	16	15	16	15	15	16	16	15	16	16	16
Effect of U18	16	19	19	19	19	19	19	19	19	18	18	18	18
Effect of U19	18	18	18	17	18	18	16	17	18	19	19	19	19

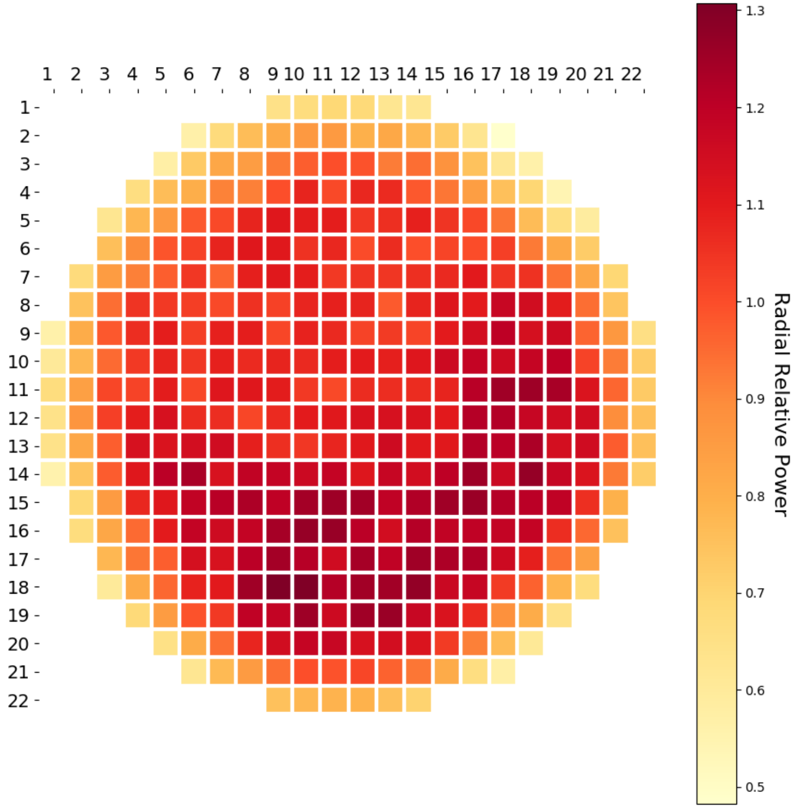
Efficient/Accurate Simulation: ROM Application to CANDU Example

CANDU Bundle Model and Core Configuration



Parameter	Dimension
Lattice pitch (square)	28.575 cm
Length of bundle	49.53 cm
Core length	594.36 cm
Core radius	379.7 cm
Channel count	380
Fuel bundles per channel	12
Fuel type	Natural Uranium
Fuel bundle type	37-element
Heavy Water Moderator Purity	99.97 wt% D_2O
Heavy Water Coolant Purity	99.20 wt% D_2O
# LZCs	14
# SORs	28
# ARs	21

- 37 fuel-pin bundle model by NEWT (and Serpent for comparison) in 37 depletion steps
- 300 Sampler runs

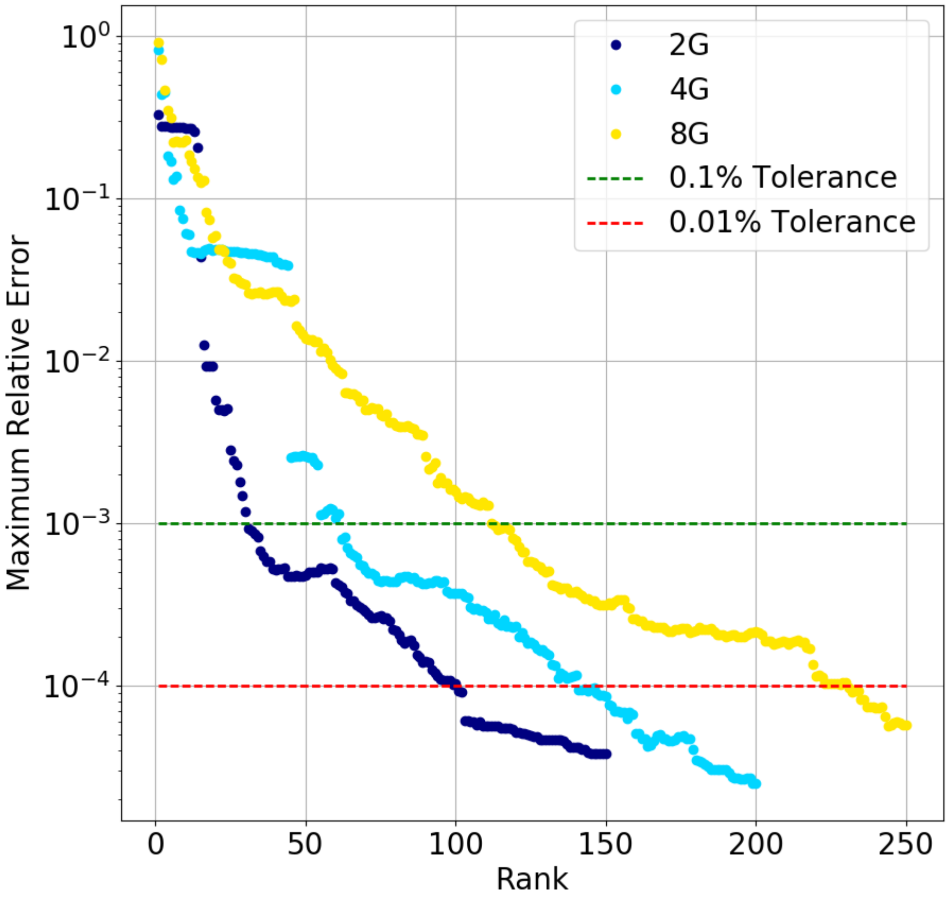


- CANDU-6 full core model
- NESTLE-C core simulator

Efficient/Accurate Simulation: ROM Application to CANDU Example

Active DOFs of FG Covariance in 2, 4, and 8G structure

Group Structure	0.1% Tolerance	0.01% Tolerance
2G	30 DOFs	100 DOFs
4G	60 DOFs	140 DOFs
8G	120 DOFs	230 DOFs



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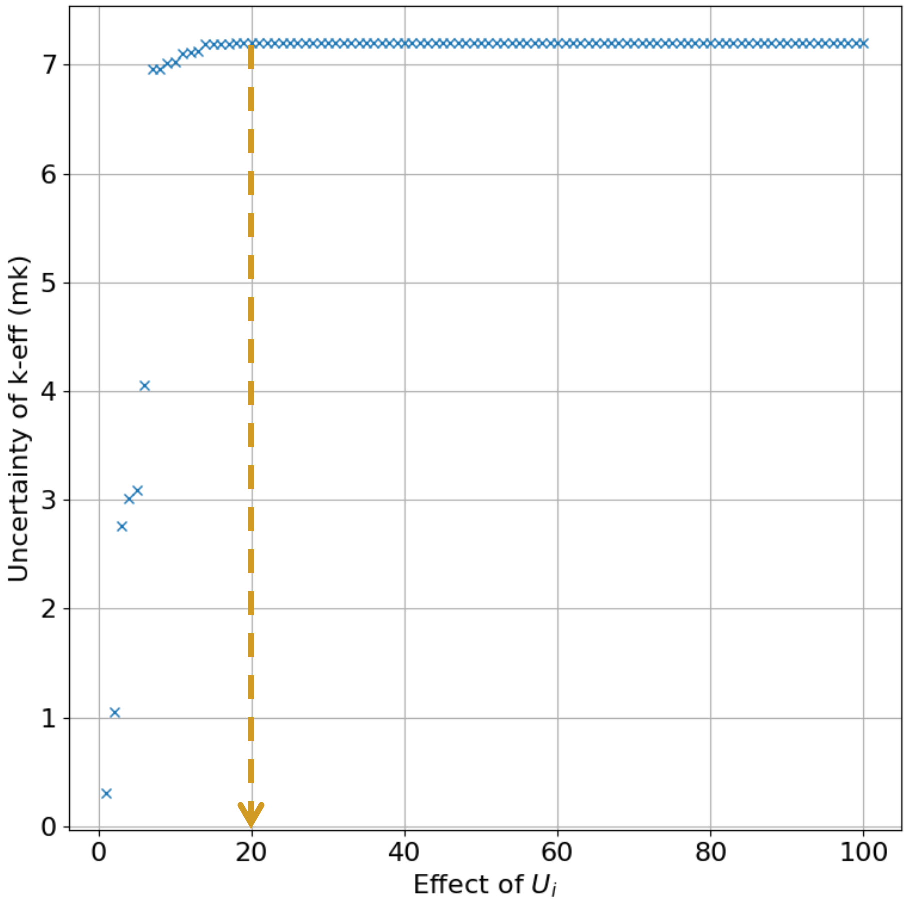
Uncertainty of Core k-eff

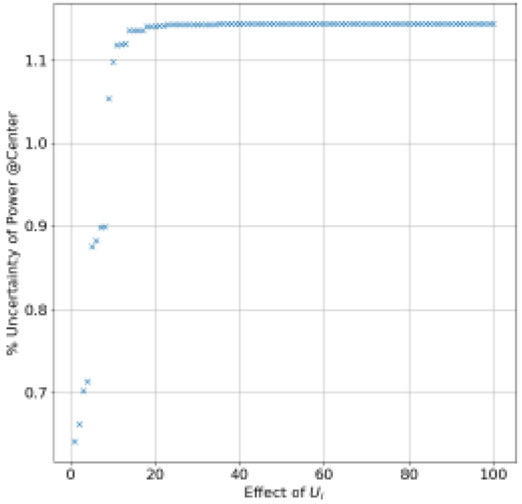
- Core k-eff sensitive to few active DOFs, much smaller than nominal cross-section dimensionality.



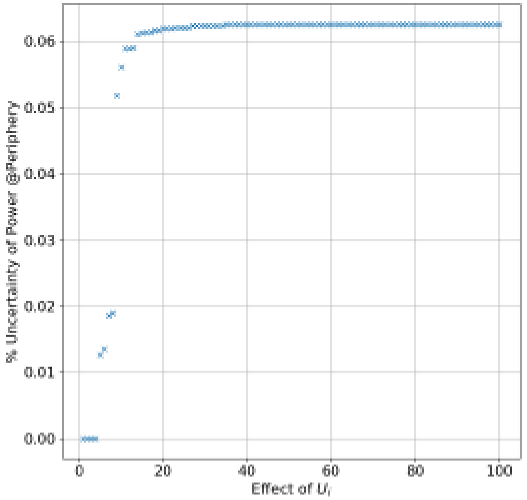
Efficient/Accurate Simulation: ROM Application to CANDU Example

Uncertainty of Core Power Distribution

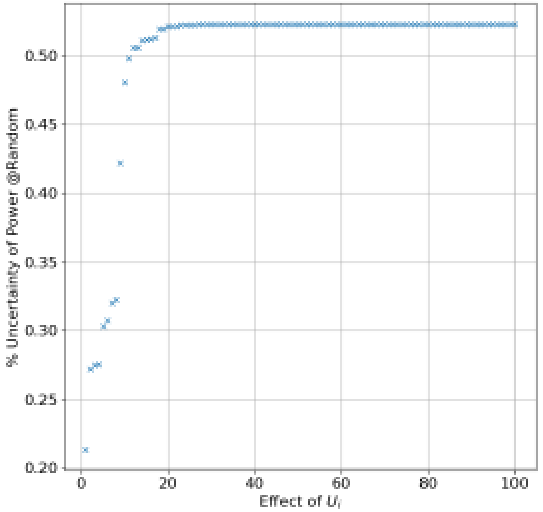
- ROM-based core power uncertainty at three different positions:
  - in the center
  - on the periphery
  - at a random mesh point
- Rank is insensitive to type of response, i.e., k-eff, flux, power, etc.



