SAND2016-4990C

Uncertainty quantification studies of stand-alone and coupled CTF

Russell Hooper
&
Vince Mousseau
Sandia Labs

Collaborators:
Sandia Labs: Brian Adams, Noel Belcourt
North Carloina State Univ.: Ralph Smith, Nathan Porter
Los Alamos Lab.: Brian Williams

CTF-3
Villigen, Switzerland
June 1, 2016

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

The **C**onsortium for **A**dvanced **S**imulation of **L**ight water reactors (CASL)

CASL's *mission :* to provide forefront and usable modeling and simulation capabilities needed to address phenomena that limit the operation and safety performance of LWRs

http://www.casl.gov

Energy Innovation Hub

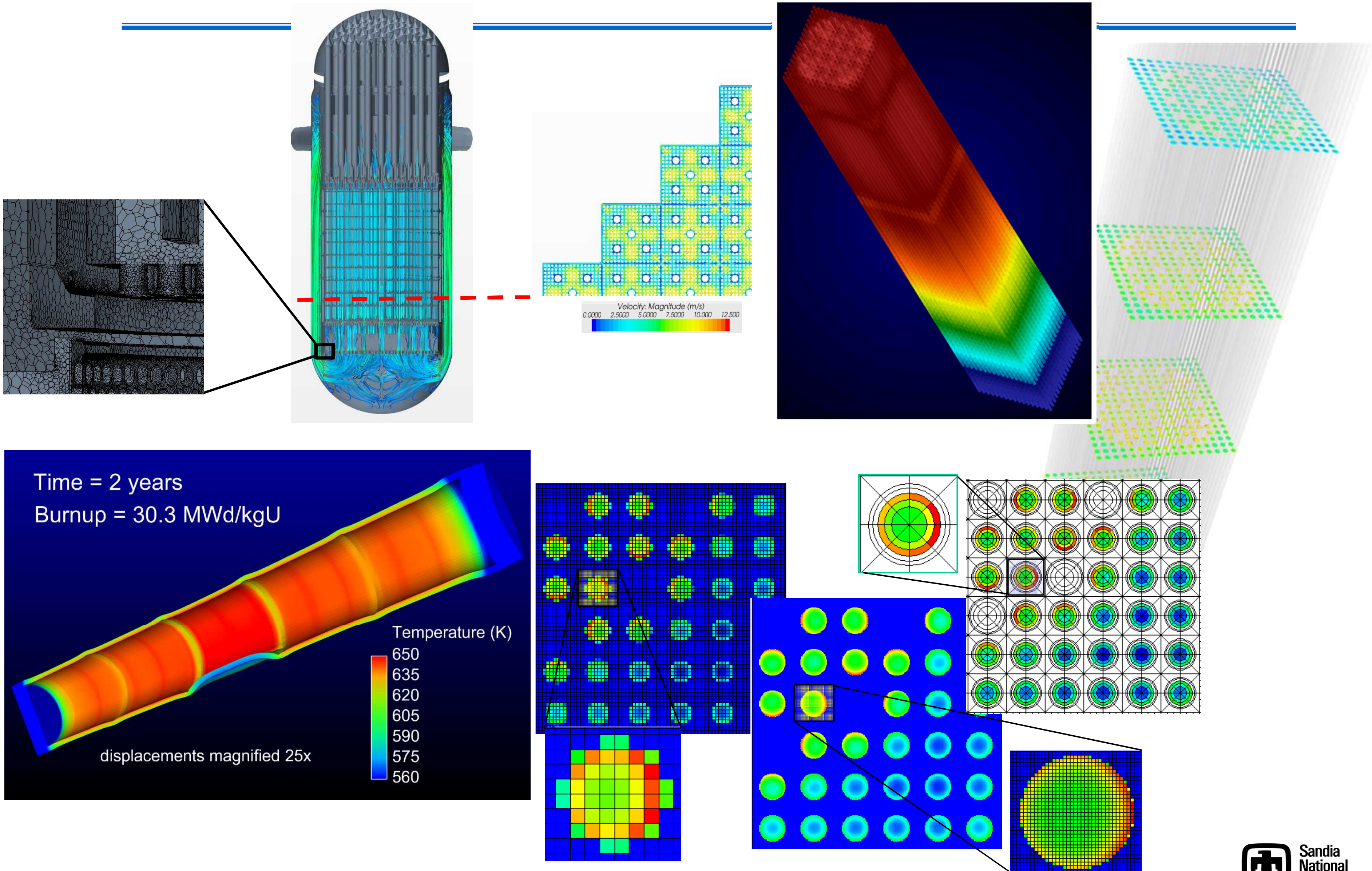
Core Partners

CASL is an outcome-oriented endeavor. Science and engineering products are of primary importance.

