Methods Development & Application of Uncertainty Quantification & Data Assimilation for Multiphysics Simulations

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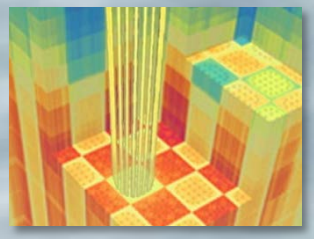
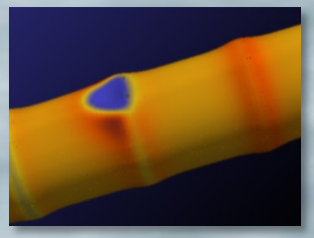
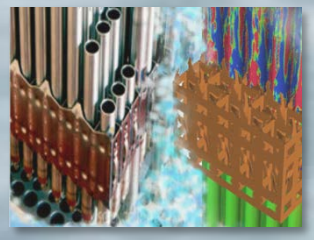






The Consortium for Advanced Simulation of LWRs
A DOE Energy Innovation Hub

CASL-U-2016-1087-000

U.S. DEPARTMENT OF ENERGY

Objective

- Develop efficient surrogate model via reduced order models for applications to uncertainty quantification and data assimilation for multphysics problems
- Verify methodologies developed
- Apply methodologies developed to VERA-CS for 3D single fuel assembly and quarter core models

Milestones

- FY15 milestone completed as scheduled on UQ for VERA-CS for 3D single fuel assembly model (with Sandia)
- FY16 milestone completed as scheduled on UQ and DA for VERA-CS for quarter core model

Significant Findings & Accomplishments

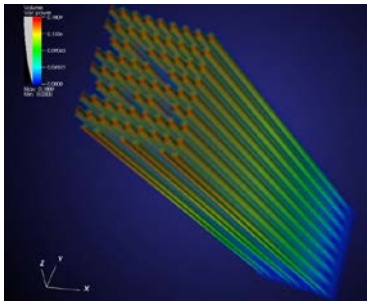
In this work:

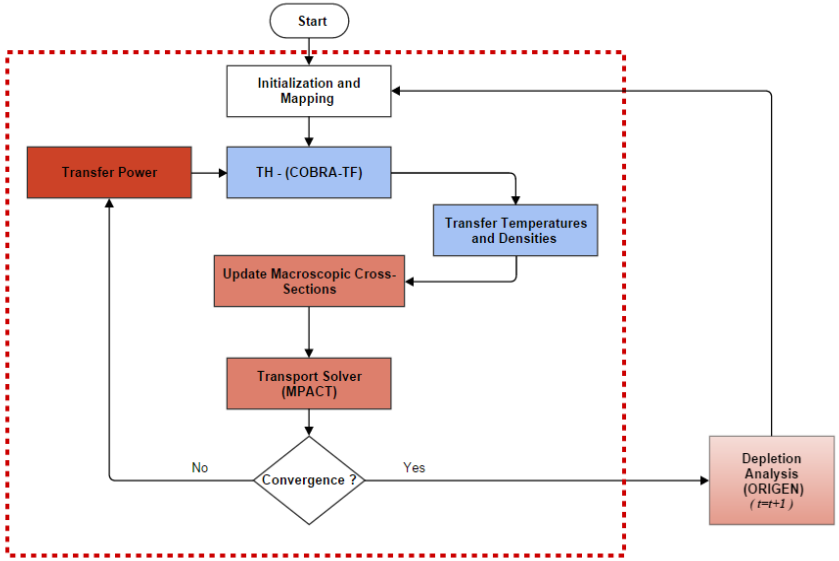
- **Gradient-free and gradient-based** reduced dimensionality based algorithms are extended to multi-physics coupled models (feedback effect).
- An efficient and integrated **multi-physics uncertainty quantification/ sensitivity** scheme was developed.
- An efficient reduced dimensionality based **data assimilation** scheme was being developed.
- An efficient reduced dimensionality based **target accuracy assessment** scheme was developed.
- Algorithms were validated via **SCALE6.1** lattice physics calculations, 3 dimensional assembly model (CASL Progression Problem 6) and core wide problem (CASL Progression Problem 9) **all with depletion with thermal-hydraulics feedback simulated via VERA-CS.**

Significant Findings & Accomplishments

Applications: UQ for VERA-CS for Single Fuel Assembly Model

- Progression problem 6 is a steady state 3-D model of a Westinghouse 17x17 fuel assembly for PWR.
- We are operating the assembly at 100% of rated power and at 600 PPM boron concentration. This is a realistic model of a fuel assembly at realistic powers and flow rates.
- The fuel is depleted to 30 GWd/MTU.
- 24 depletion steps were used: 0,0.1,0.5,1-10,12-30 GWd/MTU.