Power Uncertainty in the Center



Power Uncertainty on the Periphery

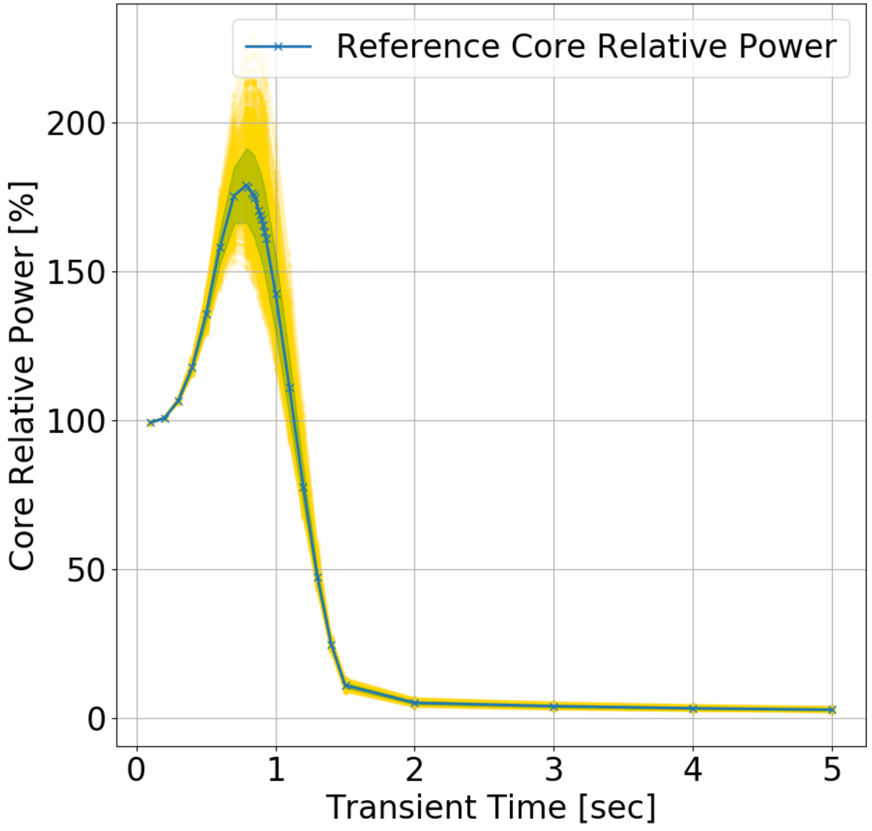


Power Uncertainty at a Random Position

Efficient/Accurate Simulation: ROM Application to CANDU Example

LOCA Core Model - UQ

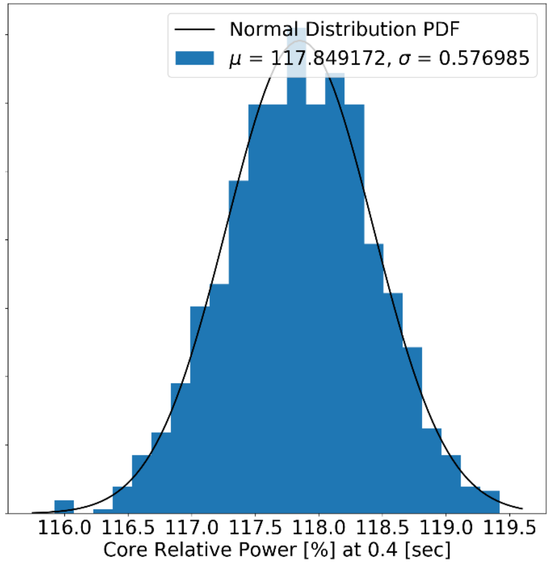
- Reference core relative power vs time marked by blue line
- Standard deviation of core power uncertainty in light blue band
- Randomized samples in gold band
- All trends can be reconstructed by same active DOFs from steady state calculations.

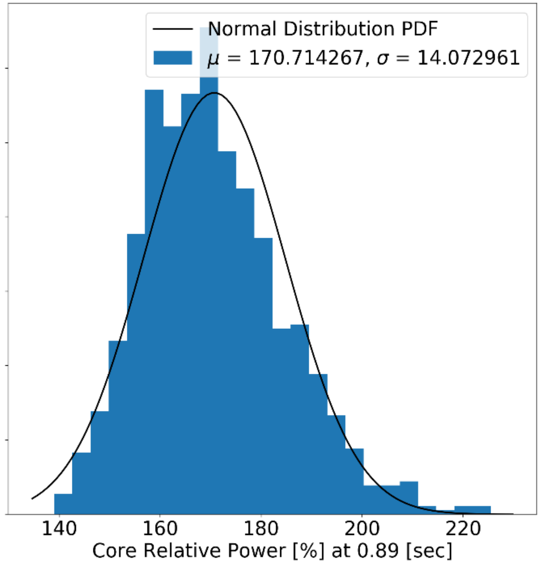


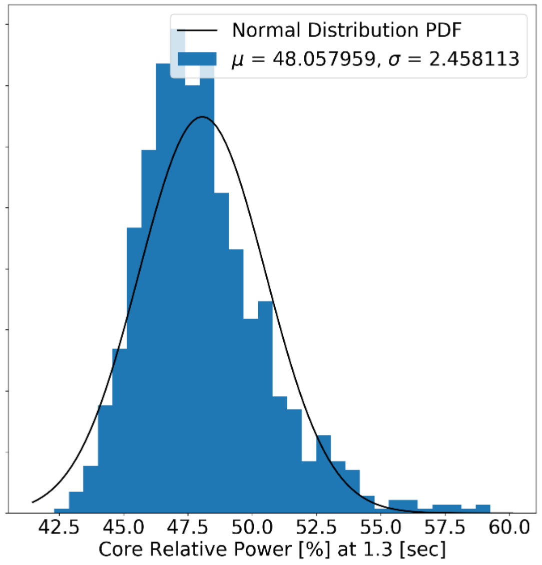
Efficient/Accurate Simulation: ROM Application to CANDU Example

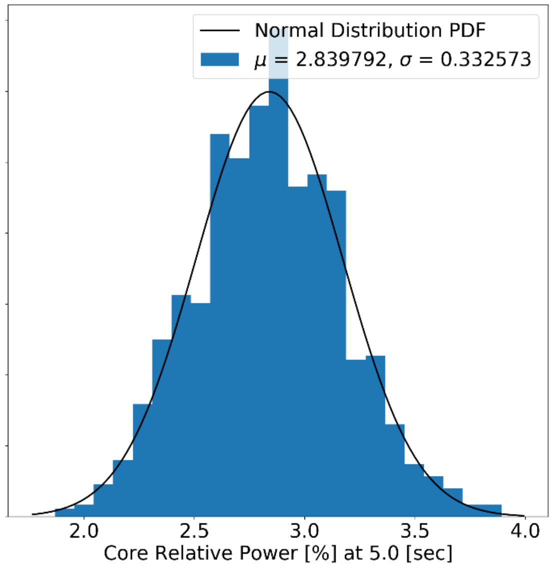
LOCA Core Model - UQ

- Uncertainties of core power at selected time steps
- Shifting from normal distribution around the peak location (0.89 sec)
- Nonlinearity in transient core model









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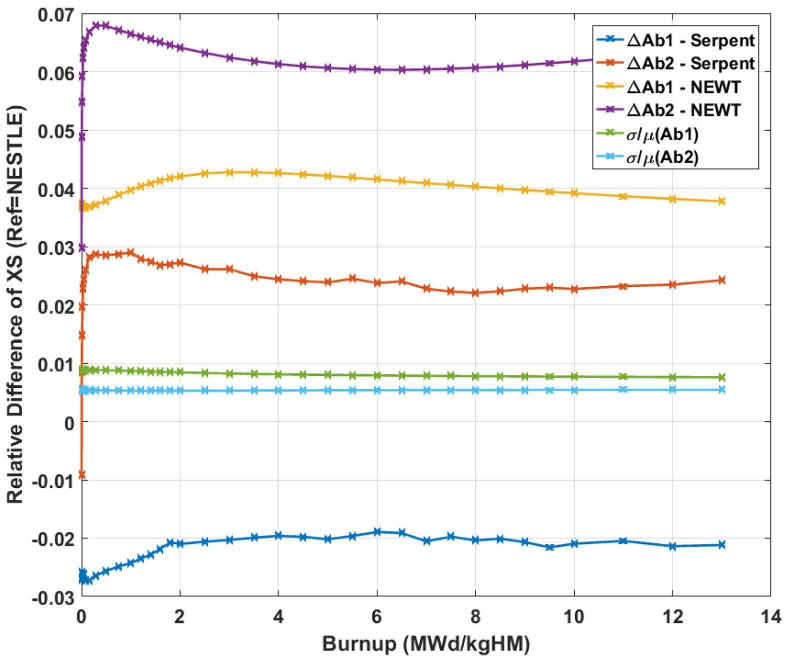
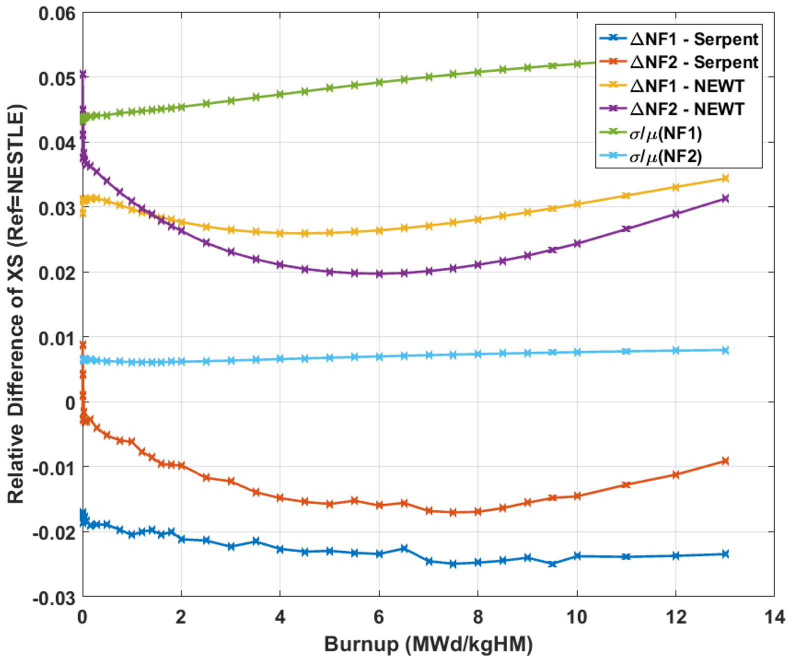
Efficient/Accurate Simulation: ROM Application to CANDU Example