Sandia National Laboratories

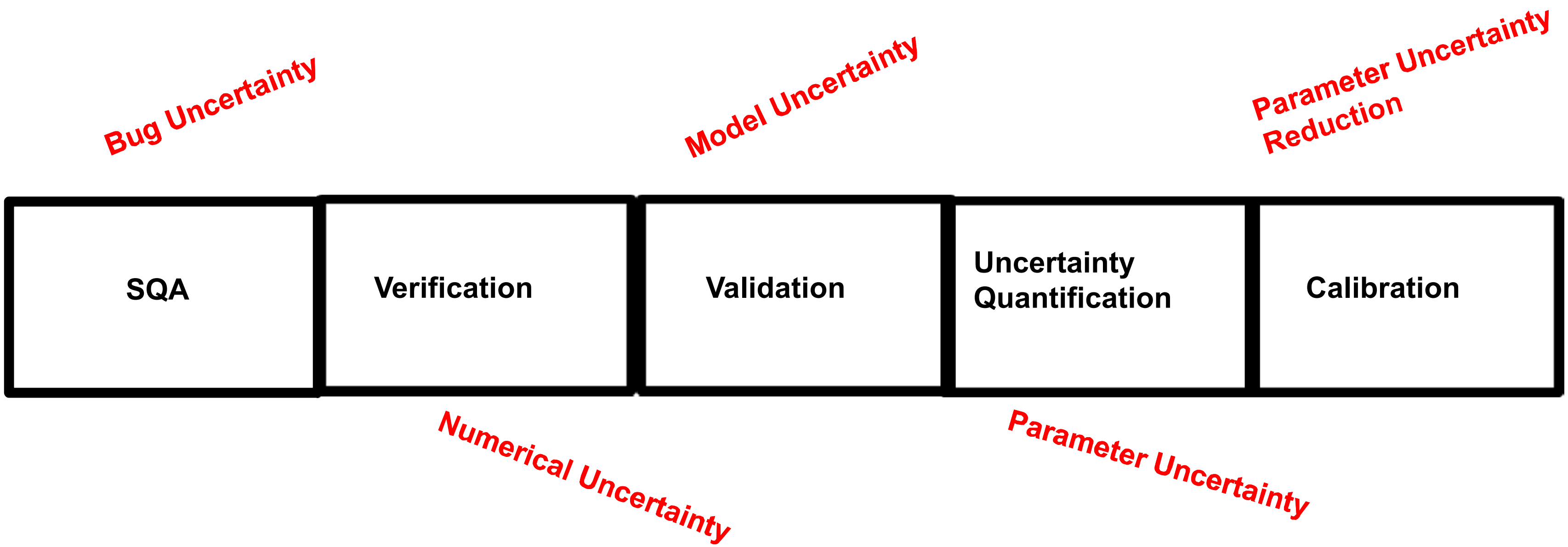
CASL Mod-Sim Challenges

Full core to assembly to subassembly to pin/pellet



Sandia National Laboratories

PCMM



- The Predictive Code Maturity Model (PCMM) is the process being employed in CASL to measure software quality and maturity.
- This is an iterative process where one continually works to increase the lowest score.

Total Uncertainty

- **Total uncertainty = numerical + model + parameter = verification + validation + uncertainty quantification**

- **A large uncertainty results from bad numerics, bad physical models, and/or large parameter uncertainties.**

- **It is unsafe to make assumptions about unmeasured uncertainties.**

- **Improved confidence in mod-sim capability is achieved from a quantitative-based holistic approach.**

Common Measures of Uncertainty

- **Verification:** $||QOI_{exact} - QOI_{computed}||$
- **Validation:** $||QOI_{experimental} - QOI_{computed}||$
- **Uncertainty Quantification:**

$$||QOI_{perturbed} - QOI_{computed}||$$

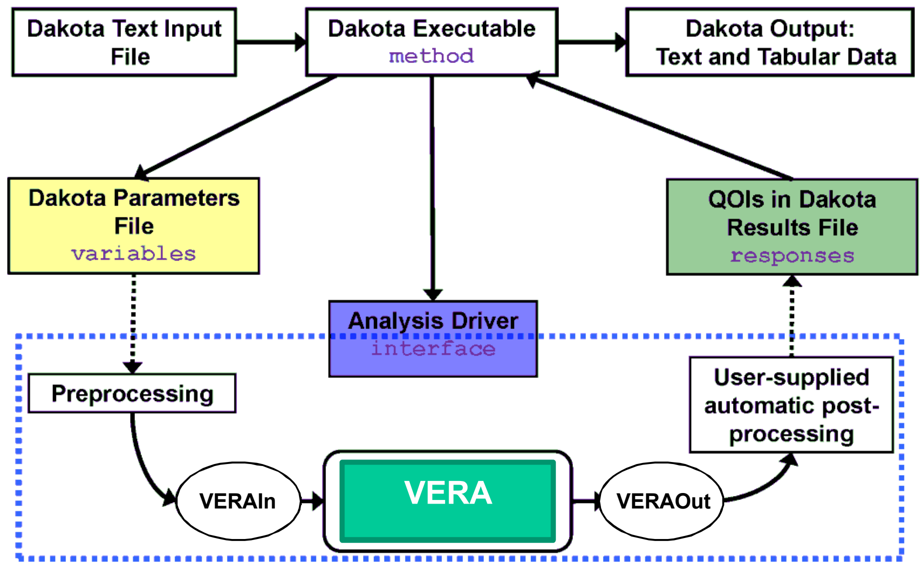
Numerical, model, and parameter uncertainty are computed in a consistent manner to allow meaningful comparisons of error and sensitivity.