Significant Findings & Accomplishments

Applications: UQ for VERA-CS for Single Fuel Assembly Model

The uncertainty in 3 responses will be estimated:

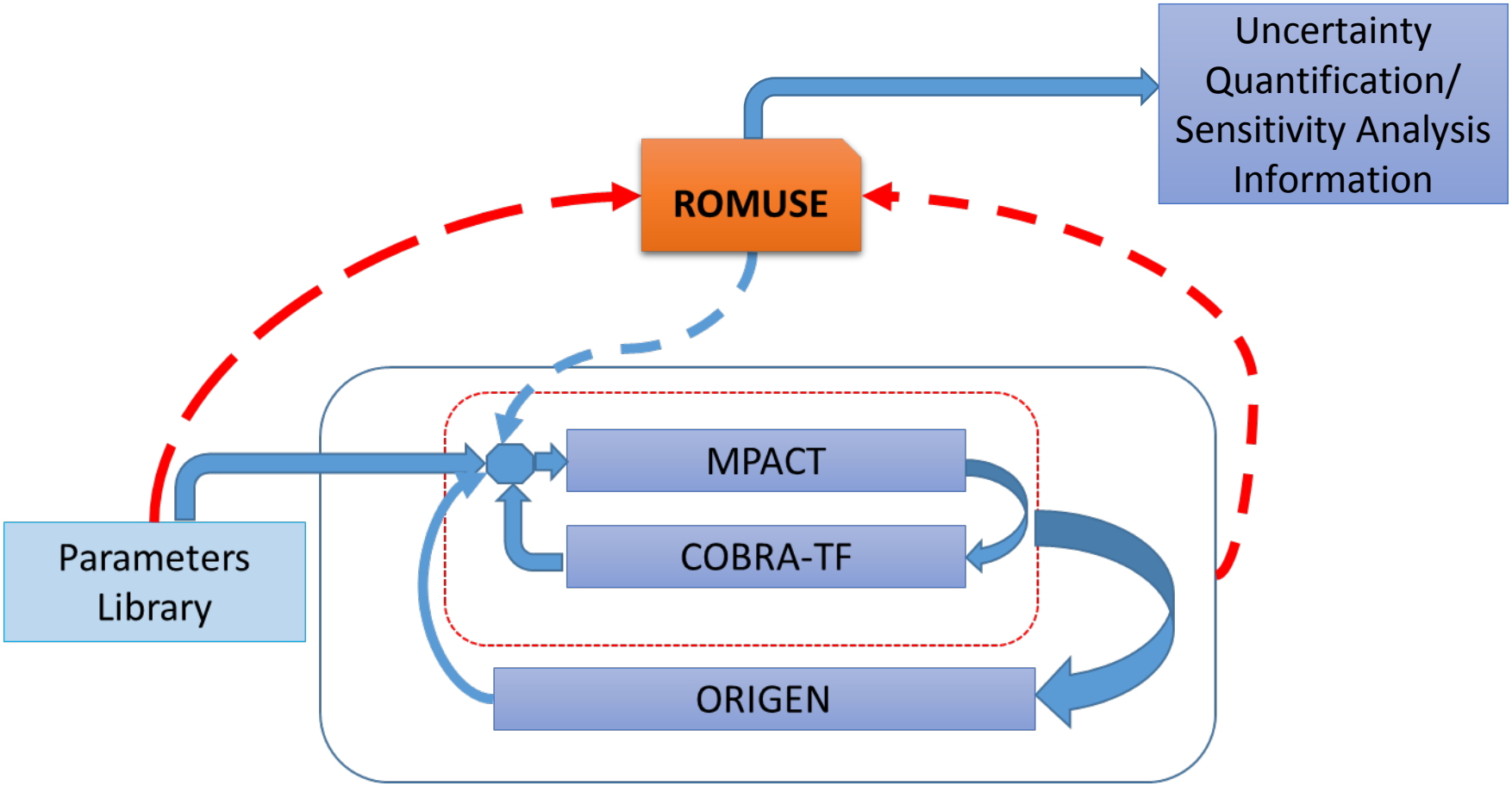
- Multiplication Factor (i.e. *keff)*
- Maximum Pin Power
- Maximum Pin Temperature

Parameter	Distribution	Uncertainty
Nuclear Data Cross-Sections	Gaussian	44 group cov library
Gap conductivity	Uniform	$\pm 50\%$
Grid Spacer Loss Coefficient	Uniform	$\pm 4\%$
Fuel Thermal Conductivity	Uniform	$\pm 10\%$

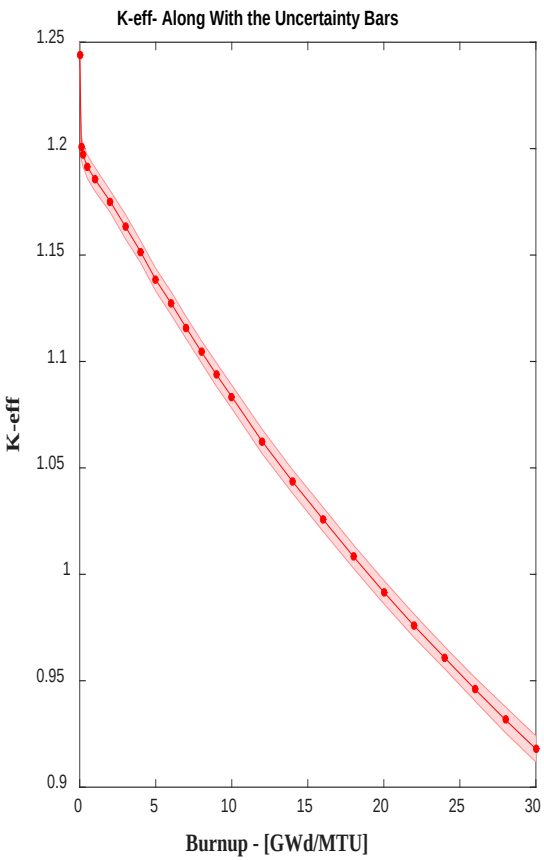
- **VERIFICATION** - Uncertainties predicted by surrogate [MCUQ – Surrogate] and **original physics models using Monte Carlo sampling** and linearized model [MP-EUQ] will be contrasted.