Modeling Discrepancy vs. Parameter Uncertainty

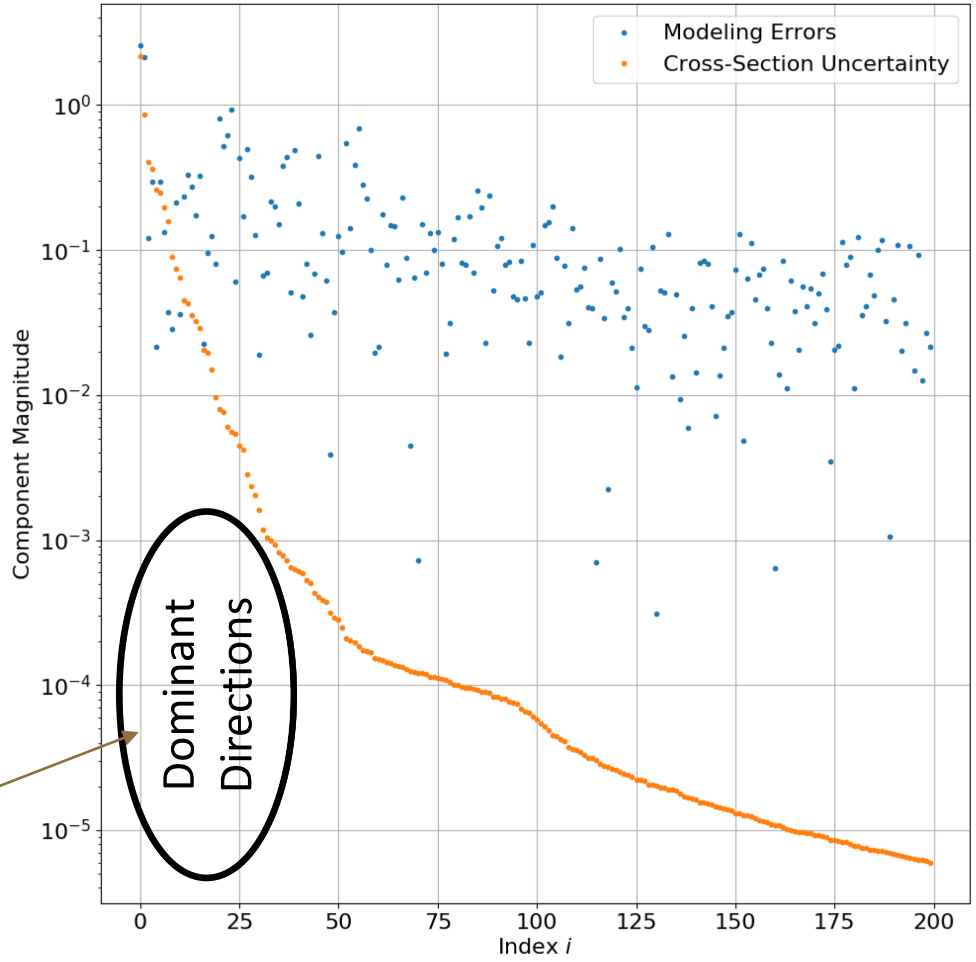




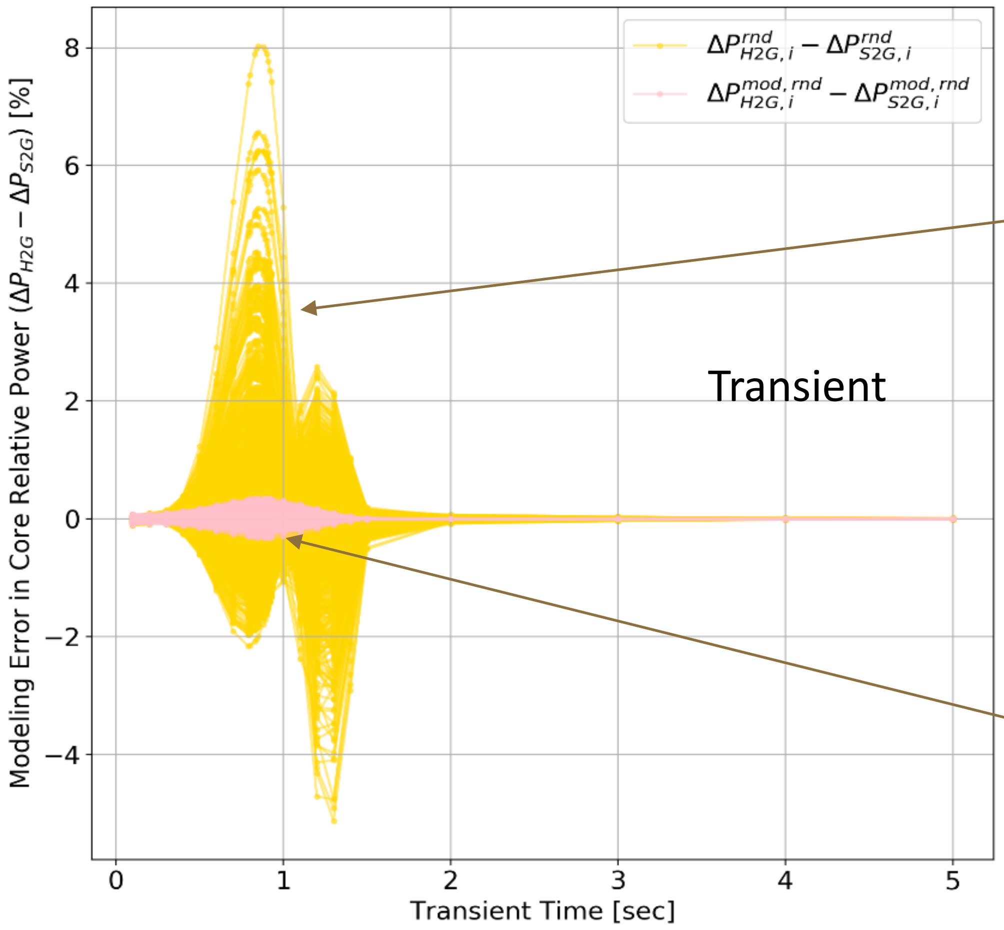
- Comparison of modeling error and cross-section uncertainty
- Modeling errors and XS standard deviations are in the same order of magnitude

Modeling Error-Preserving Sampling: NESTLE-C-based CANDU Core Case

- For Few-Group XS, this figure compares modeling errors and XS standard deviation along each of the eigen directions of covariance matrix
  - Eigen directions transform original variables into a set of uncorrelated statistical variables
- UQ analysis perturbs XS along dominant eigen directions, effectively changing modeling errors in each sampled random run
- DA adjusts XS along dominant directions, assuming modeling errors independent of XS uncertainties



Modeling Error-Preserving Sampling: NESTLE-C-based CANDU Core Case

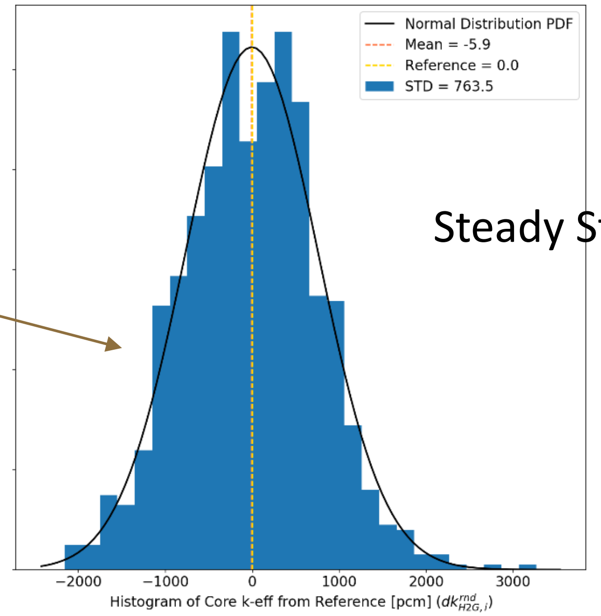


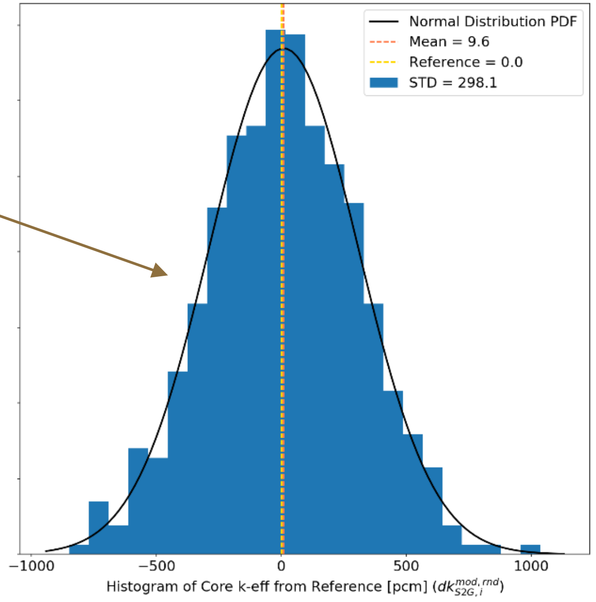
Transient

Prior Covariance-based Random sampling

Modeling Errors-preserving sampling

Steady State





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Designing “Relevant” Experiments

- To support assimilation of experimental and simulation results, model validation requires ability to design, select, and/or optimize “relevant” experiments using quantitative metrics.

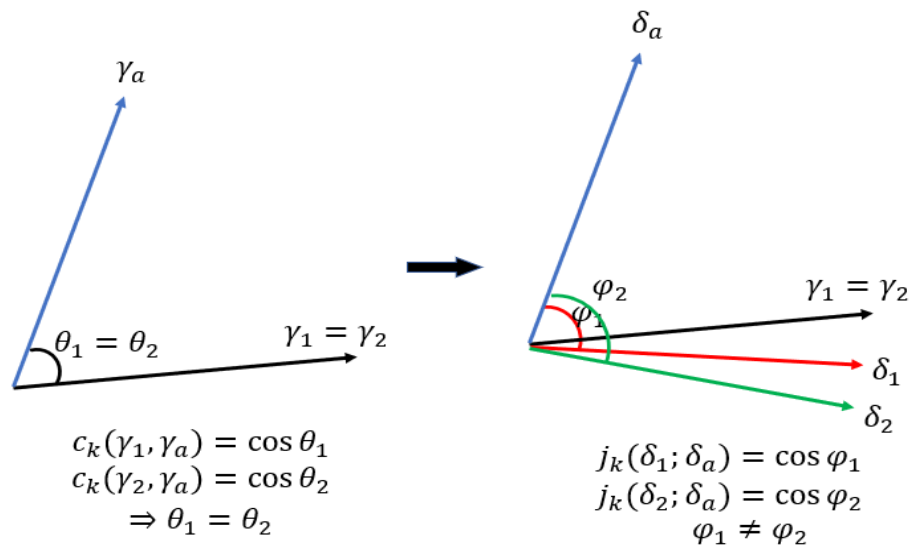
- Similarity index c_k commonly employed in reactor physics community to measure “relevance”
  1. Cross-sections constitutes major source of uncertainty in neutronic calculations
  2. Similarity based on “common” sources of uncertainties only
  3. Relies on first-order variations in given response, e.g., k-eff, with respect to cross-section variations, i.e., sensitivity profiles
  4. Similarity index, c_k, measures angle between sensitivity profiles of an experiment and application as weighted by cross-section prior covariance matrix

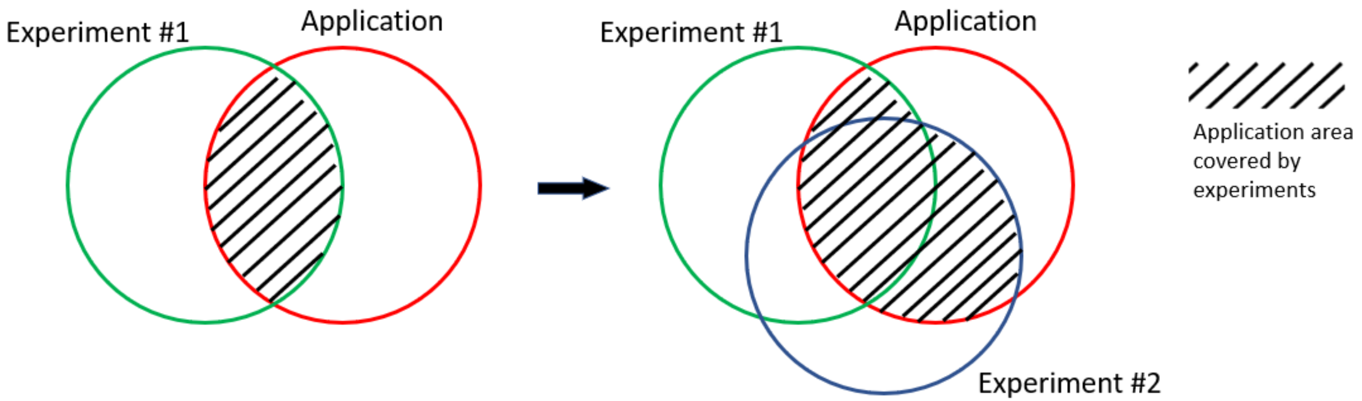
$$c_k = \frac{s_e^T \boldsymbol{C}_{\alpha\alpha} s_a}{\sqrt{s_e^T \boldsymbol{C}_{\alpha\alpha} s_e}\sqrt{s_a^T \boldsymbol{C}_{\alpha\alpha} s_a}}$$

where
- s_e : sensitivity profile of experiment
- s_a : sensitivity profile of application
- $\boldsymbol{C}_{\alpha\alpha}$: Cross-section covariance matrix