General Strategy

- Quantify all modes of uncertainty
- Quantitatively compare the different forms of uncertainty
- Work to reduce the largest uncertainties
- Predictive Capability Maturity Model will be employed by CASL.

Dakota Driver

- DAKOTA is the software package that will be used to deliver tools to improve the PCMM analysis.
- DAKOTA has been strong in uncertainty quantification and calibration and MVA1 MVA2re improving its ability to do verification and validation.



- Adapters to manipulate parameters in:
  - High-level user input
  - Auxiliary data, e.g., model form
  - Offline generated input data such as cross section

Dakota enables V MVA3 analyses in CASL

Slide 8

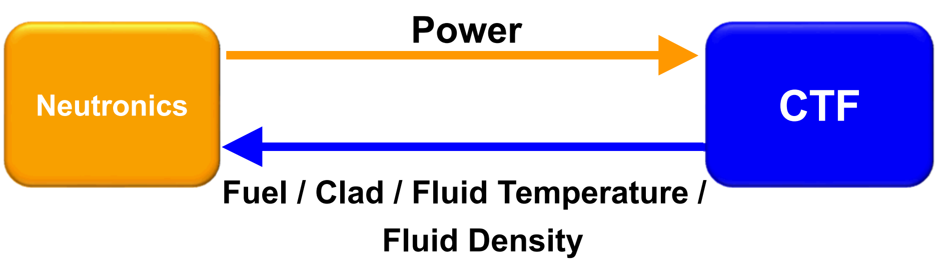
MVA1 changed so to and
Mousseau, Vincent Andrew, 5/23/2016

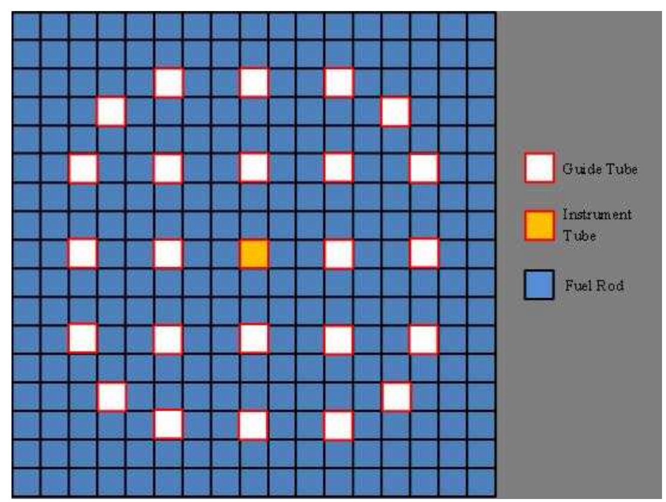
MVA2 Shoud we replace code input with "VERAIN" and code output with "VERAOUT"?
Mousseau, Vincent Andrew, 5/23/2016

MVA3 remove core since it has multiple meanings in this talk
Mousseau, Vincent Andrew, 5/23/2016

VUQ Analysis of Cobra-TF for Problem of Interest

- **Simulation of a single PWR assembly**
  - **Hot Full Power, T/H feedback**
  - **Boron concentration of 1300 ppm, 100% power**
  - **Power supplied by neutronics held constant**
- **Dittus Bolter parameter variation**
- **Quantity of Interest is maximum fuel temperature**
- **Results are based on random samples of the parameter distributions.**
- **A 95% credible interval is calculated similar to Wilks** MVA4



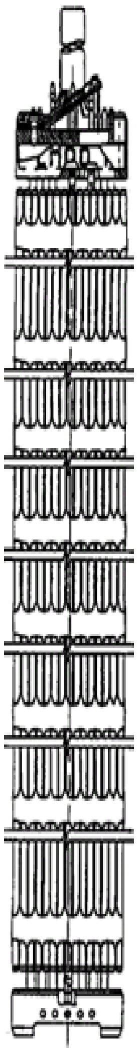


Slide 9

MVA4 Compare with Wilks which most of them use.
Mousseau, Vincent Andrew, 5/23/2016