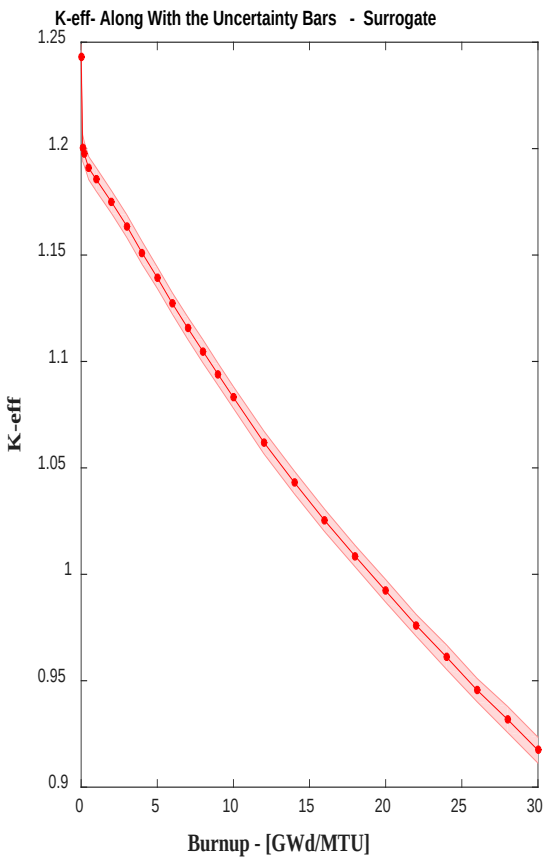
Significant Findings & Accomplishments

Applications: UQ for VERA-CS for Single Fuel Assembly Model



Joint uncertainty → *k-eff*





Burnup dependent k_{eff} along with uncertainty ±σ due to joint samples (left: MCUQ. Right: Surrogate Form).

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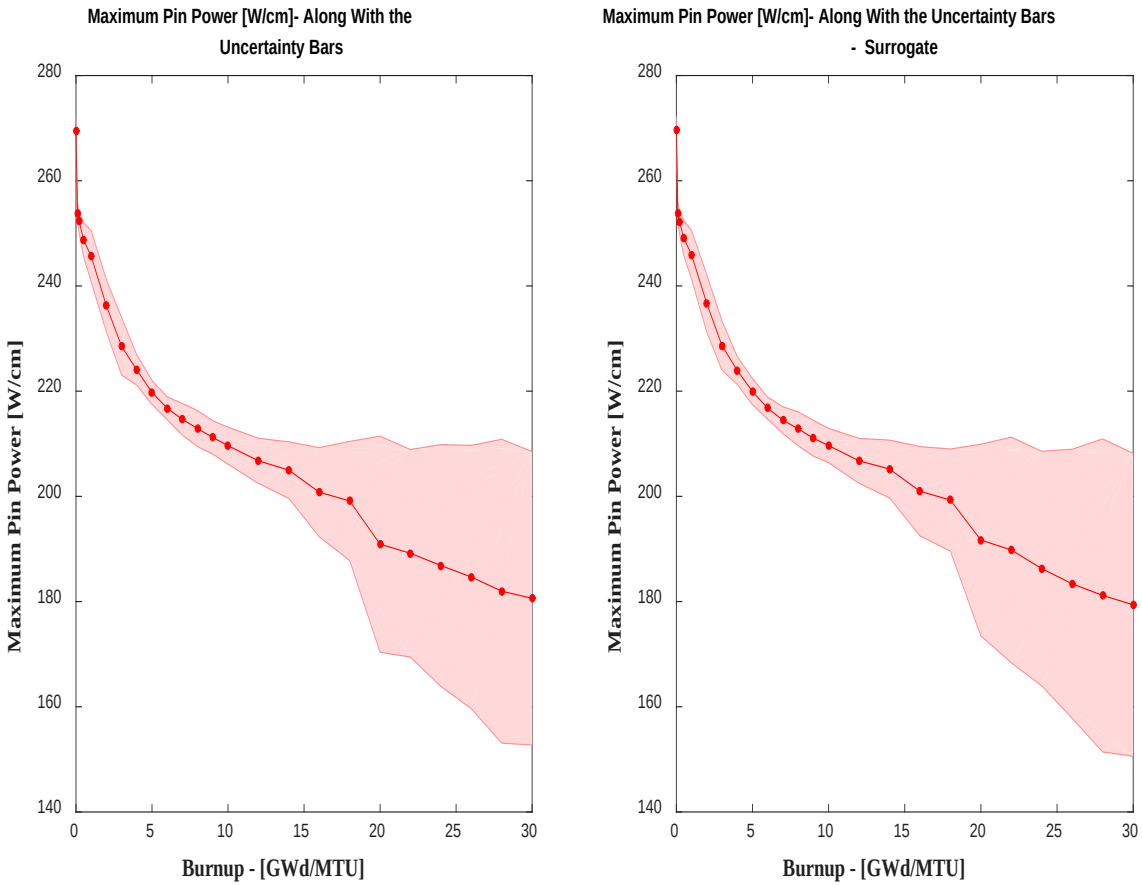
Joint uncertainty → *Max. Pin Power*



