A Study of Uncertainty Quantification of CIPS

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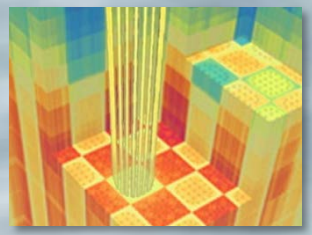
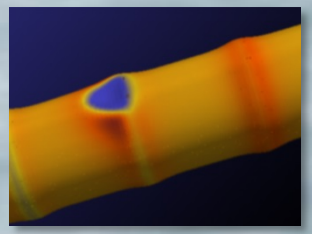
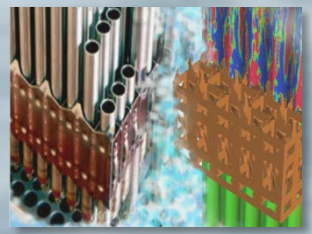
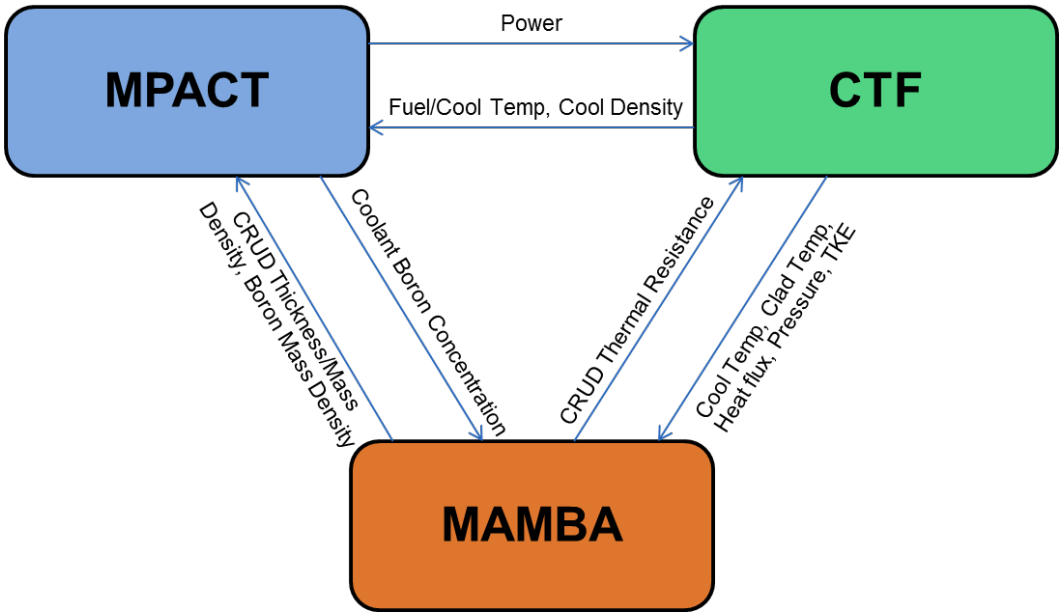






Initial Scope: UQ CIPS Challenge Problem

- Quarter-core CIPS (QoIs: max_crud_thickness & total_boron)
  - Depletion (36 state points)
  - Each run ~65,000 core-hours on Titan (10,960 cores for 6+ hours)
- Wilks UQ (95/95 → 59 runs)
- Validation data available



Initial Observations

- ✓Need stable VERA code
- ✓Need stable run environment (modules/TPLs)
- ✓Need credible baseline (values and performance)

- Dakota concurrency can overwhelm filesystem
- Perturbations to empirical expressions (curve fits) must respect coefficient correlations (joint variation)
- Small crud thickness can exaggerate sensitivity, i.e. sensitivity normalized by baseline thickness

Rescoped: UQ CIPS Challenge Problem

- Quarter-core CIPS (QoIs: max_crud_thickness & total_boron)
  - Depletion (36 state points)
  - Each run ~65,000 core-hours on Titan (10,960 cores for 6+ hours)
- Wilks UQ (95/95 → 59 runs)

- More tractable companion problem
  - Establish and sanity check Dakota-based UQ workflow on Titan
  - Apply PCMM to downselect parameters for full study
  - Identify and address potential issues
- Representative 17x17 single assembly problem
  - BCs correspond to interior region where CRUD is expected
  - Not amenable to validation against experimental data