Cobra-TF Solution Verification

CTF-only: With Spacer Grids*



Spacer Grid Challenge

*** Grid locations were shifted to produce equal mesh spacing between all grids.**

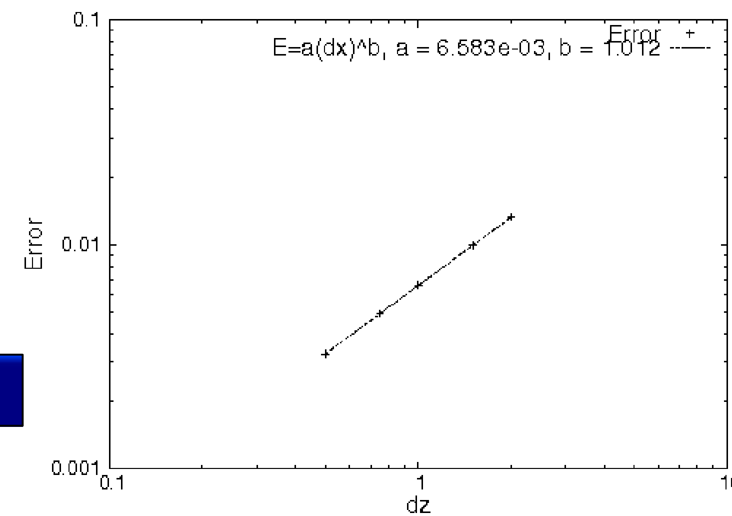
Mesh factor, f	Δz (cm)	#Axial elements	Tot. Press. (bar)
0.5	4.036	72	1.16843
0.75	6.054	48	1.1701
1.0	8.072	36	1.17176
1.5	12.108	24	1.17508
2.0	16.144	18	1.17845

Error Model:

$$E = P - \bar{P} = a\,(\Delta z)^b$$

$$b = 1.012$$

Very good agreement with theoretical 1.0



es

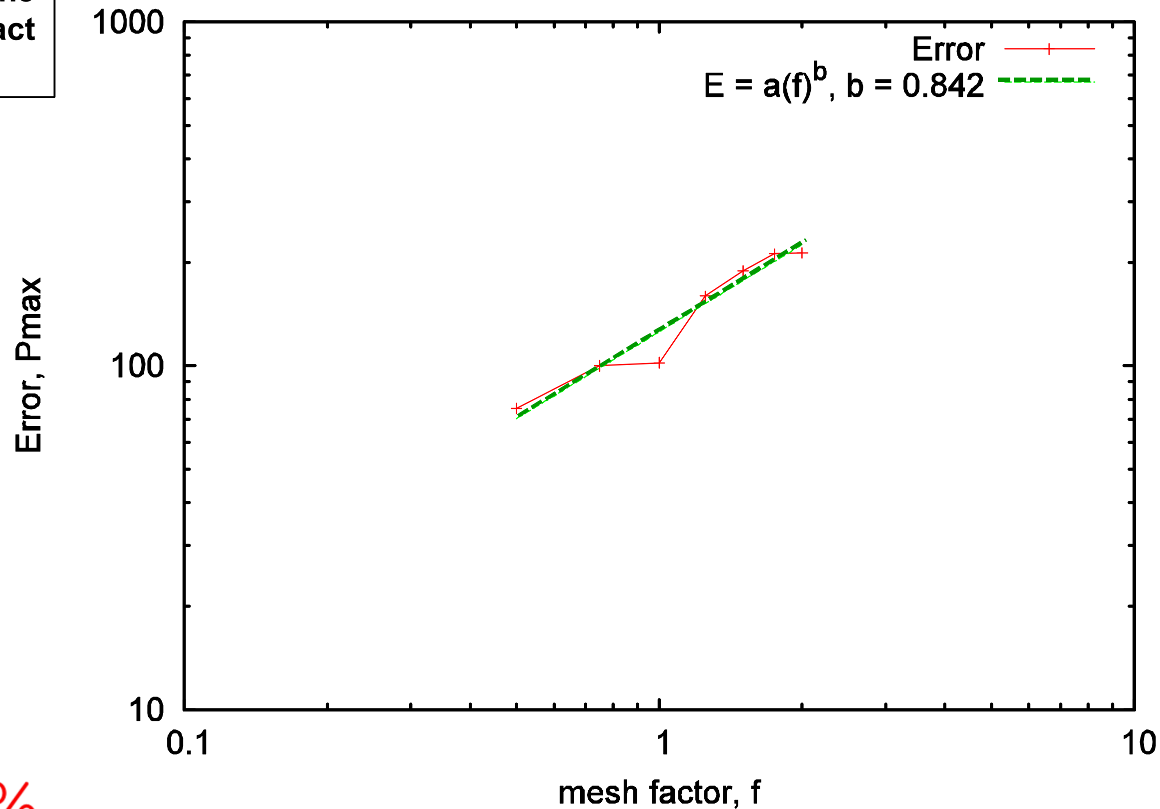
MVA5 MVA6

Coupled CTF-Neutronics Solution Verification

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

Each run requires ~600 cpu hours on ORNL's Titan

Progression Problem 6		
Mesh factor, f	#Axial elements	Max Power
0.5	92	27,882
0.75	65	27,907
1.0	50	27,909
1.25	43	27,966
1.5	37	27,995
1.75	35	28,018
2.0	30	28,019