Limitations of the similarity index, c_k

- Absence of "other non-common" uncertainties
  - Higher measurement uncertainties should degrade similarity
  - Non-Common uncertainties, such as geometry, composition, etc., can degrade similarity
- Redundancy of past experiments
  - The c_k value measures similarity between a single experiment and application
- Similarity does not translate directly into "Value" for Model Validation



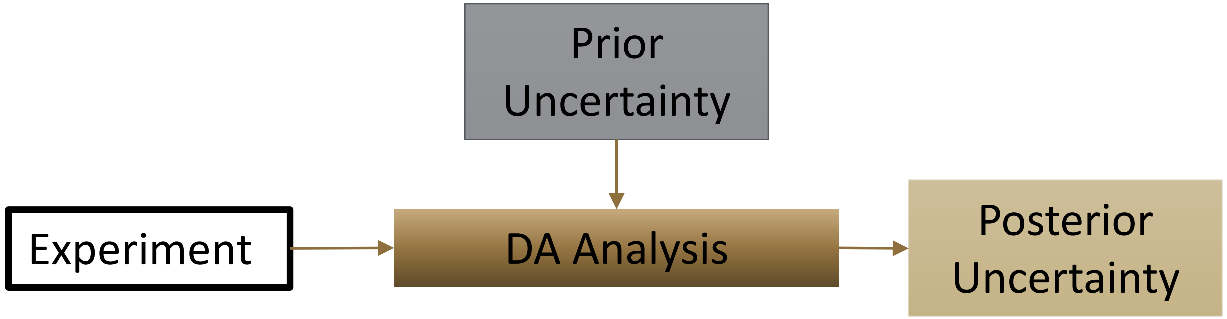


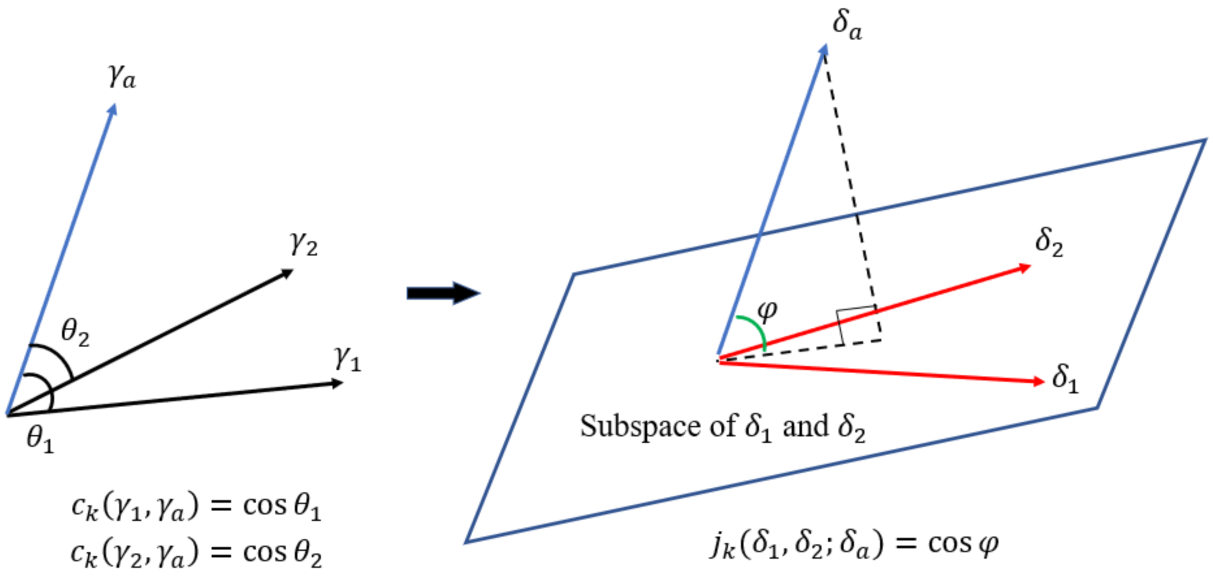
Extended similarity index, ACCRUE index, j_k

1. Employs "Value" rather than "Similarity" to measure "Relevance", with "Value" measuring reduction in uncertainty for quantity of interest.

2. Allows analyst to order experiment to reach most stable variation in assimilation results

3. Finds minimum number of experiments to reach user-defined confidence for quantities of interest

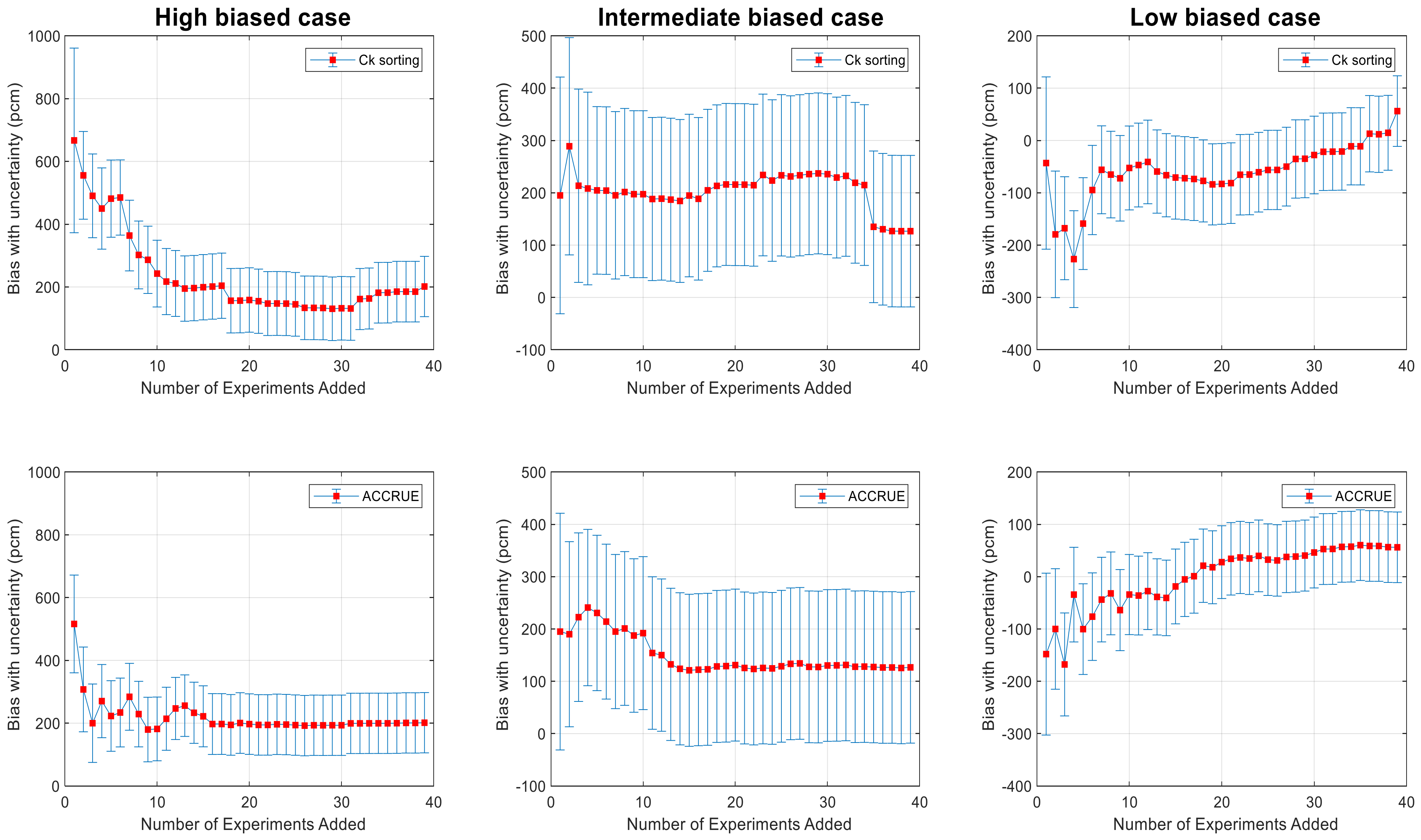




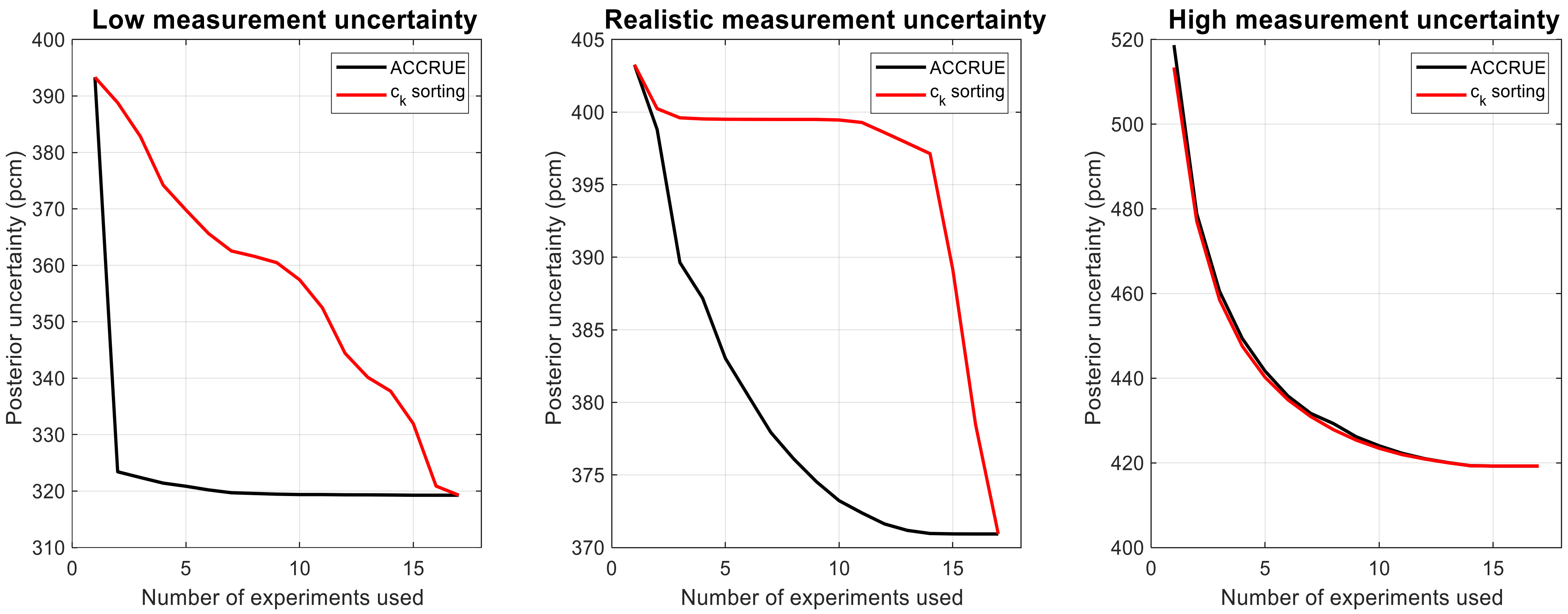
ACCRUE: Accumulated Correlation Coefficient for Relevance of Uncertainties in Experimental Validation

