Application of PCM Model Validation on Isotopic Prediction and Uncertainty Reduction

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Nuclear Model Validation

Why model validation

- ❑ Numerical simulations of nuclear models are not perfect due to approximations and uncertainties in mathematical models and data

- ❑ Biases (prediction error) and bias uncertainties (how well do we know our prediction error) need to be calculated for nuclear application in order to calculate **safety margins**
  - Criticality Safety (spent fuel storage, nuclear waste containers, reactor startups)
  - Nuclear Reactor Safety (Dynamic Safety Margin Characterization)
  - Advanced Nuclear Reactor Designs, e.g., Molten Salt Reactors

Nuclear Model Validation

Tasks and challenges

❑ Validation carries out the following tasks:

- Determine computational biases (discrepancy between predictions and measurements)
- Quantify uncertainties of responses from major sources of uncertainties
- Map biases and uncertainties to application under given conditions

❑ Current validation methods suffer from several challenges:

- Limited number of relevant benchmark experiments
- Only parameter uncertainties quantified (absence of modeling uncertainties)
- Relies heavily on parametric regression (e.g., fitting)
- Not clear when it fails and why it fails

Model Validation

Problem setup

Uncertainty

- Known
- Unimportant
- Unknown

Model Prediction

- Experiment
- Application

Measurement

- Experiment

Model Validation

Problem setup

Uncertainty

- Known
- Unimportant
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Model Prediction

- Experiment
- Application

Measurement

- Experiment

Model Validation

Problem setup

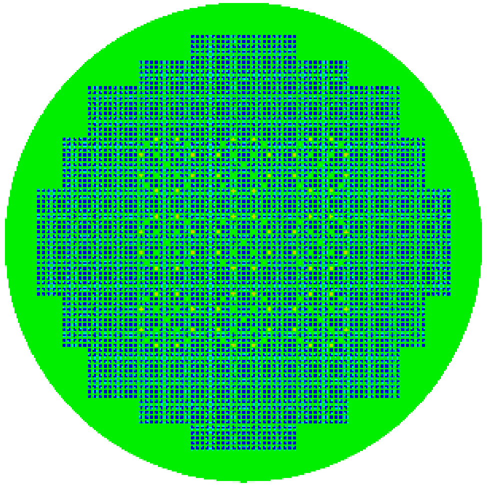
Uncertainty

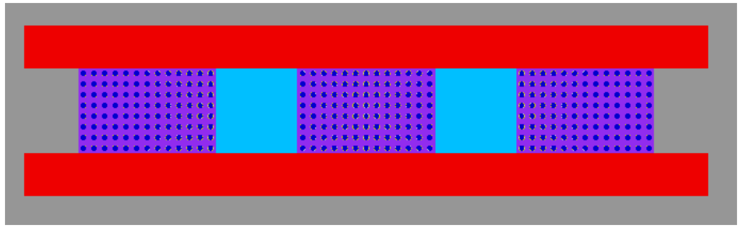
- Known
- Unimportant
- Unknown

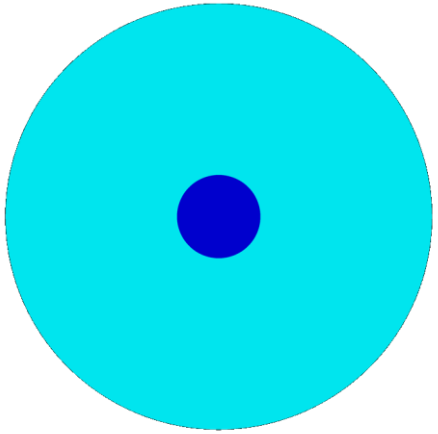
Model Prediction

- Experiment
- Application

small-scale or
separate effects experiments







Model Validation

Problem setup

Uncertainty

- Known
- Unimportant
- Unknown

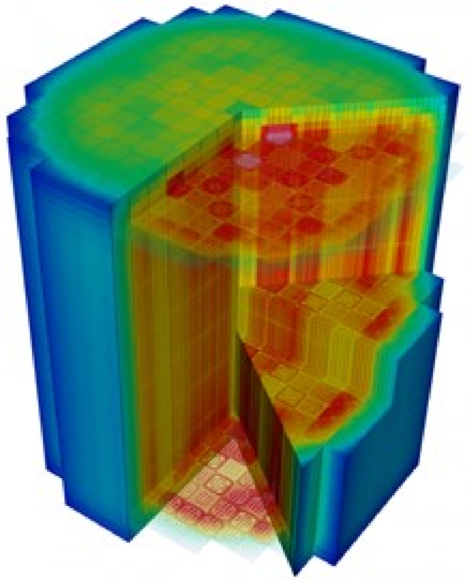
Model Prediction

- Experiment
- Application

full-scale system or design stage

Measurement

- Experiment



Model Validation

Problem setup

Uncertainty

- Known
- Unimportant
- Unknown

Model Prediction

- Experiment
- Application

Measurement

- Experiment

$$y_{cal}^{exp} = f^{exp}(x \quad , u \quad)$$

$$y_{cal}^{app} = f^{app}(x \quad , v \quad)$$

x: common physics parameters

u: control parameters for experiment

v: control parameters for application

Model Validation

Problem setup

Uncertainty

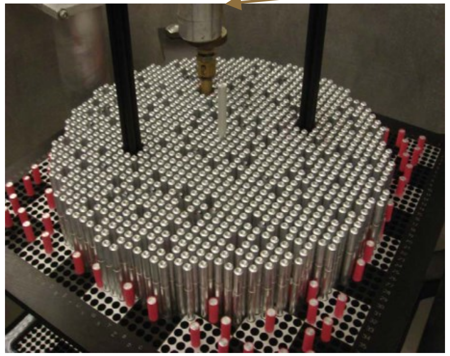
- Known
- Unimportant
- Unknown

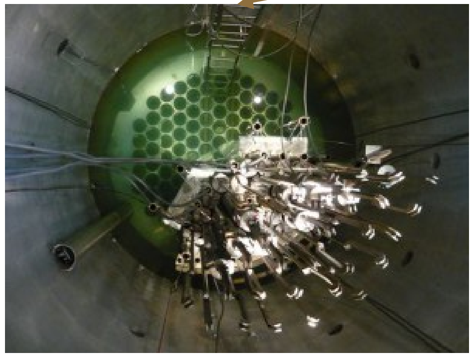
Model Prediction

- Experiment
- Application

Measurement

- Experiment





Model Validation

Uncertainty Sources

Uncertainty

- Known
- Unimportant
- Unknown

Model Prediction

- Experiment
- Application

Measurement

- Experiment

Model Validation

Uncertainty Sources

Uncertainty	Model Prediction	Measurement
Known	Experiment	Experiment
Unimportant	Application	
Unknown		