$$E_{(f=1.0)} = 102 = 0.37\%$$

Error Model: $E_{P_{\text{max}}} = P_{\text{max}} - \bar{P}_{\text{max}} = a\,(f)^b$

$$b = 0.842$$

Degraded order-of-convergence but still usable.

Slide 11

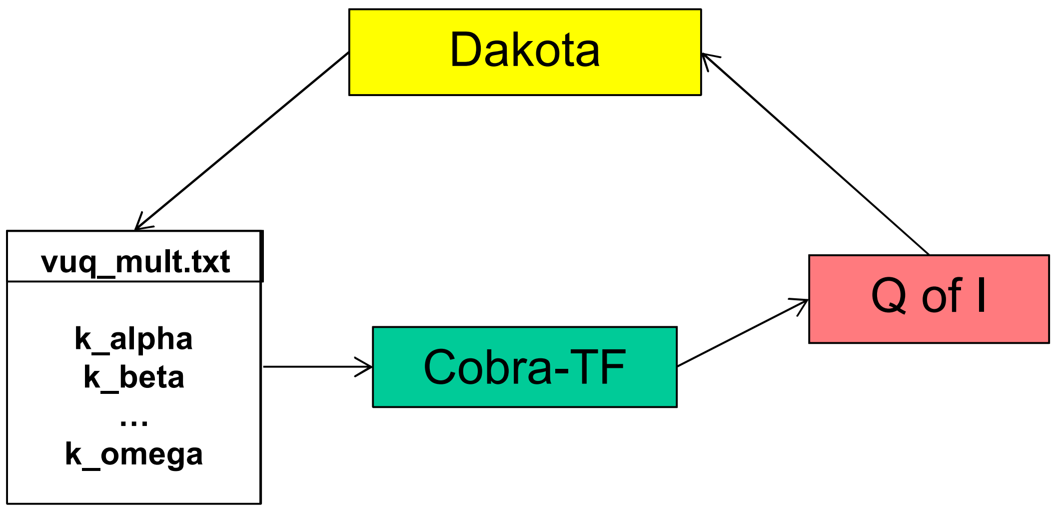
MVA5 The green line does not show up well on my monitor. You might want to change it to black.
Mousseau, Vincent Andrew, 5/23/2016

MVA6 Make sure in the talk you define "FEM Error"
Mousseau, Vincent Andrew, 5/23/2016

Cobra-TF Parameter Exposure

For general parameter perturbations:

$$\alpha = k_\alpha \alpha_0 + s_\alpha$$

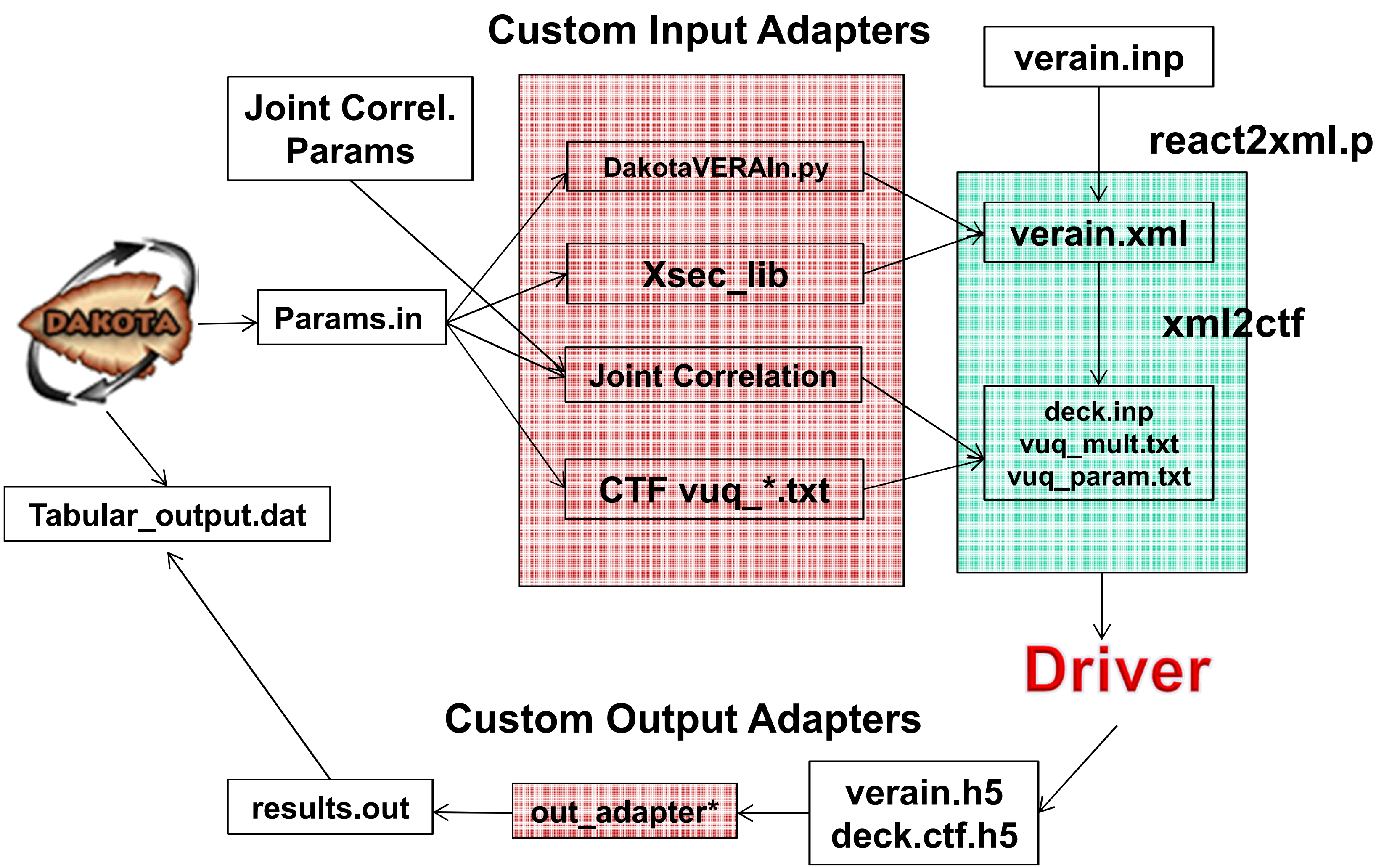


This capability enables:

- **Sensitivity studies**
- **UQ studies**
- **Parameter optimization and calibration**

Exposure of VERA Input and Cobra-TF input parameters enables VUQ analysis

Accommodating Other Parameters



CTF-only Parameter Downselect

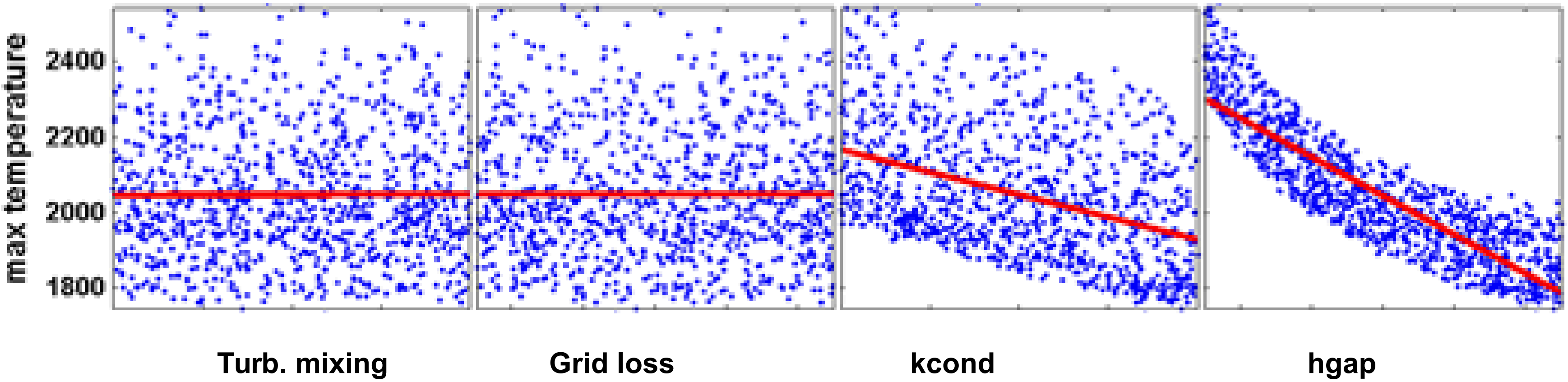
Variable Description	Multiplier	Percent Difference	Physics
Gap Conductivity	0.5	24.028	Fuel
Gap Conductivity	1.5	-8.18	Fuel
Thermal Conductivity	0.9	7.313	Fuel
Thermal Conductivity	1.1	-5.745	Fuel
Fission Heat	1.05	4.740	Input
Fission Heat	0.95	-4.626	Input
Mesh Spacing	NA	0.015	Numerical
Turbulent Mixing of Liquid Mass	0.95	0.006	Thermal Hydraulics
Turbulent Mixing of Liquid Energy	0.95	0.002	Thermal Hydraulics
Grid Spacer Loss Coefficient	0.95	0.001	Thermal Hydraulics