Burnup dependent maximum pin power along with uncertainty ±σ due to joint samples. (left: MCUQ. Right: Surrogate Form)

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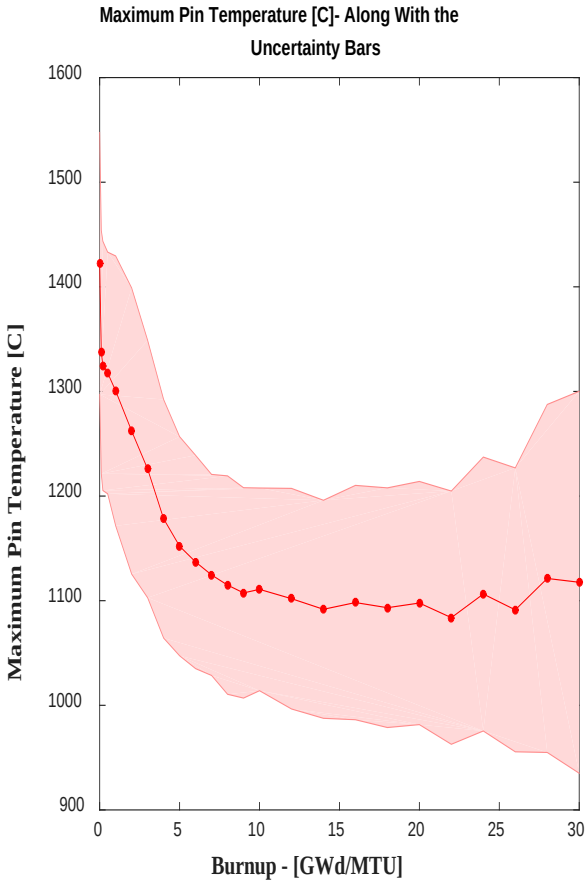
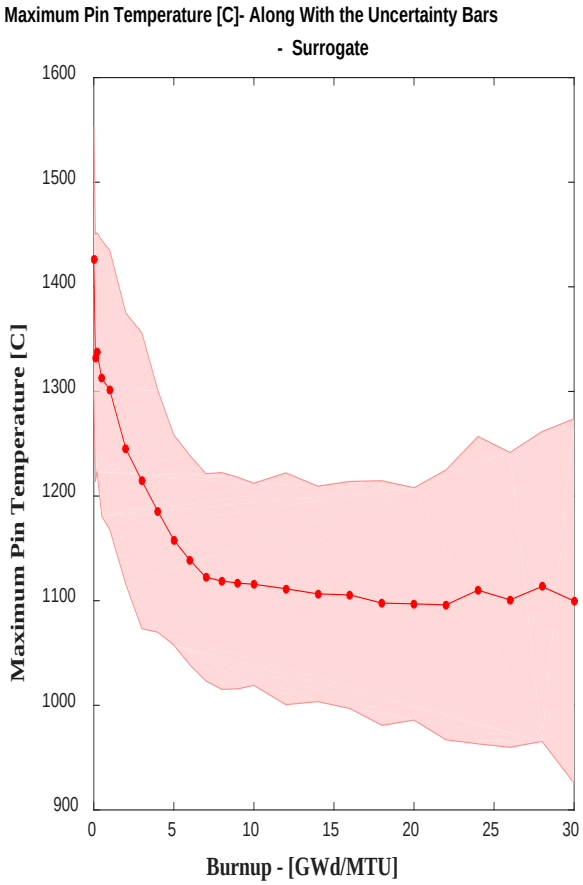
Joint uncertainty → *Max. Pin Temp.*





Burnup dependent maximum pin temperature along with uncertainty ±σ due to joint samples. (left: MCUQ. Right: Surrogate Form)

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(MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)
k-eff

Summary of the *k-eff* uncertainty results - Joint (MCUQ Vs. KL- MP-EUQ Vs. MCUQ-Surrogate)

Depletion (irradiation)	(KL-Approach) MP-EUQ r=50	3rd Order Surrogate (100 samples - 5 experiment)	Monte Carlo (100 samples – 5 experiments)
0.0 GWdMTU	589 pcm	625 pcm	606 pcm
	-	39 pcm	43 pcm
5 GWdMTU	523 pcm	525 pcm	531 pcm
	-	33 pcm	36 pcm
10 GWdMTU	488 pcm	514 pcm	524 pcm
	-	39 pcm	42 pcm
22 GWdMTU	524 pcm	552 pcm	543 pcm
	-	22 pcm	24 pcm
30 GWdMTU	591 pcm	622 pcm	641 pcm
	-	34 pcm	42 pcm

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(MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)
Maximum Fuel Pin Power

Summary of the Maximum Pin Power uncertainty results - Joint (MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)