parameter uncertainty
e.g., nuclear data uncertainty

Model Validation

Uncertainty Sources

Uncertainty	Model Prediction	Measurement
Known	Experiment	Experiment
Unimportant	Application	
Unknown		

e.g., numerical uncertainty

Model Validation

Uncertainty Sources

Uncertainty	Model Prediction	Measurement
Known	Experiment	Experiment
Unimportant	Application	
Unknown		

e.g., modeling uncertainty
other uncertainty

Model Validation

Validation process

Uncertainty

- Known $p(x)$
- Unimportant
- Unknown

Model Prediction

- Experiment $p(y_{cal}^{exp})$
- Application $p(y_{cal}^{app})$

Measurement

- Experiment

Model Validation

Validation process

Uncertainty

Known $p(x)$

Unimportant

Unknown

Model Prediction

Experiment $p(y_{cal}^{exp})$

Application $p(y_{cal}^{app})$

Measurement

Experiment $p(y_{msr}^{exp})$

Model Validation

Objective

Uncertainty

- Known $p(x)$
- Unimportant
- Unknown

Model Prediction

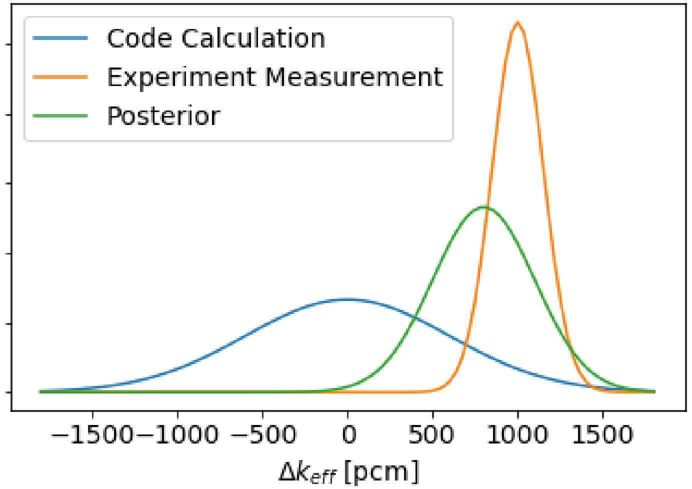
- Experiment $p(y_{cal}^{exp})$
- Application $p(y_{cal}^{app})$

Measurement

- Experiment $p(y_{msr}^{exp})$

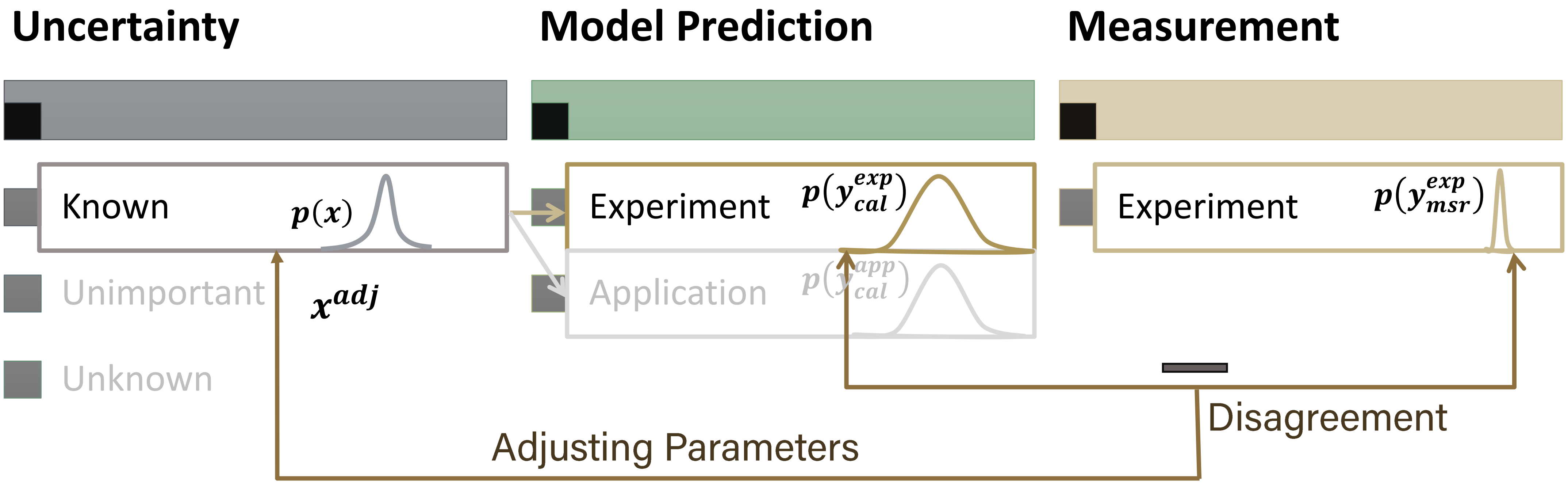
$p(y^{app})$

given application conditions ?