Overall Approach

- PIRT
- QPIRT
- Parameter Downselect & Characterization
- UQ
- Empirical validation of Wilks

PIRT
(Expert Opinion)

- Temperature uncertainty ± 5 F, normal distribution
- Pressure uncertainty ± 50 psi, normal distribution (there is also a 20 psi bias not included so the total uncertainty is ±70 psi instead)
- Coolant chemistry (to be provided later for MAMBA)
- Core Average Power uncertainty is ± 0.6%, normal distribution
- Single Assembly Power Uncertainty is ± 4%, normal distribution
- Boron uncertainty; agree with Andrew G., this is a measured value so ± 5 ppm should be acceptable, assumed uniformed distribution
- Core Average Flow uncertainty is 2%, normal distribution
- Fuel average density uncertainty is typically within ±0.5% of target (for example target 95% TD, final 95.5%), assumed normal distribution
- Fuel region average enrichment uncertainty is typically within ±0.05 wt% of target (example target 3% U235, final 3.05%), assumed normal distribution
- Local Heat Flux uncertainty is ± 3% uncertainty to account for manufacturing uncertainties, normal distribution

PIRT
Mapping to VERA Input

Parameter	f8.inp	Value	f8.xml	Value
Temperature	tinlet	F	+STATES/State_1/tinlet	C
Pressure	pressure	psia	+STATES/State_1/pressure	MPa
Power	rated, first value	MW	*CORE/rated_power	MW
Flow	rated, second value	Mlbs/hr	*CORE/rated_flow	units
Fuel avg. den.	Fuel U43 second value	-	*ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_U43/thden	-
Fuel avg. den.	Fuel BLK second value	-	*ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_BLK/thden	-
Fuel avg. enrich.	fuel U43	-	+ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_BLK/enrichments[1]	-
Fuel avg. enrich.	fuel BLK	-	+ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_BLK/enrichments[1]	-

PIRT
Code-level Parameters

VERAIn

*ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_BLK/thden
*ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_U43/thden
*CORE/rated_flow
*CORE/rated_power
+ASSEMBLIES/Assembly_B9B-128I/Fuels/F
+ASSEMBLIES/Assembly_B9B-128I/Fuels/F
+STATES/State_1/pressure
+STATES/State_1/tinlet

CTF

k_cd
k_cdfb
k_clad_avg_tmp
k_cond
k_cool_avg_den
k_cool_avg_tmp
k_eta
k_fuel_avg_tmp
k_gama
k_hgap
k_htcl
k_htcv
k_qliht
k_qradd
k_qradv
k_qvapl
k_rodqq

Nominal perturbations of +- 10%

PIRT
Code-level Parameters

VERAIn

*ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_BLK/thden
*ASSEMBLIES/Assembly_B9B-128I/Fuels/Fuel_U43/thden
*CORE/rated_flow
*CORE/rated_power
+ASSEMBLIES/Assembly_B9B-128I/Fuels/F
+ASSEMBLIES/Assembly_B9B-128I/Fuels/F
+STATES/State_1/pressure
+STATES/State_1/tinlet

CTF

k_cd
k_cdfb
k_clad_avg_tmp
k_cond
k_cool_avg_den
k_cool_avg_tmp
k_eta
k_fuel_avg_tmp
k_gama
k_hgap
k_htcl
k_htcv
k_qliht
k_qradd
k_qradv
k_qvapl
k_rodqq

MAMBA

k_Bthresh
k_Cpor
k_crud_solid
k_delta_r
k_fac
k_Hc
k_kp2
k_mit0
k_Nc
k_rc
k_Tsat

(k_Bfract)

Nominal perturbations of +- 10%

PIRT
Cross-Sections “Parameters”

Xsec Filename
mpact47g_70s_v4.0_pert_1.fmt
mpact47g_70s_v4.0_pert_10.fmt
mpact47g_70s_v4.0_pert_100.fmt
mpact47g_70s_v4.0_pert_11.fmt
mpact47g_70s_v4.0_pert_12.fmt
mpact47g_70s_v4.0_pert_13.fmt
mpact47g_70s_v4.0_pert_14.fmt
mpact47g_70s_v4.0_pert_15.fmt
mpact47g_70s_v4.0_pert_16.fmt
mpact47g_70s_v4.0_pert_17.fmt
mpact47g_70s_v4.0_pert_18.fmt
mpact47g_70s_v4.0_pert_19.fmt
mpact47g_70s_v4.0_pert_2.fmt
mpact47g_70s_v4.0_pert_20.fmt
mpact47g_70s_v4.0_pert_21.fmt
mpact47g_70s_v4.0_pert_22.fmt
mpact47g_70s_v4.0_pert_23.fmt
mpact47g_70s_v4.0_pert_24.fmt
mpact47g_70s_v4.0_pert_25.fmt
mpact47g_70s_v4.0_pert_26.fmt