Depletion (irradiation)	(KL-Approach) MP-EUQ r=50	3rd Order Surrogate (100 samples - 5 experiment)	Monte Carlo (100 samples – 5 experiments)
0.0 GWdMTU	2.03 [W/cm]	2.76 [W/cm]	2.32 [W/cm]
	-	0.09 [W/cm]	0.11 [W/cm]
5 GWdMTU	2.22 [W/cm]	2.48 [W/cm]	2.94 [W/cm]
	-	0.10 [W/cm]	0.13 [W/cm]
10 GWdMTU	2.38[W/cm]	3.31 [W/cm]	3.94 [W/cm]
	-	0.11 [W/cm]	0.13 [W/cm]
22 GWdMTU	15.21 [W/cm]	20.52 [W/cm]	20.55 [W/cm]
	-	0.09 [W/cm]	0.1 [W/cm]
30 GWdMTU	23.45 [W/cm]	30.15 [W/cm]	29.76 [W/cm]
	-	0.11 [W/cm]	0.13 [W/cm]

(MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)
Maximum Fuel Pin Temperature

Summary of the Maximum Pin Temperature uncertainty results - Joint (MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)

Depletion (irradiation) time (days)	(KL-Approach) MP-EUQ r=50	3rd Order Surrogate (100 samples - 5 experiment)	Monte Carlo (100 samples – 5 experiments)
0.0 GWdMTU	92 [C]	99 [C]	112 [C]
	-	8 [C]	10 [C]
5 GWdMTU	79[C]	90 [C]	95 [C]
	-	6 [C]	11[C]
10 GWdMTU	70 [C]	81 [C]	78 [C]
	-	7 [C]	14[C]
22 GWdMTU	90 [C]	101 [C]	106[C]
	-	7 [C]	10[C]
30 GWdMTU	101 [C]	119 [C]	139 [C]
	-	13 [C]	21 [C]

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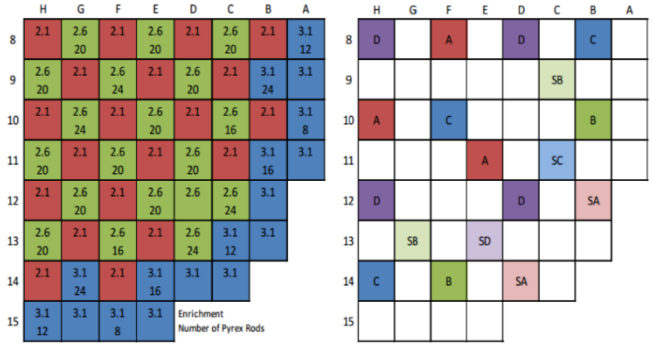
Significant Findings & Accomplishments

Applications: UQ and DA for VERA-CS for Quarter Core Model

Case Study: CASL Progression Problem 9 (A Core Problem)

- Problem 9 is a full core Watts Bar Nuclear 1 (WBN1) with neutronics coupled to thermal hydraulics feedback.
- In this problem both fuel and burnable absorbers are depleted throughout the first cycle.
- However, due to computational resources limitation, this case study will perform the uncertainty quantification study upon a part of cycle 1 using a few depletion steps. Specifically, the core is depleted to 160 effective full power days (EFPD) via 9 depletion steps (0, 9, 32, 45, 60, 80, 100, 120, 160 EFPD).



Core layout in quarter symmetry

Efficient Methods for Data Assimilation

- **Algorithm**

✓ Enhance the identifiability. Find a unique solution tied to certain physical constraints.

✓ Reduce the computational cost (Less DOFs to search along).

Step 1. Determine the DOFs satisfying a set of physics constraints. GF-MPRFA

↓

Step 2. Determine the intersections of spaces from Step1

↓

Step 3. Construct a reduced order model.

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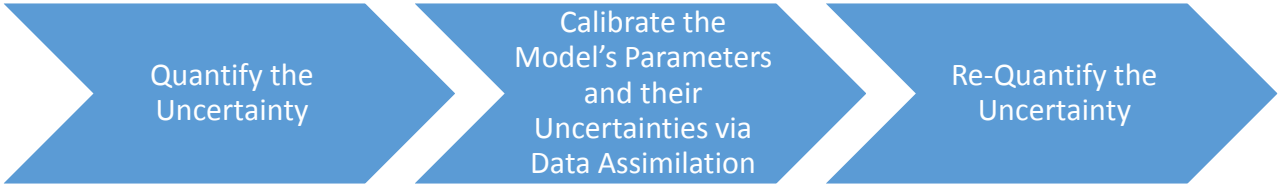
Step 4. Solve the DA problem for the surrogate and along the DOFs determined in Step 2.

What is the Plan ?!



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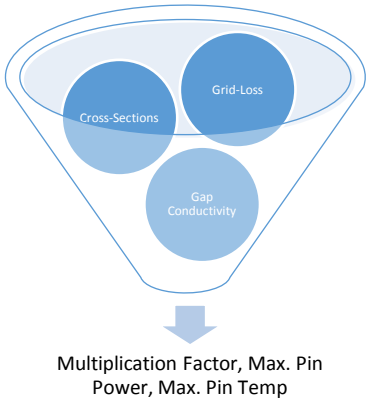
CASL Progression Problem # 9 - UQ

The uncertainty in 3 responses will be estimated :

- Multiplication Factor (i.e. k_{eff}).
- Maximum Pin Power.
- Maximum Pin Temperature.