Model Validation

Calibration-based Techniques

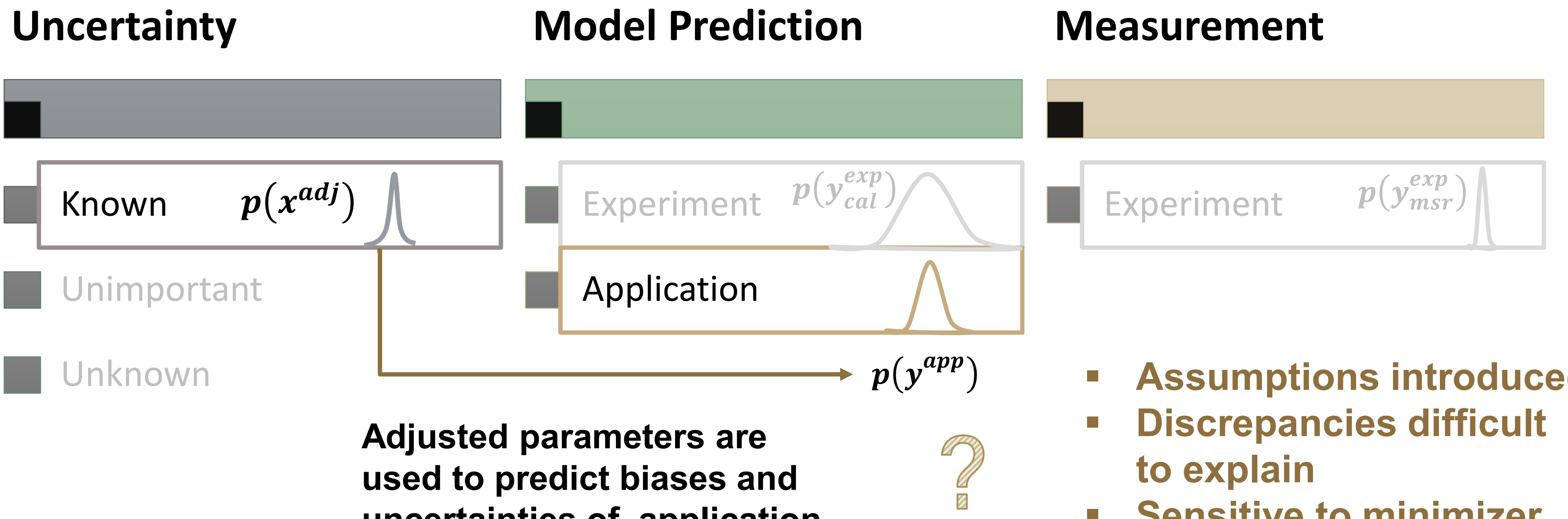


$$\min_{x} \left\| y_{msr}^{exp} - f^{exp}(x, u) \right\|$$

Discrepancies between predicted and measured responses, including their 1st order derivatives, adjust model parameters to minimize the discrepancies

Model Validation

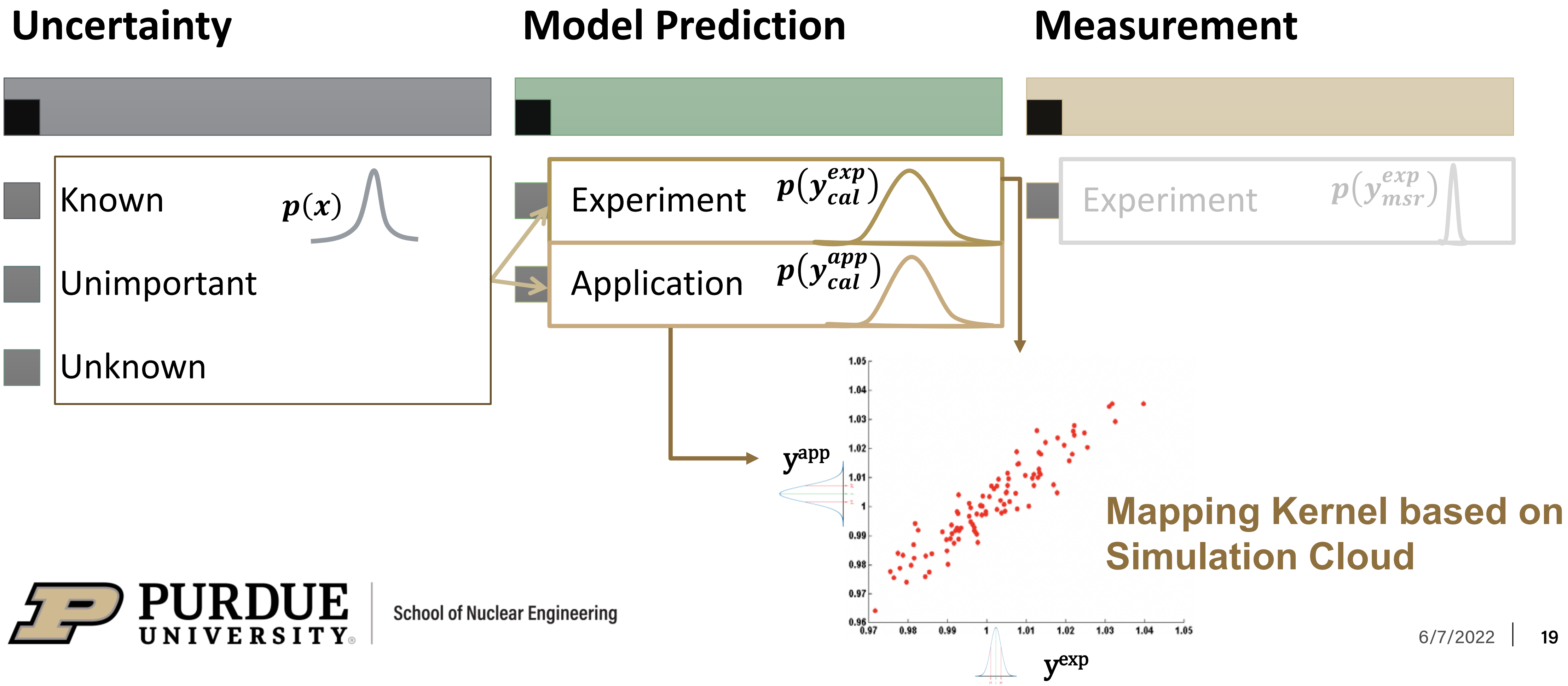
Calibration-based Techniques



Adjusted parameters are used to predict biases and uncertainties of application

- **Assumptions introduced**
- **Discrepancies difficult to explain**
- **Sensitive to minimizer**