QPIRT
(DAKOTA Centered Parameter Study)

VERAIn	+STATES/State_1/tinlet	-14.58%
	+STATES/State_1/tinlet	13.08%
	+STATES/State_1/pressure	-75.19%
	+STATES/State_1/pressure	102.91%
	*CORE/rated_power	-16.28%
	*CORE/rated_power	14.58%

CTF	k_rodqq	-40.84%
	k_rodqq	34.25%

MAMBA	k_Cpor	-11.68%
	k_Cpor	30.72%
	k_Tsat	1787.21%
	k_Tsat	-60.61%
	k_mit0	68.51%
	k_mit0	-51.31%
	k_crud_solid	-59.11%
	k_crud_solid	-65.75%
	k_RtcB	-63.23%
	k_RtcB	-63.23%

Relatively Unimportant Parameters

	Max Crud	Total Boron
Xsec Filename		
mpact47g_70s_v4.0_pert_1.fmt	-0.03%	0.24%
mpact47g_70s_v4.0_pert_10.fmt	-0.08%	-0.27%
mpact47g_70s_v4.0_pert_100.fmt	-0.52%	-0.37%
mpact47g_70s_v4.0_pert_11.fmt	-0.01%	0.48%
mpact47g_70s_v4.0_pert_12.fmt	0.09%	0.40%
mpact47g_70s_v4.0_pert_13.fmt	-0.14%	0.46%
mpact47g_70s_v4.0_pert_14.fmt	-0.19%	0.34%
mpact47g_70s_v4.0_pert_15.fmt	0.18%	0.81%
mpact47g_70s_v4.0_pert_16.fmt	-0.44%	-0.76%
mpact47g_70s_v4.0_pert_17.fmt	-0.31%	-0.29%
mpact47g_70s_v4.0_pert_18.fmt	-0.12%	0.25%
mpact47g_70s_v4.0_pert_19.fmt	0.08%	-0.69%
mpact47g_70s_v4.0_pert_2.fmt	0.15%	0.11%
mpact47g_70s_v4.0_pert_20.fmt	-0.29%	-0.89%
mpact47g_70s_v4.0_pert_21.fmt	-0.25%	0.12%
mpact47g_70s_v4.0_pert_22.fmt	-0.49%	-0.14%
mpact47g_70s_v4.0_pert_23.fmt	0.22%	0.79%
mpact47g_70s_v4.0_pert_24.fmt	-0.05%	-0.37%
mpact47g_70s_v4.0_pert_25.fmt	-0.02%	0.21%
mpact47g_70s_v4.0_pert_26.fmt	0.06%	0.18%

- CTF: HGAP & KCOND

Candidate Parameters

VERAIn	+STATES/State_1/tinlet	Boiling
	*CORE/rated_power	
	+STATES/State_1/pressure	
	*CORE/rated_flow	
CTF	k_rodqq	Heat Xfer
	k_rodqq	
MAMBA	k_Bthresh	
	k_Cpor	
	k_crud_solid	
	k_delta_r	
	k_fac	
	k_Hc	
	k_kp2	
	k_mit0	
	k_Nc	
	k_rc	
	k_Tsat	

Consistent with CTF values?

Parameter Characterization

VERAIn: Normal

	Mean	Std. Dev.
+STATES/State_1/tinlet	291.33	1.39
*CORE/rated_power	1.0	0.02
+STATES/State_1/pressure	15.51	0.241
*CORE/rated_flow	1.0	0.02

MAMBA: Uniform

k_Bthresh	± 1%
k_Cpor	± 1%
k_crud_solid	± 1%
k_delta_r	± 1%
k_fac	± 1%
k_Hc	± 1%
k_kp2	± 1%
k_mit0	± 1%
k_Nc	± 1%
k_rc	± 1%
k_Tsat	± 1%