Parameter's Uncertainty

Parameter	Distribution	Uncertainty
Nuclear Data Cross-Sections	Gaussian	44 group cov library
Gap conductivity	Uniform	$\pm 50\%$
Grid Spacer Loss Coefficient	Uniform	$\pm 4\%$



Uncertainties predicted by surrogate [MCUQ – Surrogate] and original physics models using Monte Carlo sampling and linearized model [MP-EUQ] will be contrasted.

(MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)
k-eff

Summary of the *k-eff* uncertainty results - Joint (MCUQ Vs. KL- MP-EUQ Vs. MCUQ-Surrogate)

Depletion (irradiation)	MP-EUQ r=60	2nd Order Surrogate 500 samples	Monte Carlo 50 samples
0.0 EFPD	0.389 %	0.425 %	0.401 %
	-	0.019 %	0.063 %
9 EFPD	0.399 %	0.395 %	0.417 %
	-	0.021 %	0.066 %
32 EFPD	0.390 %	0.415 %	0.399 %
	-	0.025 %	0.074 %
45 EFPD	0.380 %	0.420 %	0.398 %
	-	0.019 %	0.052 %
60 EFPD	0.379 %	0.399 %	0.391 %
	-	0.032 %	0.071 %
80 EFPD	0.357 %	0.398 %	0.392 %
	-	0.023 %	0.065 %
100 EFPD	0.351 %	0.394 %	0.390 %
	-	0.023 %	0.062 %
120 EFPD	0.349 %	0.391 %	0.387 %
	-	0.023 %	0.058 %
160 EFPD	0.341 %	0.389 %	0.381 %
	-	0.026 %	0.046 %

(MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)
Maximum Fuel Pin Power

Summary of the Maximum Pin Power uncertainty results - Joint (MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)

Depletion (irradiation)	MP-EUQ r=60	2nd Order Surrogate 500 samples	Monte Carlo 50 samples
0.0 EFPD	1%	1.3 %	1.1 %
	-	0.02 %	0.19%
9 EFPD	0.6 %	1.1 %	1.04 %
	-	0.08 %	0.18 %
32 EFPD	0.9 %	1.5 %	1.4 %
	-	0.011 %	0.2 %
45 EFPD	2%	2.2 %	2.9 %
	-	0.2 %	1 %
60 EFPD	2.11 %	1.77 %	1.14 %
	-	0.14 %	0.58 %
80 EFPD	2.45 %	1.64 %	1.00 %
	-	0.20 %	0.55 %
100 EFPD	3.75 %	1.79 %	1.50 %
	-	0.1 %	0.50 %
120 EFPD	2.50 %	1.62 %	1.29 %
	-	0.11 %	0.33 %
160 EFPD	1.72 %	1.45 %	1.41 %
	-	0.07 %	0.16 %

(MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)
Maximum Fuel Pin Temperature

Summary of the Maximum Pin Temperature uncertainty results - Joint (MCUQ VS. MP-EUQ Vs. MCUQ-Surrogate)

Depletion (irradiation)	MP-EUQ r=60	2nd Order Surrogate 500 samples	Monte Carlo 50 samples
0.0 EFPD	0.05 %	7.23 %	6.53%
	-	0.07%	1.00%
9 EFPD	1.92%	5.10%	6.91%
	-	0.02%	0.40%
32 EFPD	1.82%	4.73%	4.53%
	-	0.03%	0.33%
45 EFPD	2.02%	5.15%	5.02%
	-	0.03%	0.31%
60 EFPD	2.35%	5.59%	5.58%
	-	0.08%	0.41%
80 EFPD	2.44%	5.56%	5.44%
	-	0.04%	0.39%
100 EFPD	3.00%	5.11%	5.00%
	-	0.09%	0.43%
120 EFPD	2.11%	5.46%	5.22%
	-	0.06%	0.38%
160 EFPD	2.33%	5.87%	5.67%
	-	0.07%	0.31%

Case Study: CASL Progression Problem # 9 - DA

- First, the surrogate is a second order surrogate.
- In this case study, the measured attributes are:

✓ the **multiplication factor (k_{eff})**,

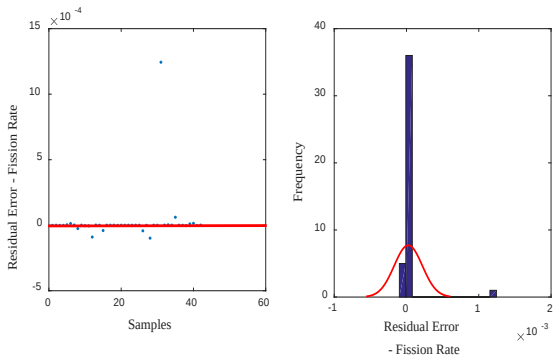
✓ and the **relative fission reaction rate 3 dimensional distribution at the (FR)**, the matrix is equivalent to measuring the fission rate over 49 axial levels and 56 fuel assemblies.