Coupled Problem Parameter Sensitivity → Downselect

Variable Description	Multiplier	Percent Difference	Physics
Gap Conductivity	0.5	21.423	Fuel
Gap Conductivity	1.5	-7.445	Fuel
Fuel Conductivity	0.9	6.807	Fuel
Fuel Conductivity	1.1	-5.405	Fuel
Fission Heat	1.05	4.436	Coupling
Fission Heat	0.95	-4.354	Coupling
Cross Sections	NA	0.739	Neutronics
Wall Heat Transfer	0.95	0.610	Thermal Hydraulics
Wall Heat Transfer	1.05	-0.495	Thermal Hydraulics
Fuel Temperature	0.95	0.254	Coupling
Fuel Temperature	1.05	-0.236	Coupling
Cross Sections	NA	-0.198	Neutronics
Moderator Density	1.05	-0.106	Coupling
Mesh Spacing	NA	0.050	Numerical
Moderator Density	0.95	0.085	Coupling
Moderator Temperature	0.95	0.034	Coupling
Moderator Temperature	1.05	-0.032	Coupling

40+ initial VUQ parameters reduced to 7 via sensitivity analysis

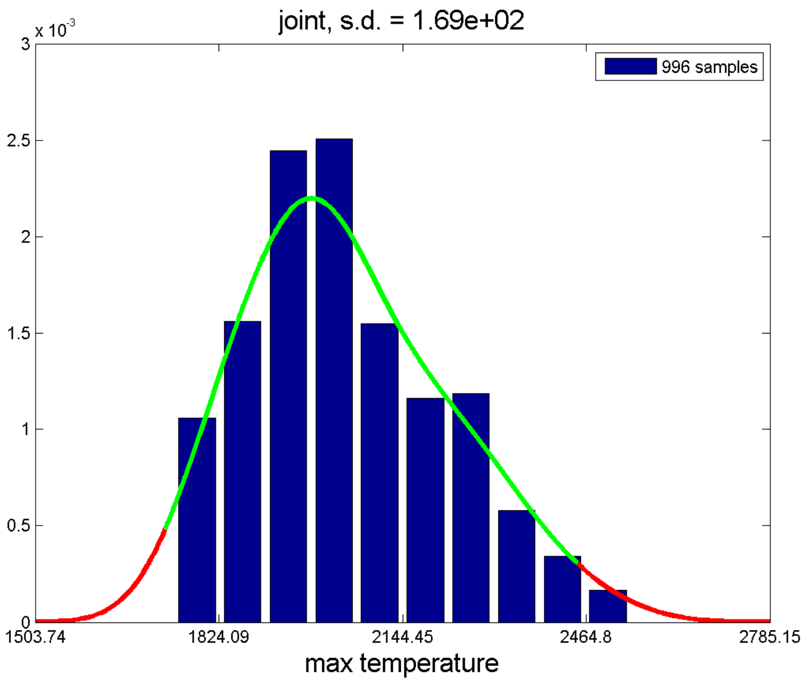
Coupled Problem Parameter Sensitivity → Downselect



Variable	Minimum	Nominal	Maximum
Thermal Conductivity Multiplier	0.9000	1.0000	1.1000
Gap Conductivity W/m^2K	2839.2	5678.3	8517.5
Dittus-Boelter	**	**	**
Cross-Sections	**	**	**