PCM-based Validation



Model Validation

PCM-based Validation

Uncertainty

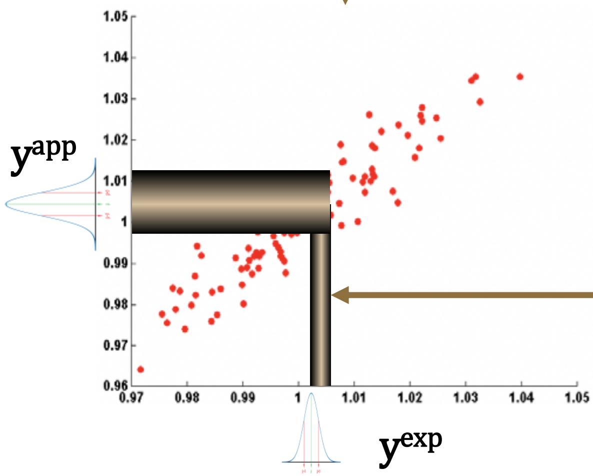
- Known $p(x)$
- Unimportant
- Unknown

Model Prediction

- Experiment $p(y_{cal}^{exp})$
- Application $p(y_{cal}^{app})$

Measurement

- Experiment $p(y_{msr}^{exp})$



Physics-guided Coverage Mapping

Objective of PCM

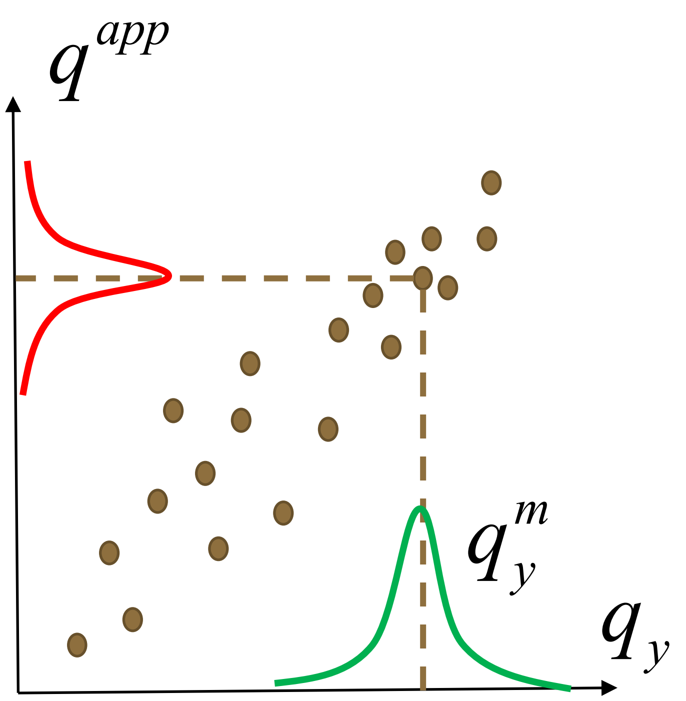
- ❑Provide reliable mapping of biases and uncertainties incorporating both experimental and application conditions
- ❑Overcome some of the challenges with current validation approaches
- ❑Determine relationship between application and all available experiments using information theory principles
- ❑Add information from each experiment, albeit small if not strongly relevant to application

Physics-guided Coverage Mapping

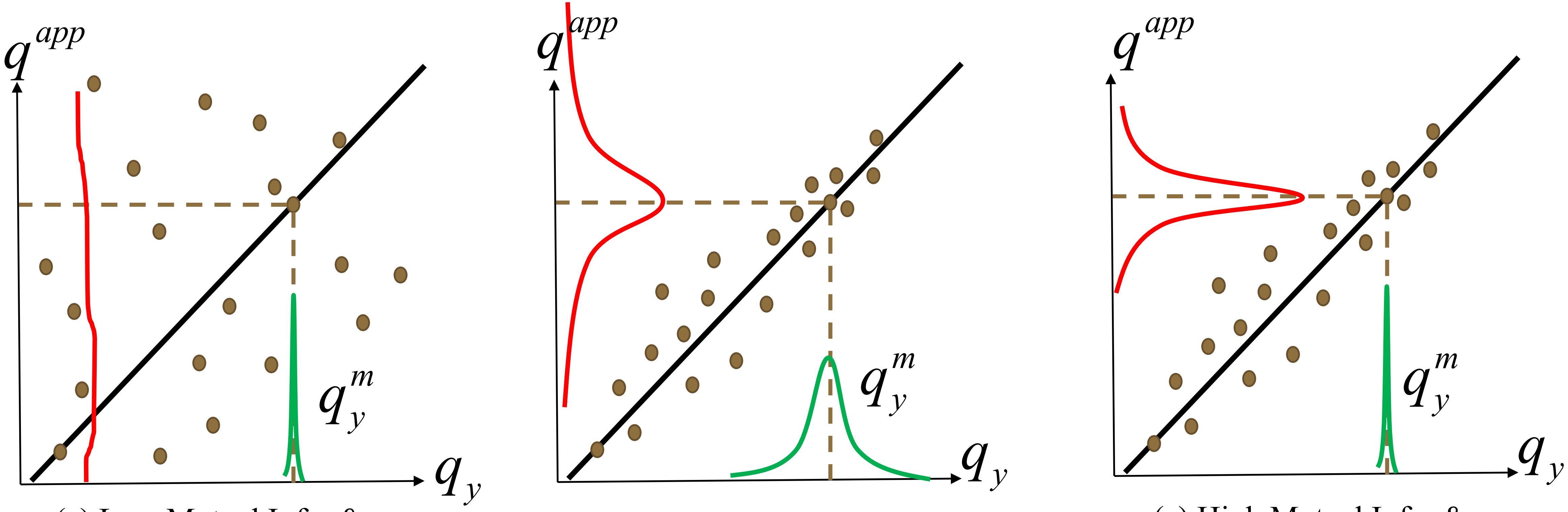
Find Mapping Kernel between Application and Experimental Responses

- 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

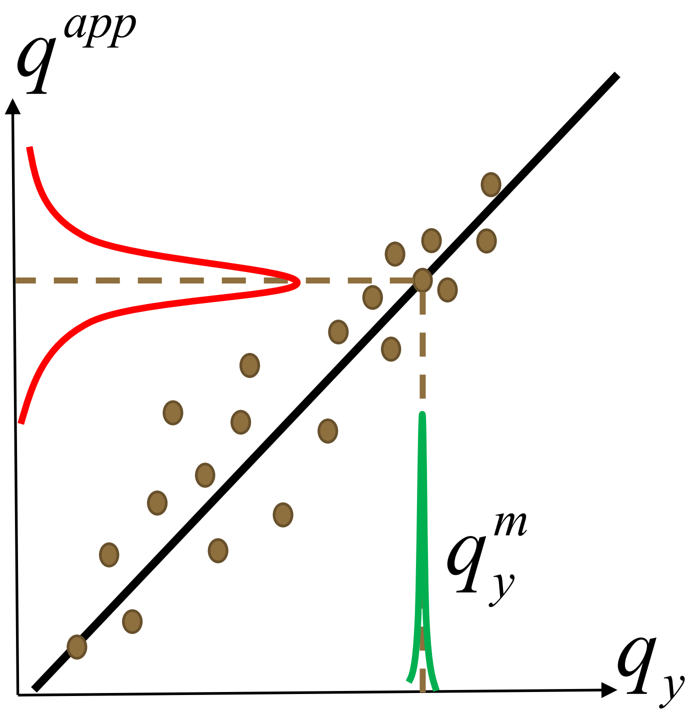
(c) High Mutual Info. & Perfect Measurements

Physics-guided Coverage Mapping

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

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

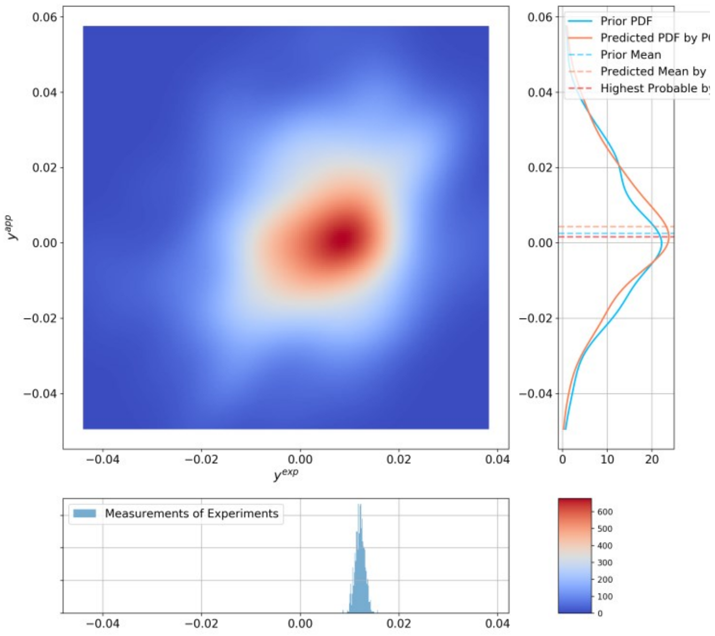
Allows one to compare different experimental setups, and sensor types before conducting the experiment.