- Allows inclusion of multiple experiments with different levels of relevance, and experimental uncertainties

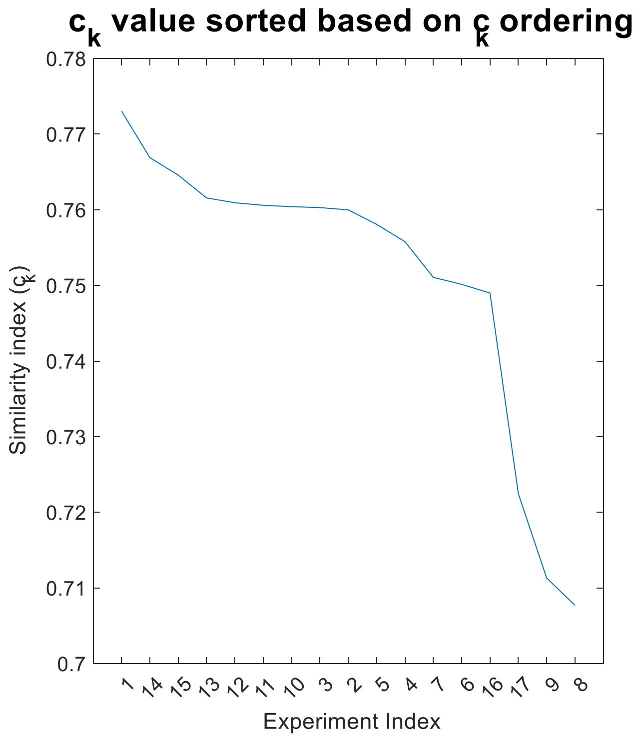
- Provides a quantitative assessment of new experiments and/or sensors.

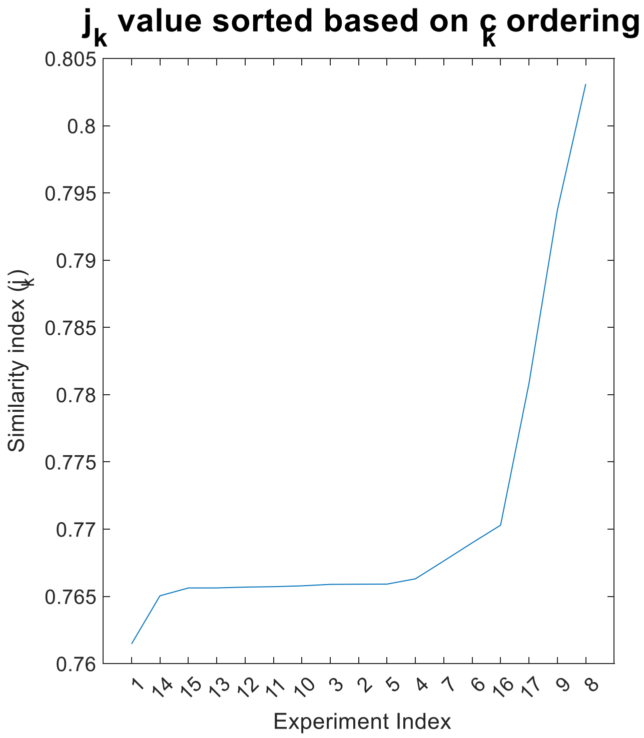


c_k- vs. j_k-Sorting



c_k- vs. j_k-Sorting

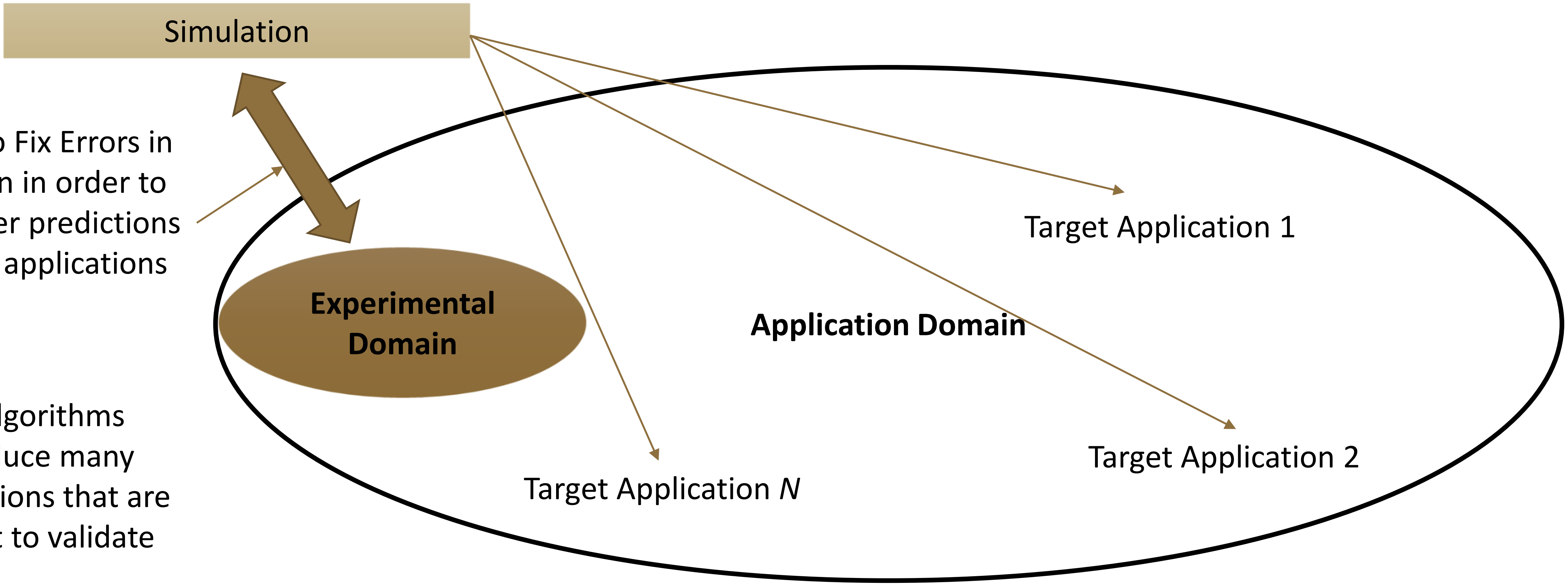




Low relevance experiments do contain information about application of interest, which could be ignored with a threshold ck approach.

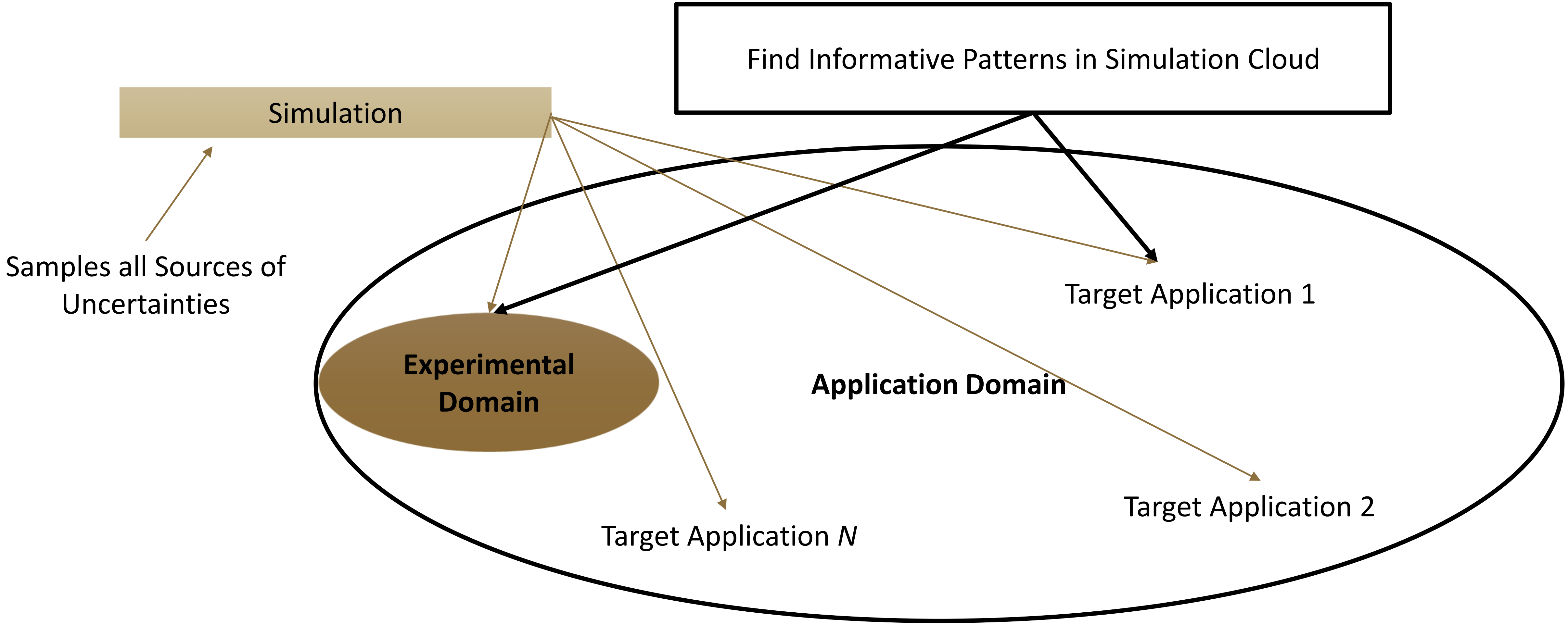
Mapping Uncertainties via Classical DA Techniques

DA tries to Fix Errors in Simulation in order to make better predictions for target applications



DA Algorithms introduce many assumptions that are difficult to validate

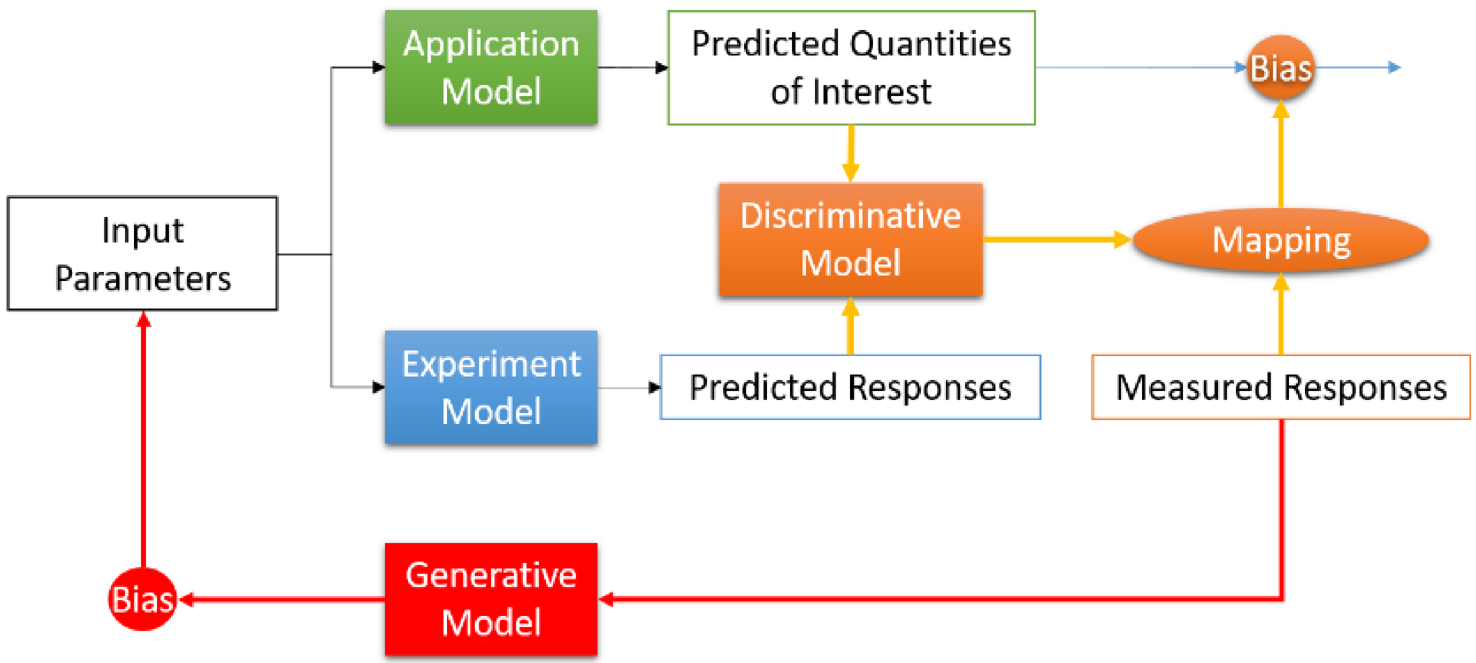
Mapping Uncertainties via Machine Learning