- **Synthetic data** will be used instead of real data. Using the synthetic data implies that the actual solution of the data assimilation problem is known a priori enabling the data assimilation method to be verified.
- **Five depletion steps** are used to generate the synthetic measurements of interest. Hence, each response is measured at each of the depletion step:

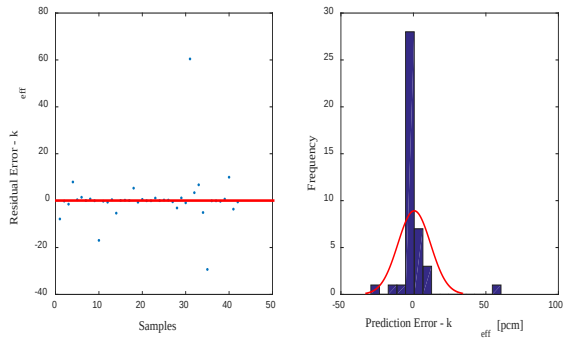
(0, 9, 32, 45, 120, 160 EFPD).

CASL Progression Problem # 9 - DA

- Referring to the figure; the parameters of interest - in this case study – are the gap conductivity (h_{gap}) and the grid loss coefficient (g_{loss}).
- In addition to that the nuclear data cross-sections will be calibrated along with the previous parameters.
- The responses of interest are the multiplication factor, and fission rate distribution
- The surrogate uncertainty is added to the measurement (observables) uncertainty.



Residual errors along with their distribution – Fission Rate at the core center.



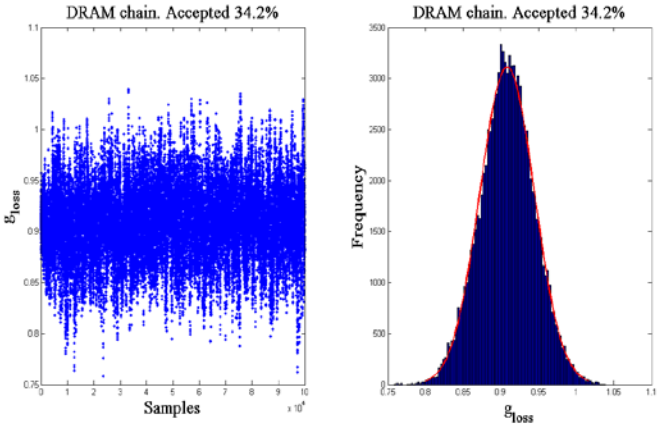
Residual errors along with their distribution - $k_{eff.}$

Surrogate Performance (2nd order / 120 runs)

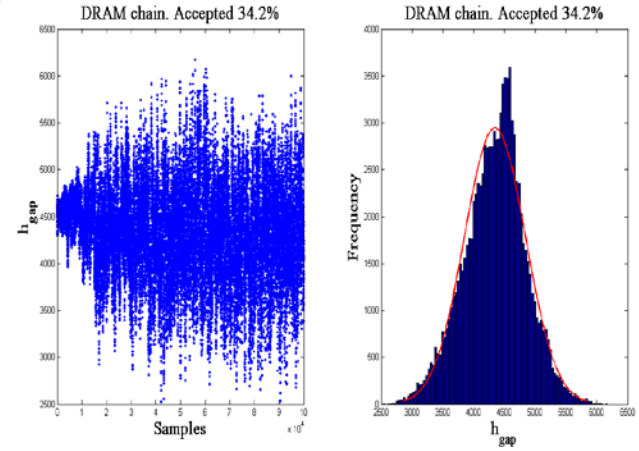
Measurements and Posteriors

Sample Measurements and their uncertainties

Measurement	0.0 EFPD	9.0 EFPD	32.0 EFPD	120.0 EFPD	160.0 EFPD
k_{eff}	1.000443 ±0.00060	1.000121 ±0.00060	1.00013 ±0.00060	0.999951 ±0.00060	0.99991 ±0.00060
FR (in core's central fuel assembly center)	1.9321 ±0.02	1.8962 ±0.02	1.8212 ±0.02	1.7612 ±0.02	1.7312 ±0.02



Chain and posterior distribution for the grid loss coefficient (g_{loss}).



Chain and posterior distribution for the gap conductivity (h_{gap})

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Problem # 9 – DA – Cross-sections Parameters

- 18 different isotope-reaction pairs are considered for calibration. Taking into account that the surrogate uses 47 group structure, the number of cross-sections parameters is 18x47 = 846.

Data assimilation results for few important parameters

Parameter	Reference Value (Reference) (± prior uncertainty)	Actual Perturbed Value	SBDA Estimated Perturbation (± posterior uncertainty)
h_{gap}	4500 ± 2250	4359.91	4109.2 ± 504.1
g_{loss}	0.907 ± 0.03628	0.9123	0.9088 ± 0.035
Σ_f^{U-235} [0.0306-0.012396] eV	1125.219 ±2.66	1258.435	1267.01 ± 1.11
Σ_f^{U-238} [2.2313-1.3534] MeV	0.8927011±0.00528	0.93246	0.9270 ± 0.00243
Σ_f^{Pu-239} [0.0306-0.012396] eV	1361.297± 16.03	1441.313	1436.2 ± 6.11
Σ_s^{H-1} [0.0306-0.012396] eV	75.346183±0.07494	82.47610	78.72 ± 0.0382
Σ_s^{O-16} [0.0306-0.012396] eV	4.329821±0.04336	4.629821	4.611 ± 0.0211