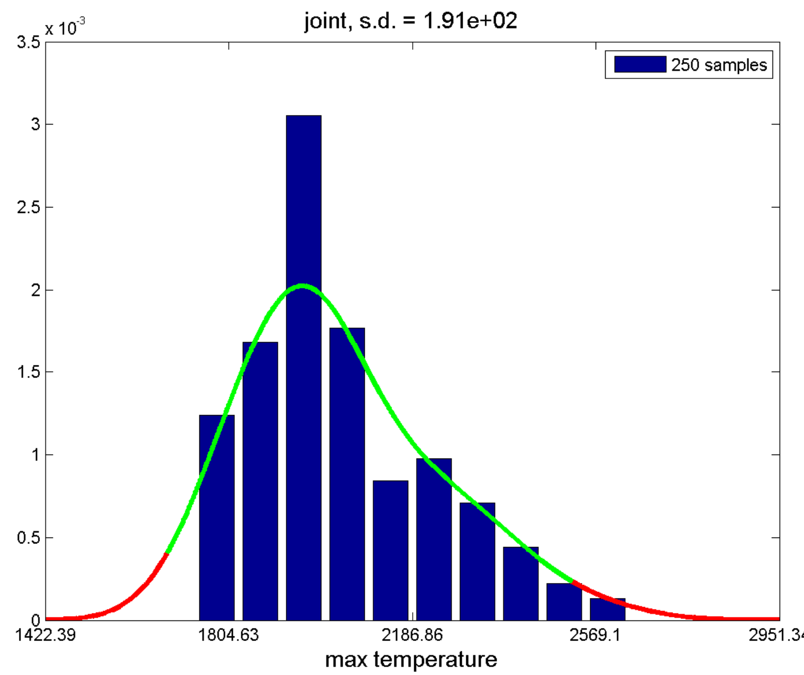
UQ Results

Coupled



MaxT = 1991.6 +- 338 C

CTF Standalone

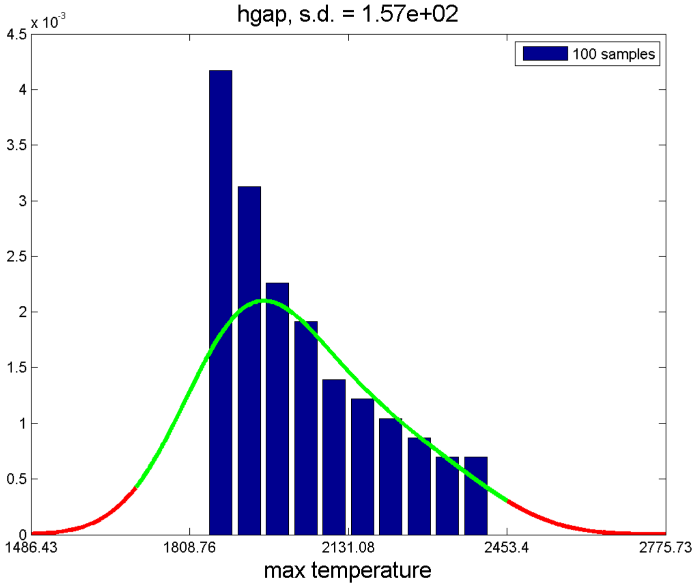


MaxT = 1991.6 +- 338 C

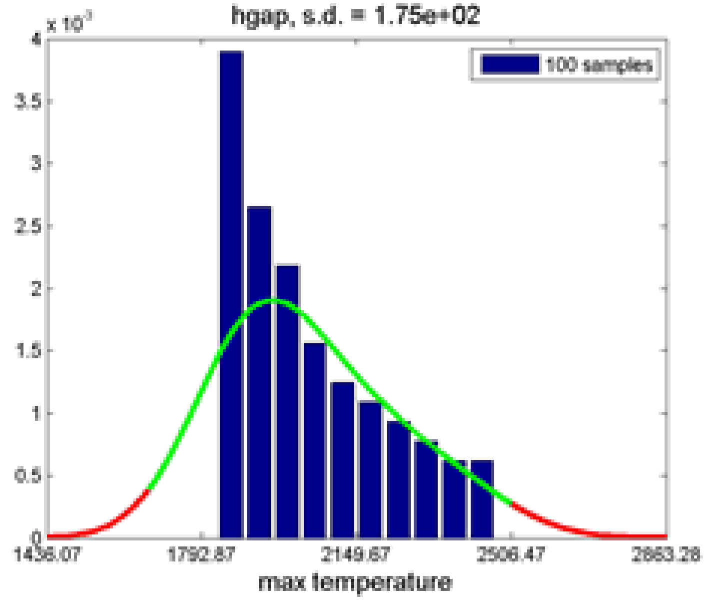
Larger Uncertainty in CTF Standalone

Single Parameter Effects, hgap

Coupled



CTF Standalone



MaxT +- 314 C

$$T_{\max} \sim {}^{1}\!/_{K}$$

MaxT +- 350 C

Larger Uncertainty in CTF Standalone

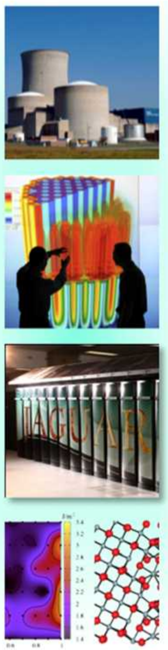
Sandia National Laboratories

Conclusions

- **The CASL project is employing a holistic view of uncertainty.**
- **Quantification of uncertainty includes**
  - numerical uncertainty quantified by verification
  - Model uncertainty quantified by validation
  - Parameter uncertainty measured by a variety of methods
- **The key to uncertainty quantification is constructing parameter distributions. We have a Bayesian method named DRAM to build these parameter distributions.**
- **This approach to uncertainty quantification is easily defendable and readily improved by incorporation of new validation data.**

Extra Slides

Parameter Uncertainty



- Wilkes is the standard (93 runs), multivariate MC using uniform dist within best-judgment ranges

- Dittus-Boelter
- McAdams
- X-secs

- Do forward UQ using these improved parameter input distributions.

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

CASL
Consortium for Advanced Simulation of LWRs

Sandia National Laboratories