Mapping Uncertainties via Machine Learning

Vapnik's principle

"when solving a problem of interest, do not solve a more general problem as an intermediate step"

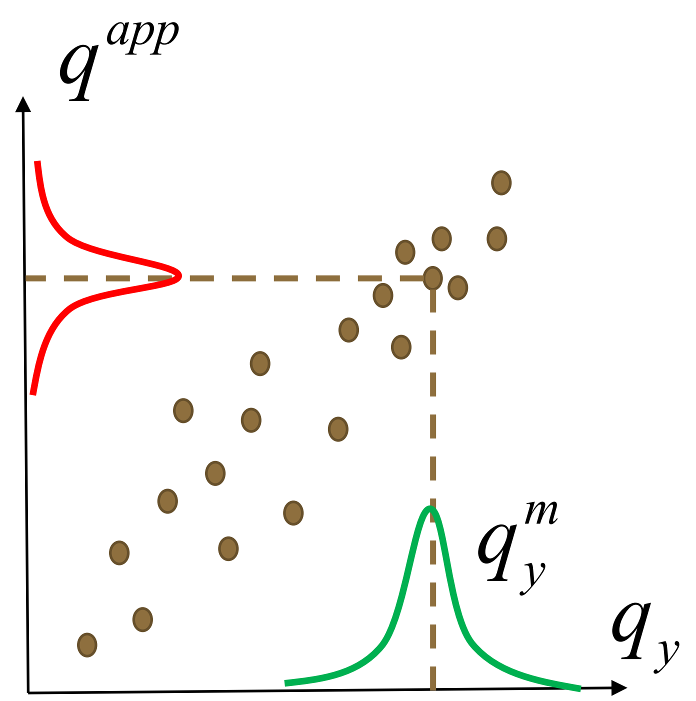


Physics-guided Coverage Mapping

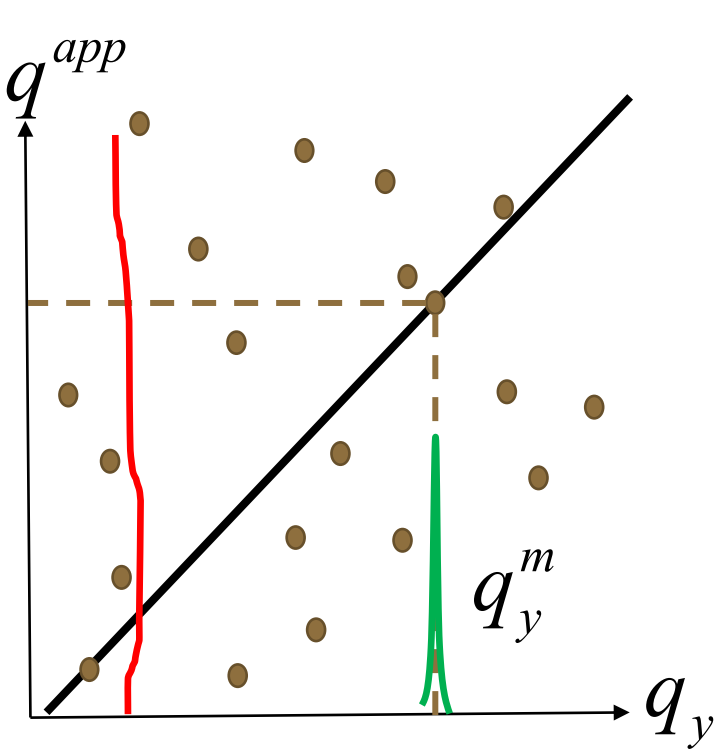
Find Mapping Kernel between Application and Experimental Responses

- Direct mapping between application quantity of interest and experimental responses (do not need to be same type)
- All sources of uncertainties can be included via sampling, both simulation and measurements
- Cloud of results harvested for highest-informing correlations between application quantities of interest and experimental responses (search guided by quantitative metric, mutual information)
  - Assumption-free approach for measuring information content, due to C. Shannon 1945

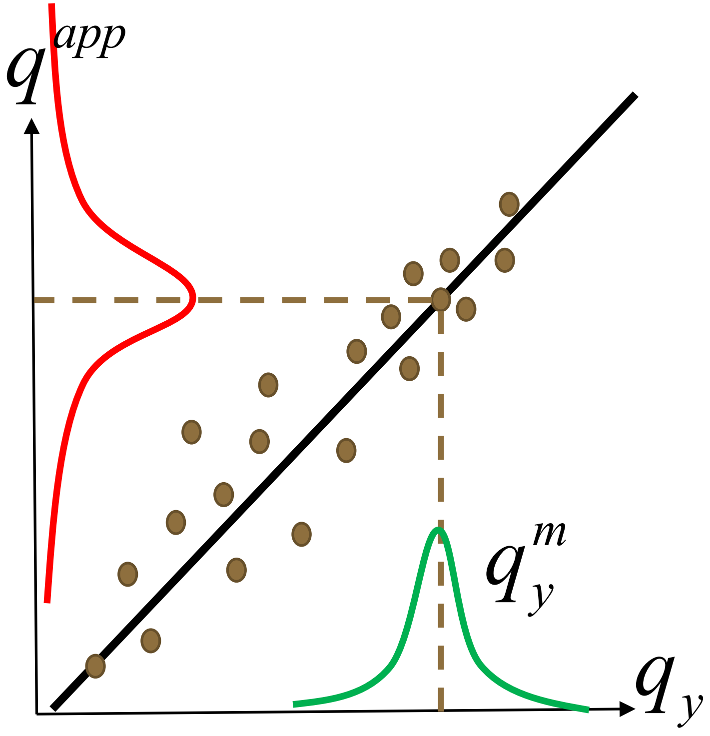
$$P^{PCM}\left(q^{app}\right)=\int P\left(q^{app},q_y\right)P\left(q_y^m\right)dq_y$$



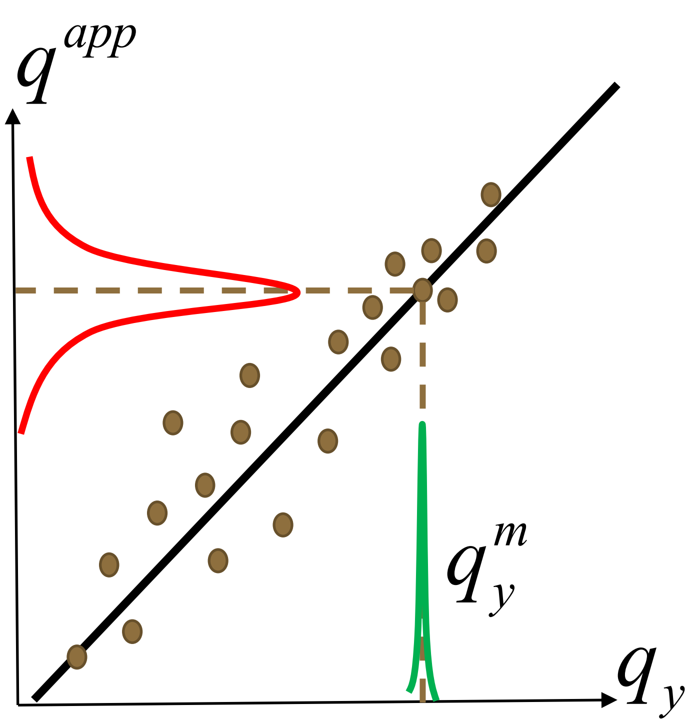
Physics-guided Coverage Mapping



(a) Low Mutual Info. & Perfect Measurements



(b) High Mutual Info. & Uncertain Measurements



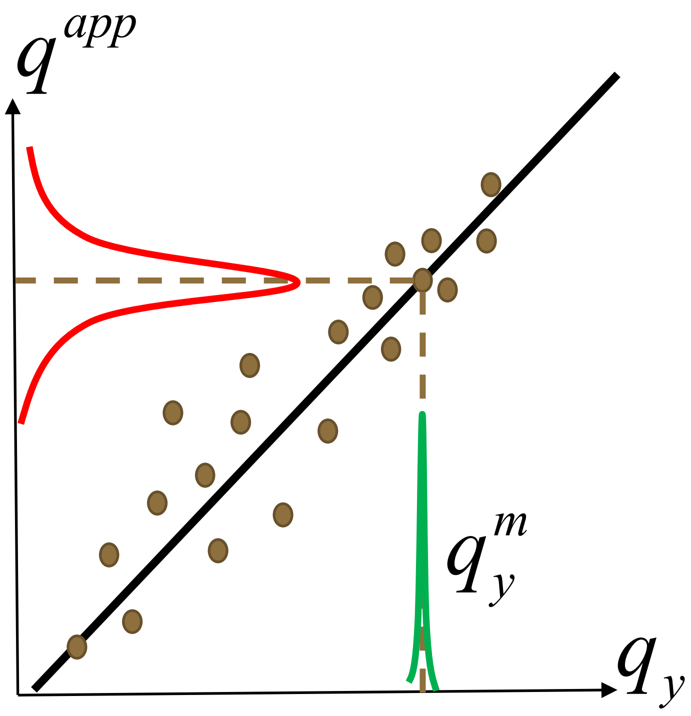
(c) High Mutual Info. & Perfect Measurements

Physics-guided Coverage Mapping

Can define reduction in entropy assuming perfect (or varying level of uncertainty for) measurements

$$r\left(q^{app}\right)=\frac{H\left(P^{PCM}\left(q^{app}\right)\right)}{H\left(P^{Prior}\left(q^{app}\right)\right)}$$

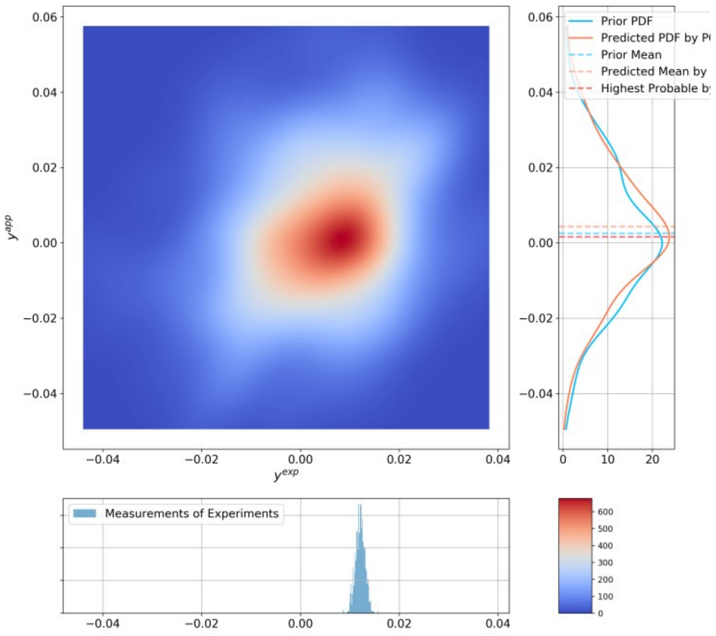
Allows one to compare different experimental setups, and sensor types before conducting the experiment.