Posterior Uncertainty Quantification

Multiplication factor-UQ

Depletion	Standard Deviation	2nd order Surrogate – Monte Carlo - Original	2nd order Surrogate Monte Carlo – Updated
0 EFPD	σ_k	0.425 %	0.210 %
	σ_{σ_k}	0.019 %	0.012 %
9 EFPD	σ_k	0.395 %	0.189 %
	σ_{σ_k}	0.021 %	0.011 %
32 EFPD	σ_k	0.415 %	0.188 %
	σ_{σ_k}	0.025 %	0.014 %
45 EFPD	σ_k	0.420 %	0.192 %
	σ_{σ_k}	0.019 %	0.009 %
60 EFPD	σ_k	0.399 %	0.193 %
	σ_{σ_k}	0.032 %	0.008 %
80 EFPD	σ_k	0.398 %	0.199 %
	σ_{σ_k}	0.023 %	0.011 %
100 EFPD	σ_k	0.394 %	0.200 %
	σ_{σ_k}	0.023 %	0.018 %
120 EFPD	σ_k	0.391 %	0.201 %
	σ_{σ_k}	0.023 %	0.017 %
160 EFPD	σ_k	0.389 %	0.205 %
	σ_{σ_k}	0.026 %	0.015 %

Maximum Fuel Pin Power-UQ

Depletion	Standard Deviation	2nd order Surrogate – Monte Carlo - Original	2nd order Surrogate Monte Carlo – Updated
0 EFPD	σ_{mp}	1.3 %	0.3 %
	$\sigma_{\sigma_{mp}}$	0.02 %	0.011 %
9 EFPD	σ_{mp}	1.1 %	0.32 %
	$\sigma_{\sigma_{mp}}$	0.08 %	0.025 %
32 EFPD	σ_{mp}	1.5 %	0.31 %
	$\sigma_{\sigma_{mp}}$	0.011 %	0.008 %
45 EFPD	σ_{mp}	2.2 %	0.4 %
	$\sigma_{\sigma_{mp}}$	0.2 %	0.1 %
60 EFPD	σ_{mp}	1.77 %	0.43 %
	$\sigma_{\sigma_{mp}}$	0.14 %	0.05 %
80 EFPD	σ_{mp}	1.64 %	0.47 %
	$\sigma_{\sigma_{mp}}$	0.20 %	0.09 %
100 EFPD	σ_{mp}	1.79 %	0.45 %
	$\sigma_{\sigma_{mp}}$	0.1 %	0.07 %
120 EFPD	σ_{mp}	1.62 %	0.42 %
	$\sigma_{\sigma_{mp}}$	0.11 %	0.064 %
160 EFPD	σ_{mp}	1.45 %	0.37 %
	$\sigma_{\sigma_{mp}}$	0.07 %	0.043 %

Maximum Fuel Pin Temperature-UQ

Depletion	Standard Deviation	2nd order Surrogate – Monte Carlo - Original	2nd order Surrogate Monte Carlo – Updated
0 EFPD	σ_{mt}	7.23 %	1.9 %
	$\sigma_{\sigma_{mt}}$	0.07%	0.06%
9 EFPD	σ_{mt}	5.10%	2.0%
	$\sigma_{\sigma_{mt}}$	0.02%	0.04%
32 EFPD	σ_{mt}	4.73%	1.9%
	$\sigma_{\sigma_{mt}}$	0.03%	0.01%
45 EFPD	σ_{mt}	5.15%	1.8%
	$\sigma_{\sigma_{mt}}$	0.03%	0.02%
60 EFPD	σ_{mt}	5.59%	1.7%
	$\sigma_{\sigma_{mt}}$	0.08%	0.05%
80 EFPD	σ_{mt}	5.56%	1.78%
	$\sigma_{\sigma_{mt}}$	0.04%	0.02%
100 EFPD	σ_{mt}	5.11%	1.8%
	$\sigma_{\sigma_{mt}}$	0.09%	0.02%
120 EFPD	σ_{mt}	5.46%	1.9%
	$\sigma_{\sigma_{mt}}$	0.06%	0.01%
160 EFPD	σ_{mt}	5.87%	2.0%
	$\sigma_{\sigma_{mt}}$	0.07%	0.02%

Plans Going Forward [future work to be completed elsewhere]

- Integration of ROMUSE within DAKOTA
- Completion of CIPS UQ utilizing capabilities developed
- Refinement of current work (not now planned)
  - Examination of correlation of T-H and neutronics parameters after DA based upon current analysis
  - Improvement of surrogate model form (e.g. GPM)
  - Repeat of DA & posteriori-UQ based upon utilization of WB-Unit 1-Cycle 1 plant follow data
  - Extension of DA to include startup physics test measurements
  - Addressing multicycle propagation of uncertainties
  - Improvement in efficiency in generating surrogate model

Budget Status [Abdel-Khalik Taxable & Nontaxable Accounts]

- Starting 10/1/14 to Present
  - Budget Increment = $75K
  - Expenditures = $70K [*PJT salary charged elsewhere*]
  - Carry-over Increment = $5K

- From Day One to Present
  - Carry-over Total = $21K

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