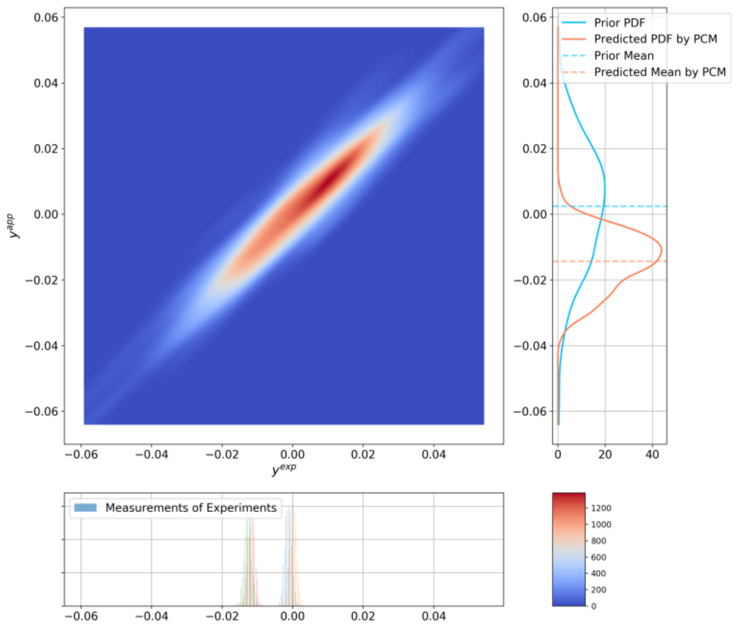
(c) High Mutual Info. & Perfect Measurements

PCM for Isotopic Validation

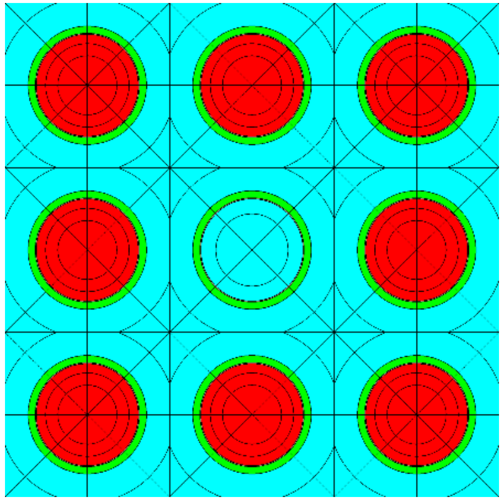
Application:
How to predict isotopics from different irradiation history, lattice types, reactor types, sources of uncertainties, etc.