UQ Results Summary

- PCMM (PIRT, QPIRT, Parameter Downselect & Characterization)
  - 8 VERAIn (→4); ~~40 CTF~~; 34 Mamba1D (→ 11); ~~200 Xsecs~~
  - VERAIn: Normal; Mamba1D: uniform +-1%

- UQ (799 MC samples)
  - Empirical validation of Wilks using MC samples

Conf. > 99.9999%

Probability Level	Max Crud Thickness (μm)	Total Boron (mg)
0.70	112.22	7.4348e+04
0.75	127.33	9.1038e+04
0.80	138.47	1.0113e+05
0.85	149.74	1.1896e+05
0.90	164.77	1.3816e+05
0.95	179.82	1.6346e+05

Wilks UQ
(Dakota 6.4+)

```
method
    sampling
    sample_type random
    probability_levels = 0.90 0.95 0.99
    wilks
        [one_sided_upper | one_sided_lower | two_sided ]
        order [int]
        confidence_level [Real]
```

```
Wilks Statistics for Two-Sided 9.5000000000e+01% Confidence Level, Order = 2 for response_fn_2:

    Coverage Level     Lower Bound        Upper Bound     Number of Samples
    --------------  -----------------  -----------------  -----------------
   7.5000000000e-01  1.7447858600e-01   5.9077759785e-01         29
   8.0000000000e-01  1.6351498895e-01   6.4617674595e-01         37
   8.5000000000e-01  1.3098323538e-01   7.7210396929e-01         50
   9.0000000000e-01  1.0844818668e-01   7.7210396929e-01         76
   9.5000000000e-01  4.1010698188e-02   8.2489197460e-01         153

Wilks Statistics for Two-Sided 9.5000000000e+01% Confidence Level, Order = 2 for response_fn_3:

    Coverage Level     Lower Bound        Upper Bound     Number of Samples
    --------------  -----------------  -----------------  -----------------
   7.0000000000e-01  5.3830621737e-01   9.6156687420e-01         24
   7.5000000000e-01  5.3830621737e-01   9.6156687420e-01         29
   8.0000000000e-01  5.1606410347e-01   1.0097142573e+00         37
   8.5000000000e-01  5.1548979886e-01   1.3069283455e+00         50
   9.0000000000e-01  4.0041444000e-01   1.3069283455e+00         76
   9.5000000000e-01  2.9238864946e-01   1.3069283455e+00         153
   9.9000000000e-01  2.4007409519e-01   1.3069283455e+00         773
```

Wilks UQ

- Given a quantile (probability level), confidence level, and order, determine the number of independent samples needed, eg

Probability Level	Max Crud Thickness (μm)	Total Boron (mg)
0.70	112.22	7.4348e+04
0.75	127.33	9.1038e+04
0.80	138.47	1.0113e+05
0.85	149.74	1.1896e+05
0.90	164.77	1.3816e+05
0.95	179.82	1.6346e+05

1st Order Single Assembly Results

Probability Level	Theoretical Confidence	Required Samples	Computed Confidence Max Crud	Computed Confidence Total Boron
0.70	0.95	9	0.962	0.956
0.75	0.95	11	0.959	0.956
0.80	0.95	14	0.974	0.973
0.85	0.95	19	0.952	0.959
0.90	0.95	29	0.960	0.959
0.95	0.95	59	0.953	0.957

Single Assembly Results Summary

- PCMM (PIRT, QPIRT, Parameter Downselect & Characterization)
  - 8 VERAIn (→4); ~~40 CTF~~; 34 Mamba1D (→ 11); ~~200 Xsecs~~
  - VERAIn: Normal; Mamba1D: uniform +-1%

- UQ (799 MC samples, 159 Latin hypercube samples)
  - Empirical validation of Wilks using MC samples (previous slide)
  - GP surrogate from LHS samples compares favorably with Wilks for 95/95 but degrades for 99/99

- Observations:
  - Counterintuitive dependence on exit pressure
  - Decreased robustness with joint parameter variations
  - Possible surrogate improvement by extending parameter domains (GPs perform better in interior of parameter domain)

Conclusions

- Model consistency across physics codes is important
- Parameter distributions for coarsened codes is an open challenge (Hi2Lo)
- Insight from smaller problems (single assembly) helps but does not guarantee success on large problems (quarter core)
- Dakota facilitates UQ (eg validated Wilks and comparisons)