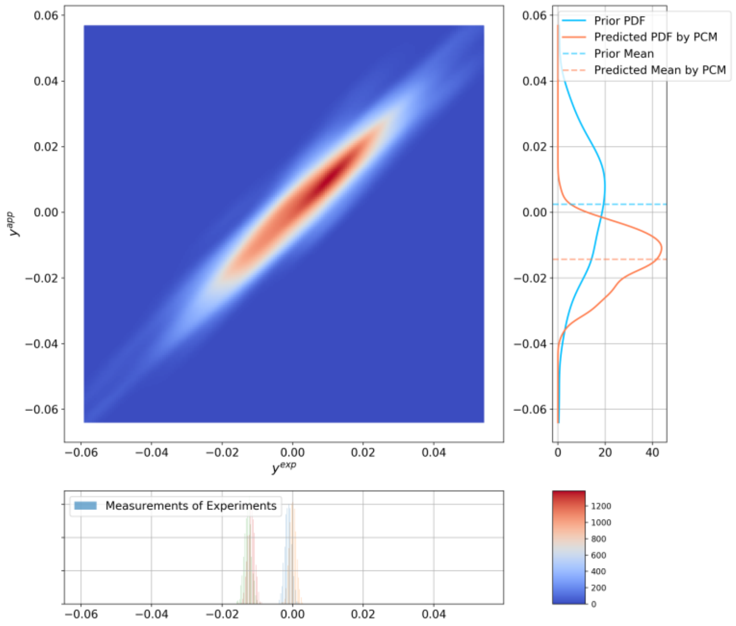
(c) High Mutual Info. & Perfect Measurements

Physics-guided Coverage Mapping: Neutronic Example

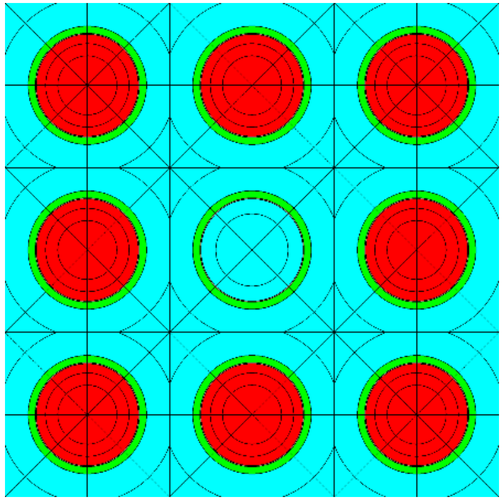
- Application: How to predict isotopics from different irradiation history, lattice types, reactor types, etc.



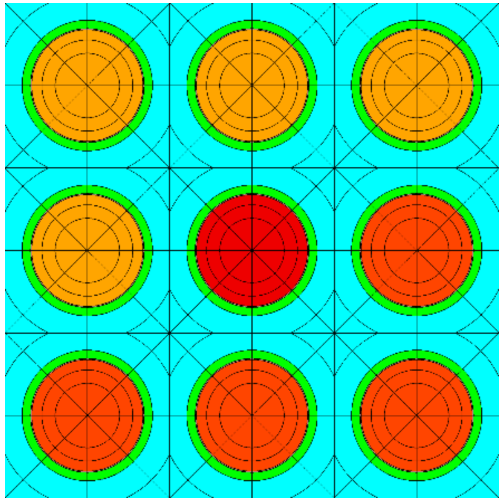
Single Predictor



Multiple Predictors



3x3 PWR Assembly by Polaris

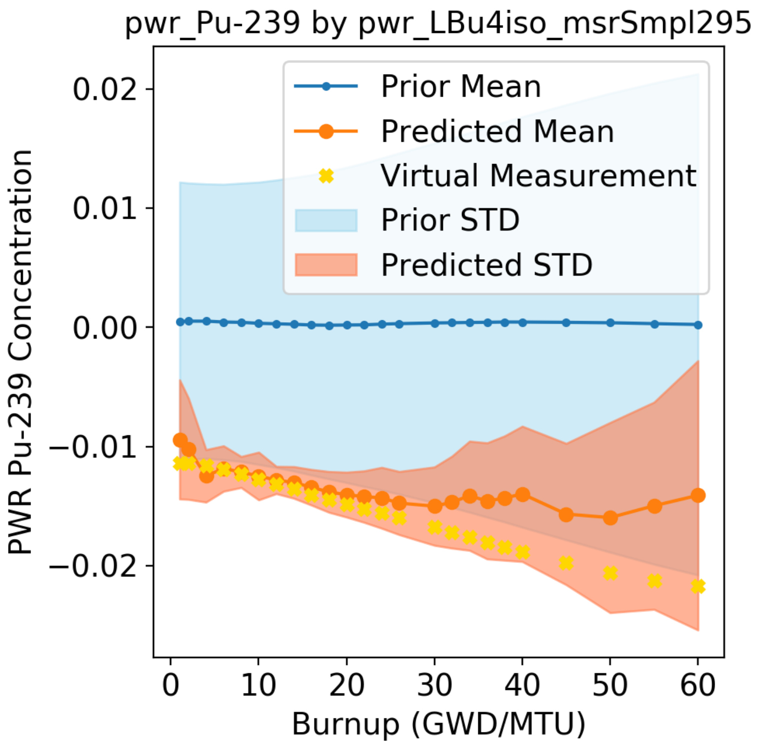


3x3 BWR Assembly by Polaris

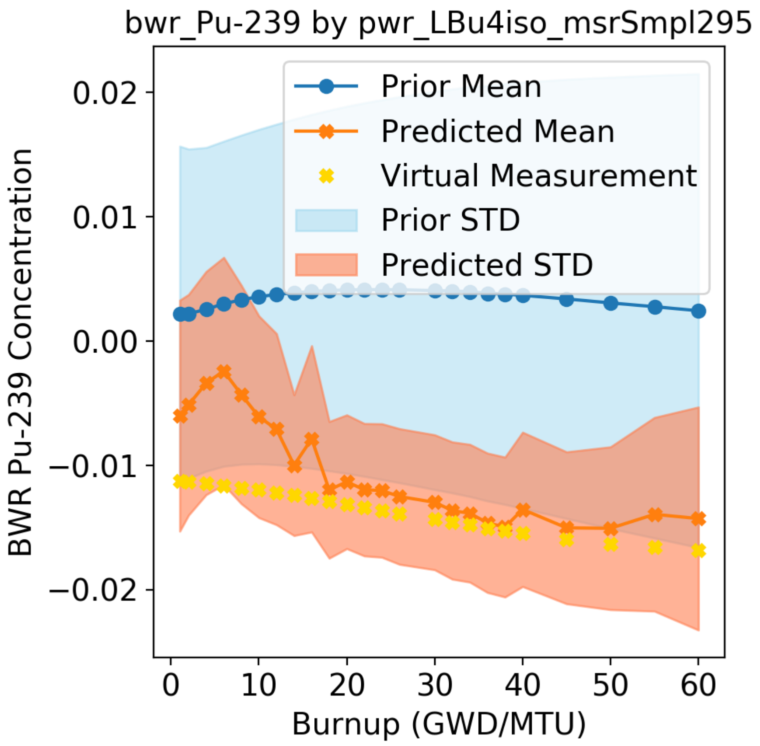
Physics-guided Coverage Mapping: Neutronic Example

- Using single predictors, i.e., measurement at single burnup.

Predict PWR using PWR



Predict BWR using PWR



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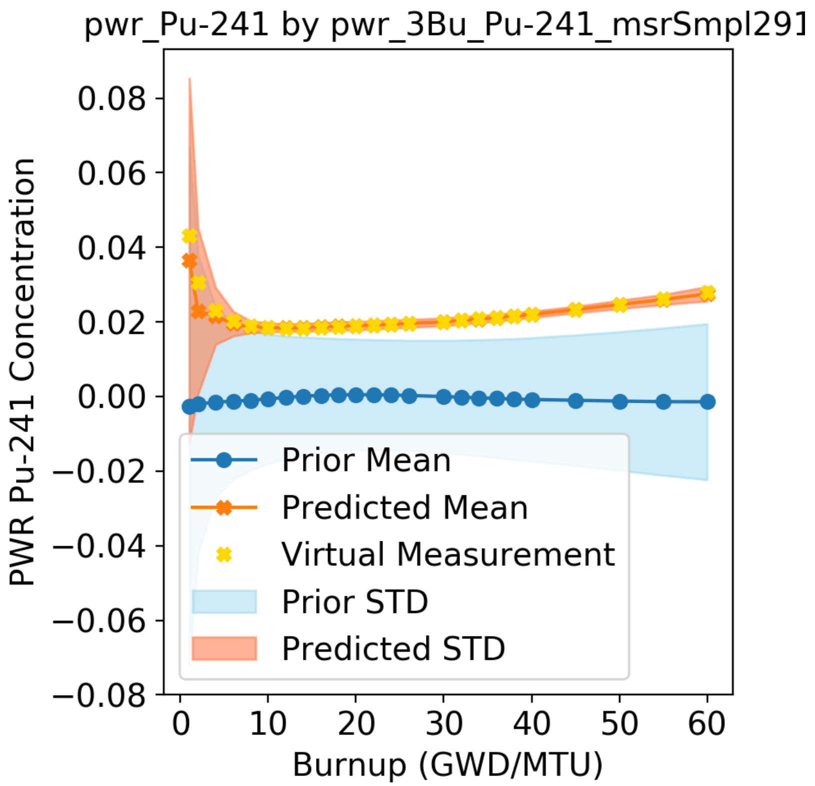
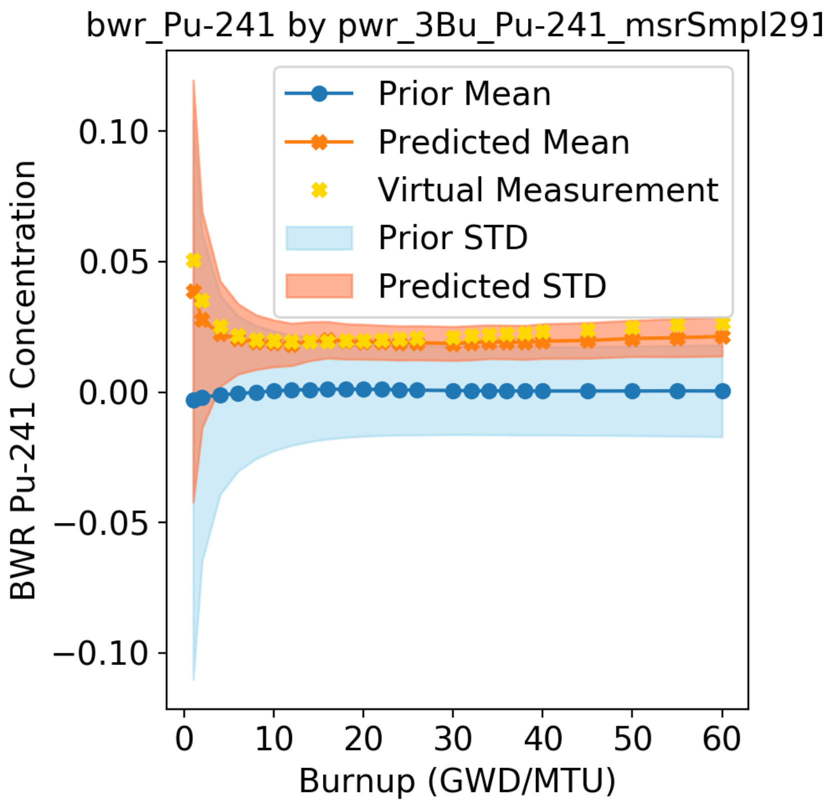
Physics-guided Coverage Mapping: Neutronic Example

- Using Multiple predictors, i.e., measurements at three different burnup values.