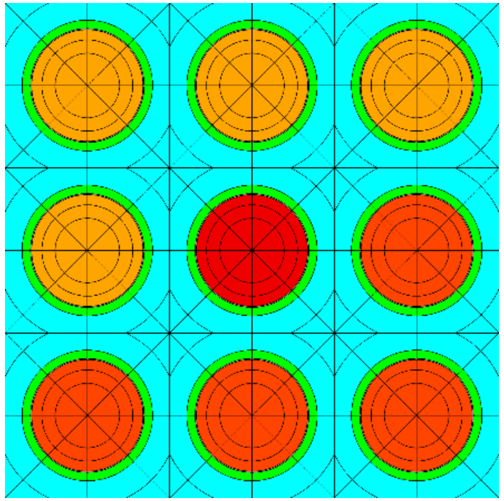
Single Predictor



Multiple Predictors



3x3 PWR Assembly by Polaris



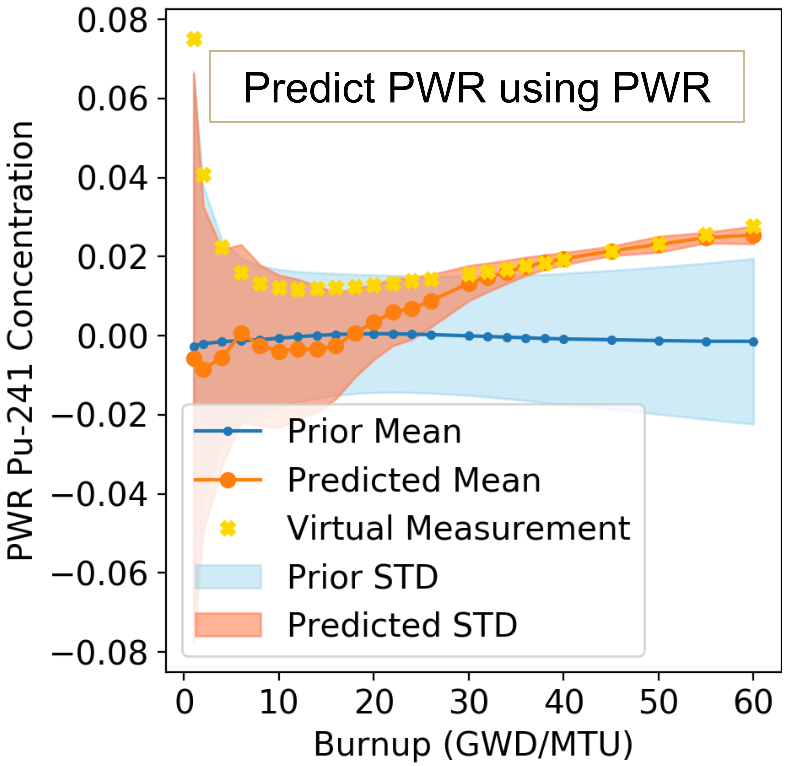
3x3 BWR Assembly by Polaris

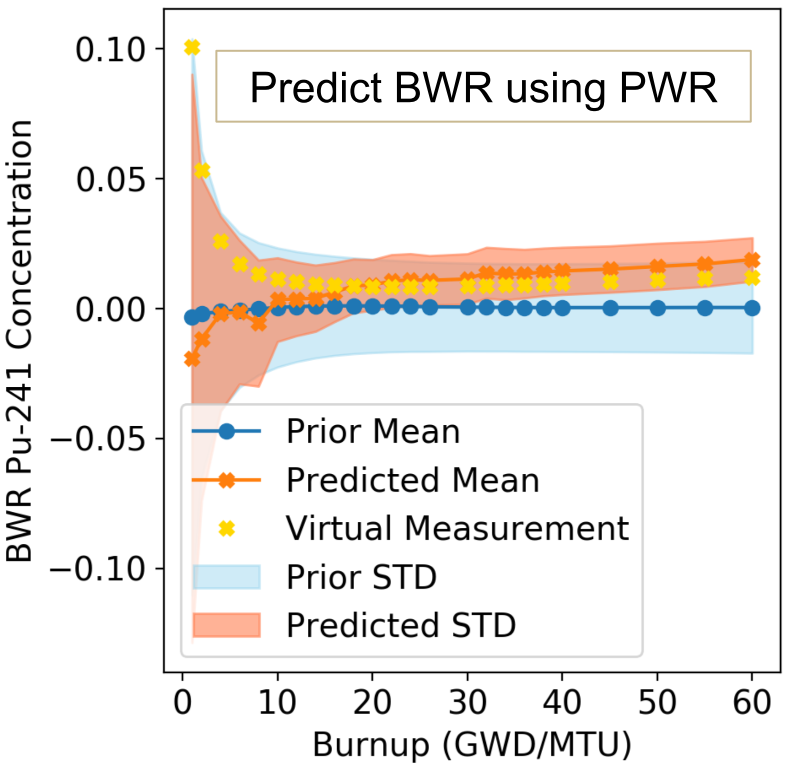
PCM for Isotopic Validation

Validation across Reactor Types

- **Application: Pu-241 concentrations across burnup**
- **Experiment: U-235, U-238, Pu-239, Pu-241 concentrations at 50 GWD/MTU from PWR**

- Best-estimate values follow measurements
- Prediction uncertainty reduced with PCM
- ~50% uncertainty reduction using validation experiments from different reactor types



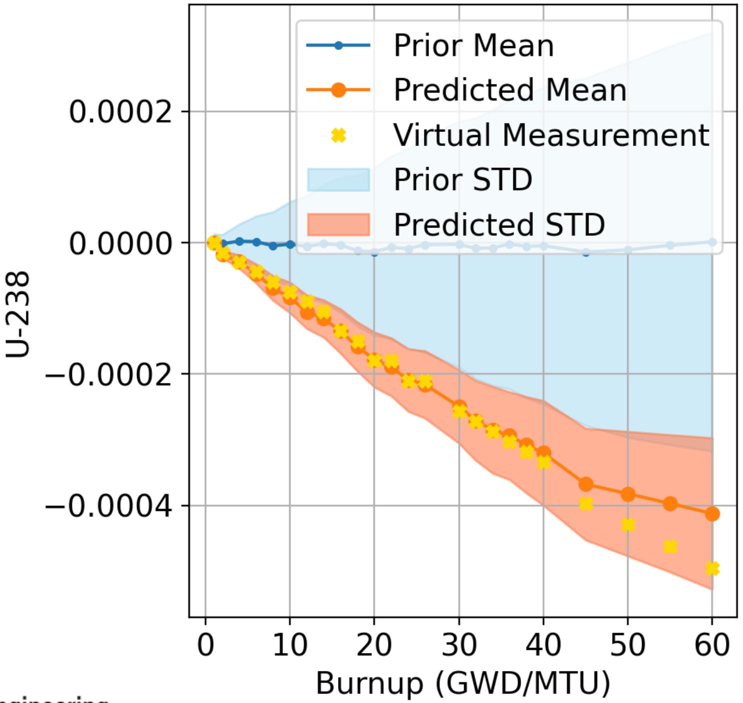


Validation with Different Uncertainty Sources

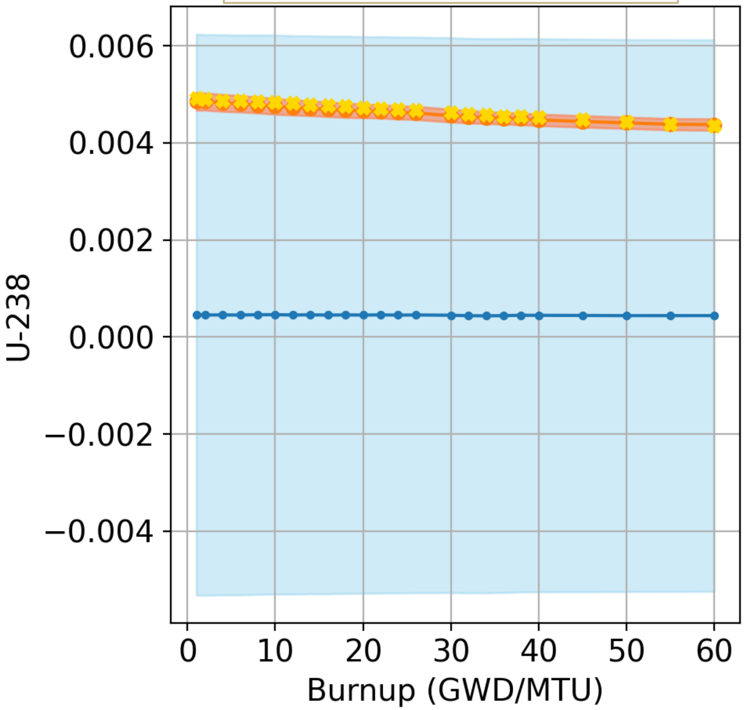
- **Application: U-238 concentrations across burnup from PWR**
- **Experiment: U-235, U-238, Pu-239, Pu-241 concentrations at 50 GWD/MTU from PWR**

- 0.01% measurement uncertainty
- 66% average uncertainty reduction with cross-section perturbed only
- 98% average uncertainty reduction with all parameters perturbed

w/ XS Perturbed



w/ All Para. Perturbed



Average Uncertainty Reduction

- Experiment: U-235, U-238, Pu-239, Pu-241 concentrations at 50 GWD/MTU
- Measurement uncertainty: 0.01%

Table. Average Uncertainty Reduction Fraction across Burnup

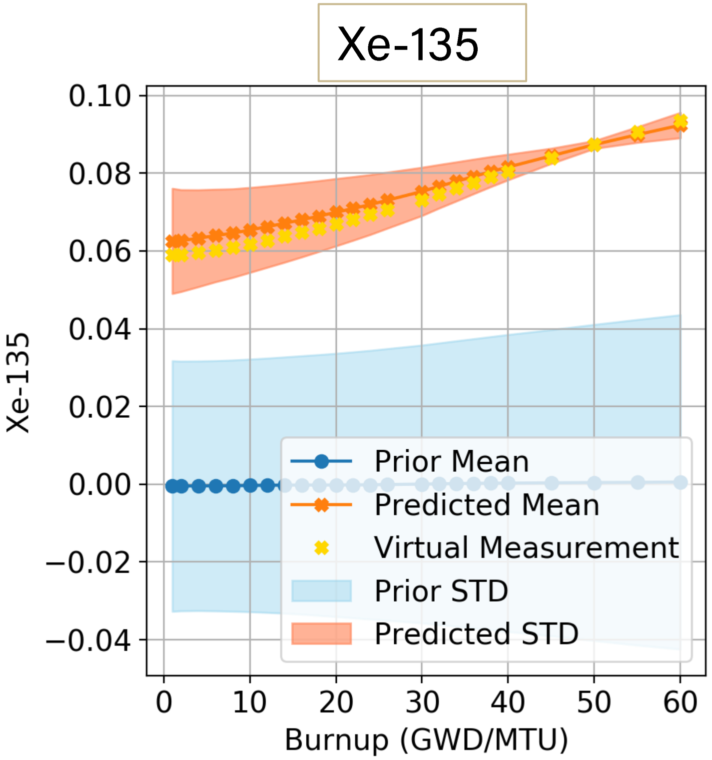
Application	w/ XS Perturbed Only	w/ All Para. Perturbed
U-235	74%	74%
U-238	66%	98%
Pu-239	84%	87%
Pu-241	63%	70%

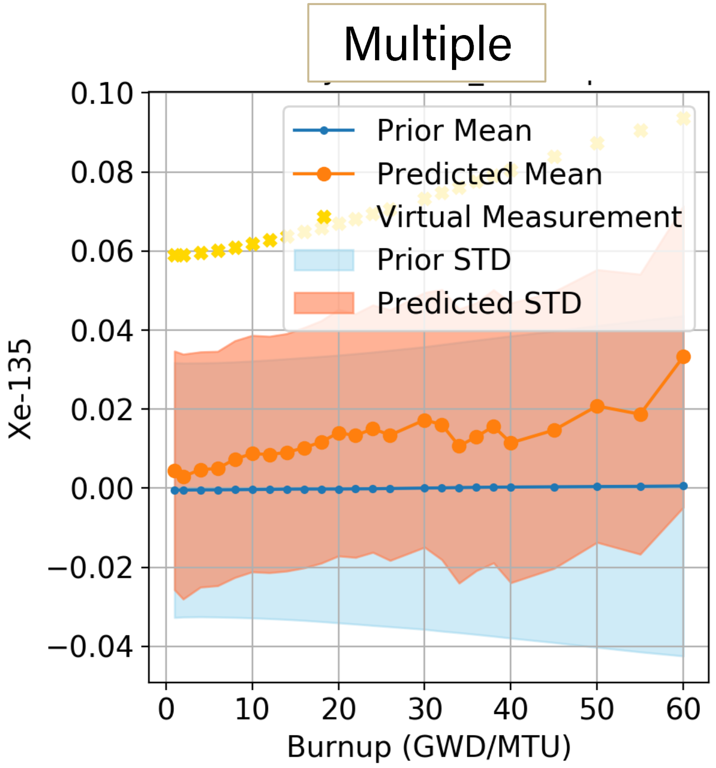
- 60-85% uncertainty reduction with cross-section perturbed only
- 70%-95% uncertainty reduction with all parameters perturbed

Fission Product Validation

- **Application: Xe-135 concentrations across burnup**
- **Experiment:**
  - **Single: Xe-135 concentration at 50 GWD/MTU**
  - **Multiple: U-235, U-238, Pu-239, Pu-241 concentrations at 50 GWD/MTU**

- PCM can be applied to fission product predictions
- Single predictor at EOC provides >70% uncertainty reduction
- Uranium and plutonium are not good predictors for fission products





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Concluding Remarks

- PCM method is a information theory-based approach guided by physics models in support of model validation
- PCM allows for transfer of biases directly from experimental domain to application domain, greatly reduces prediction uncertainties
- PCM provides a simple stochastic approach as an alternative to data assimilation/calibration-based techniques, addressing some of challenges using current validation approaches
- Future work will extend to MSR dynamic validations with liquid fuel

Acknowledgements

- Numerical models and integral experiments data are provided by Dr. Ugur Mertyurek from ORNL

THANK YOU

Questions?