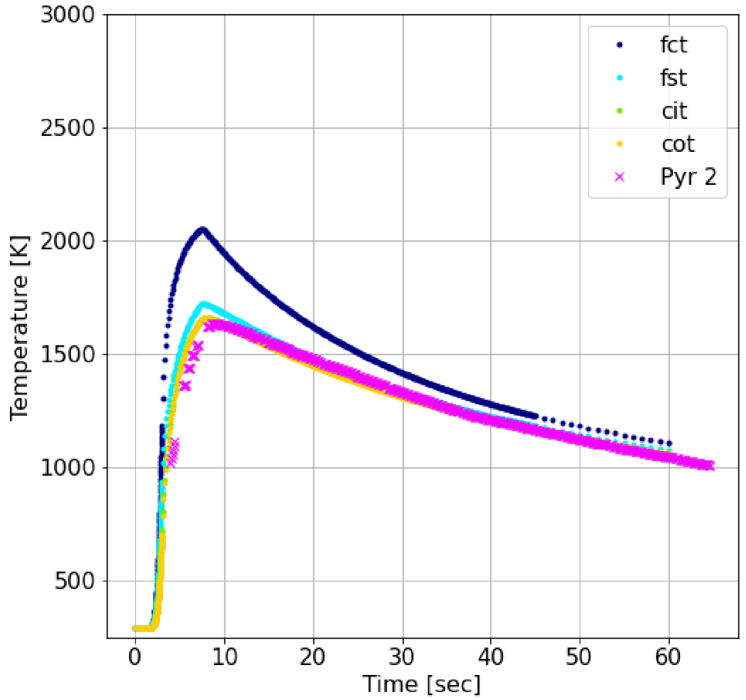




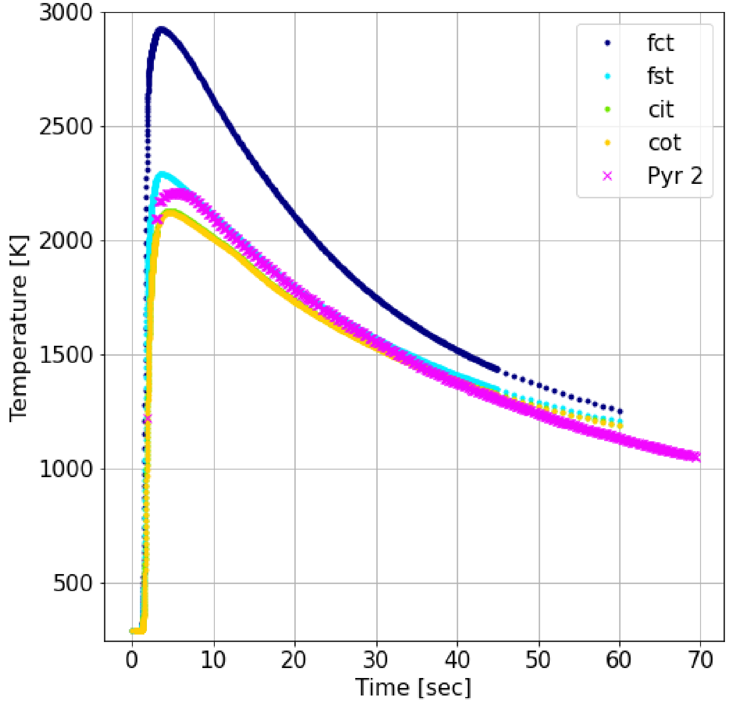
Physics-guided Coverage Mapping: INL's TREAT T/H Example

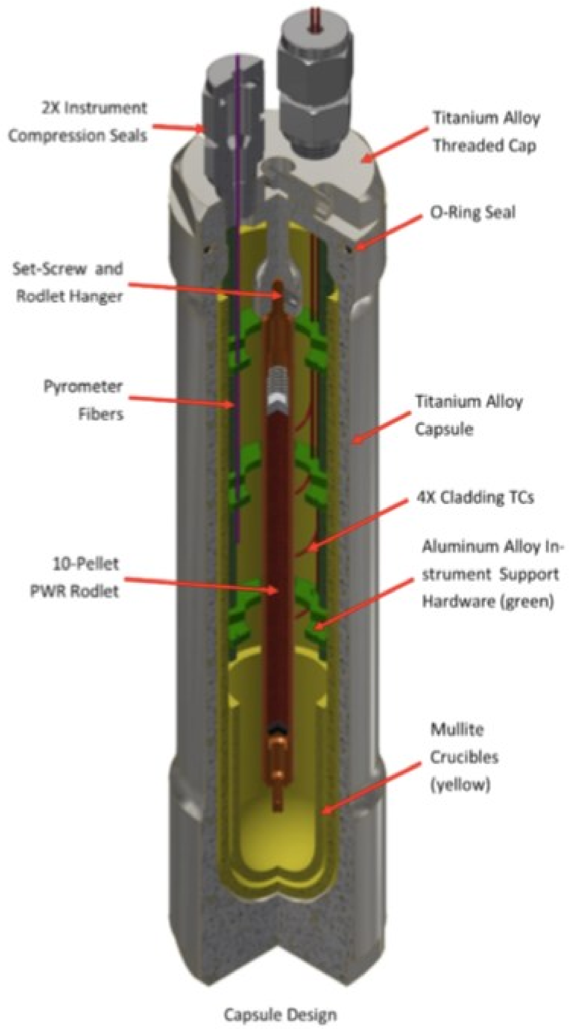
- TREAT application of SETH-C and SETH-D experiments, modeled by RELAP5-3D with fuel temperature as response, thermal parameters as sources of uncertainties

SETH-C

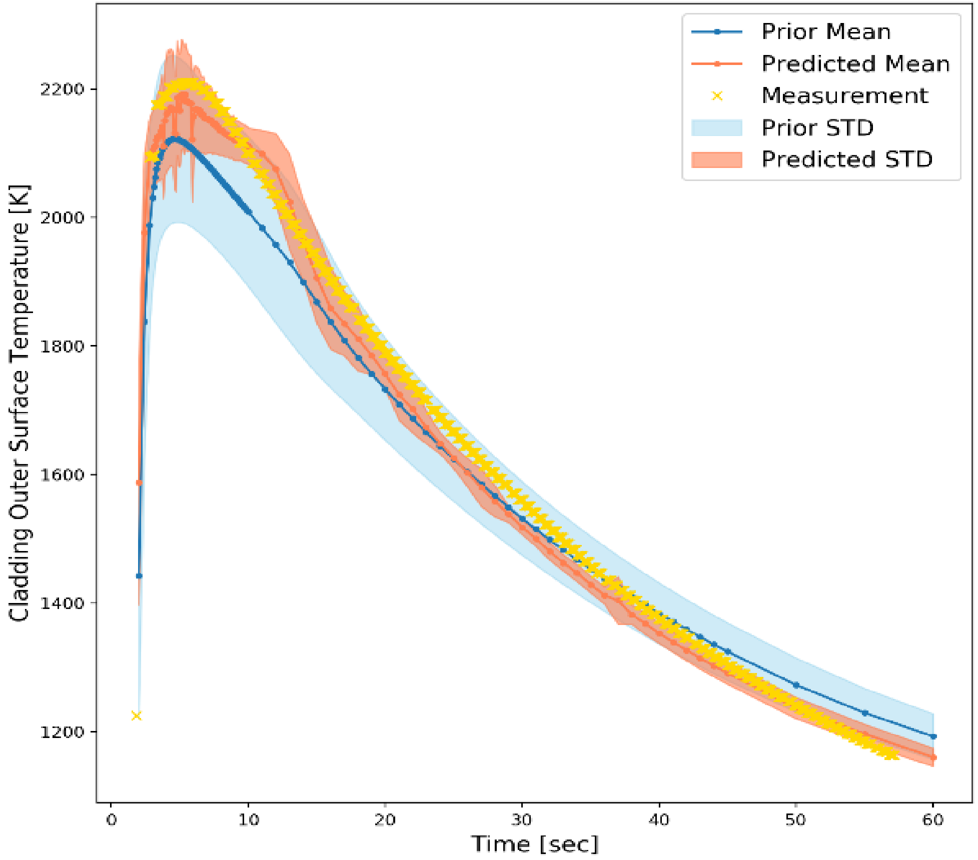


SETH-D

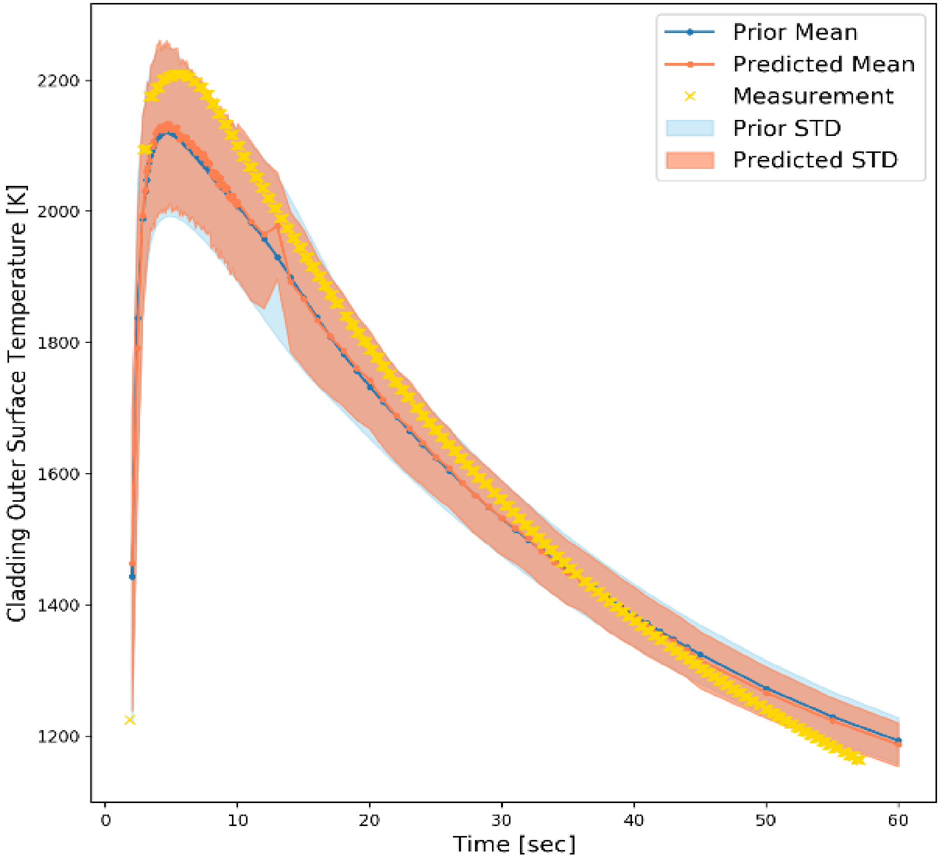




Physics-guided Coverage Mapping: INL's TREAT T/H Example



by PCM



by Gaussian-based Bayesian Inference

Thank you for your attention