Please contact
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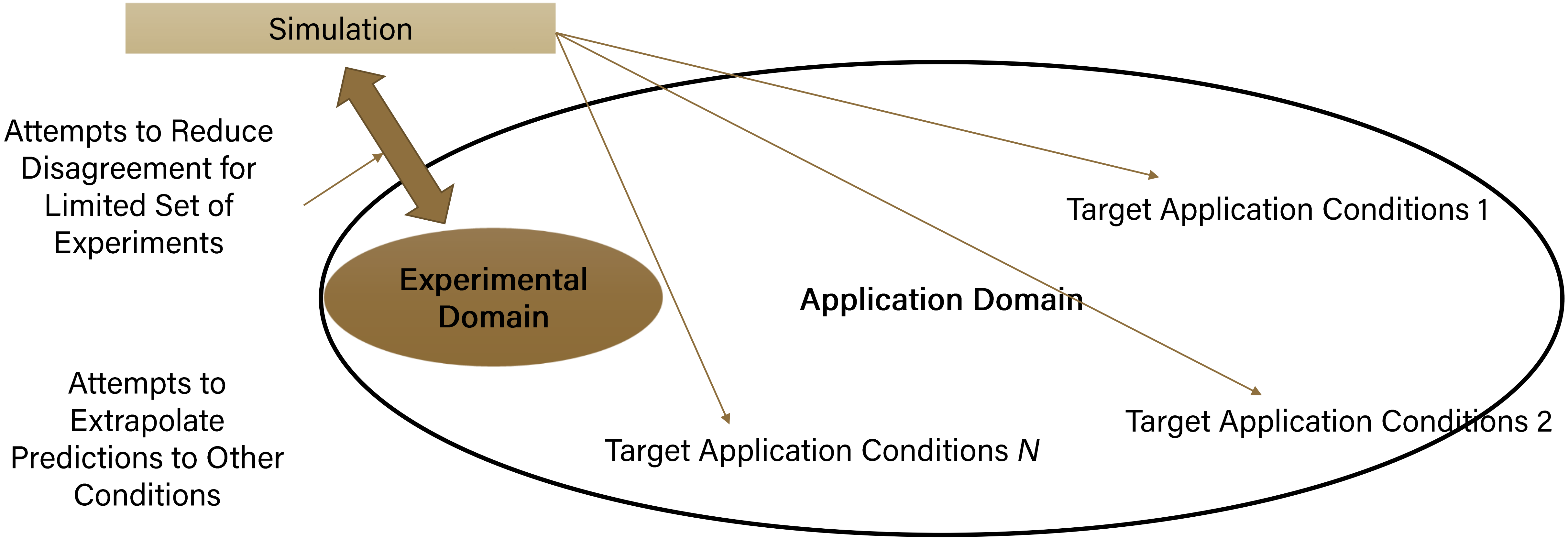
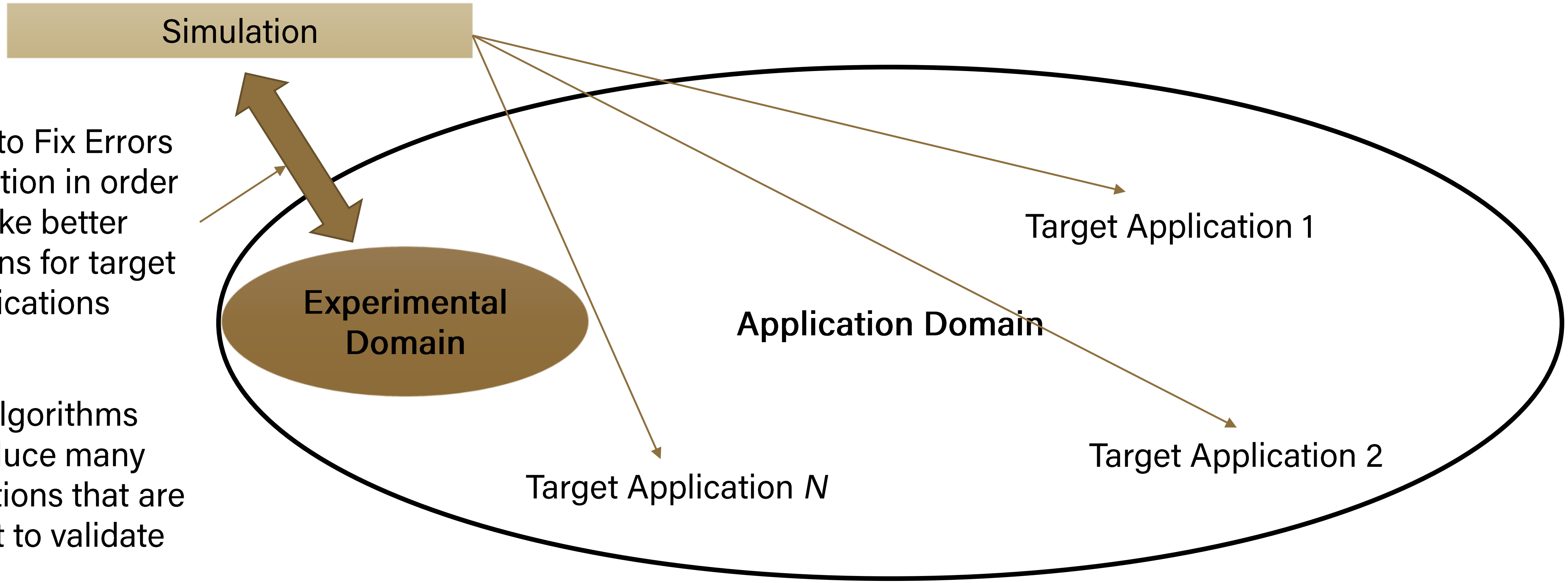
Central Problem in Model Validation



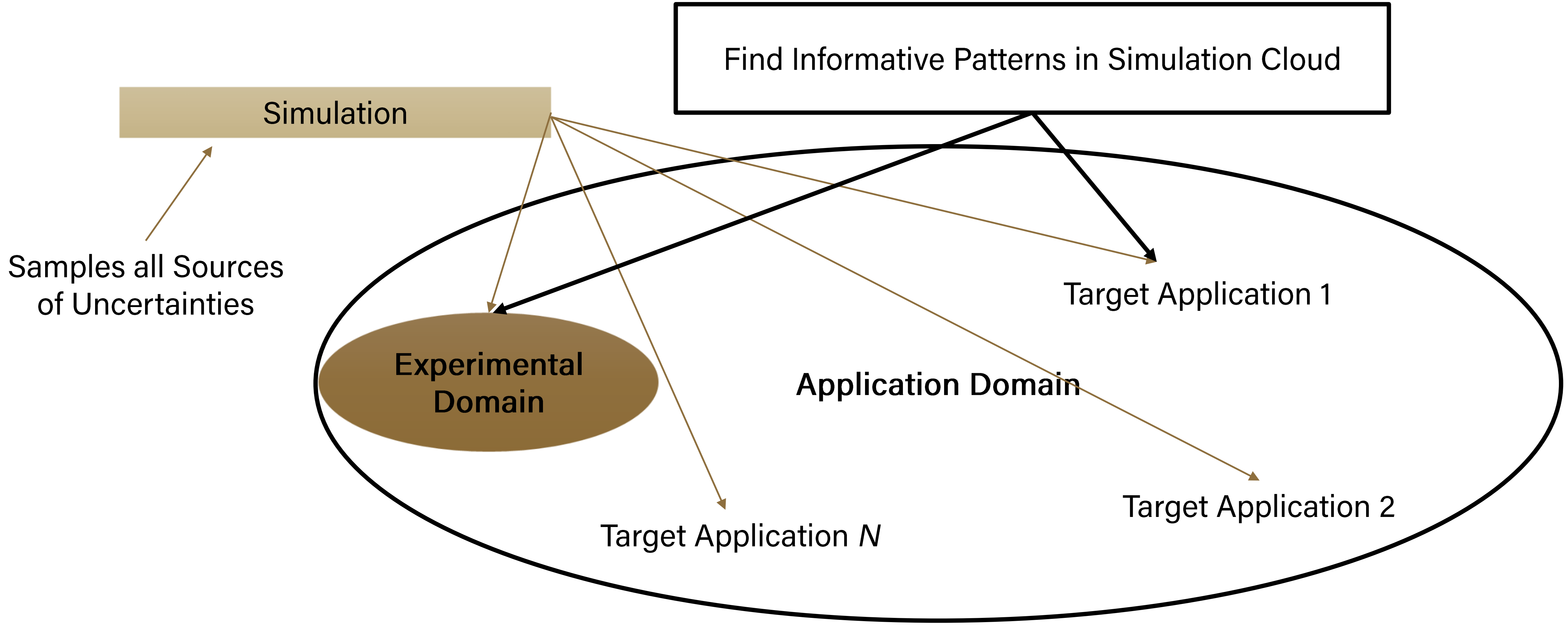
Mapping Uncertainties via Classical DA Techniques



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 PCM



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"