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CASL's approach to multi-physics UAM

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The Consortium for Advanced Simulation of Light 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

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Core Partners

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

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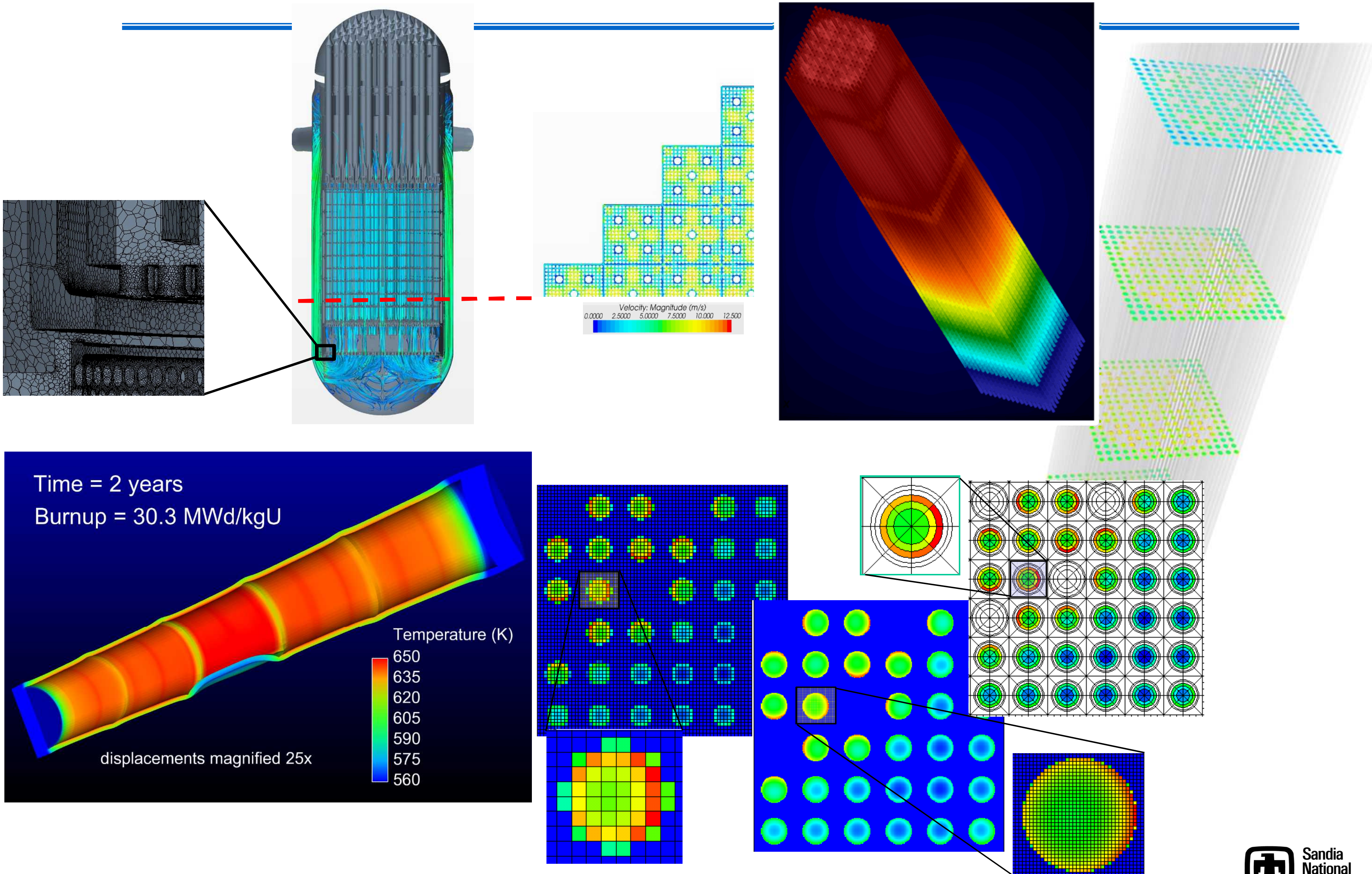
CASL Mod-Sim Challenges

Full core to assembly to subassembly to pin/pellet



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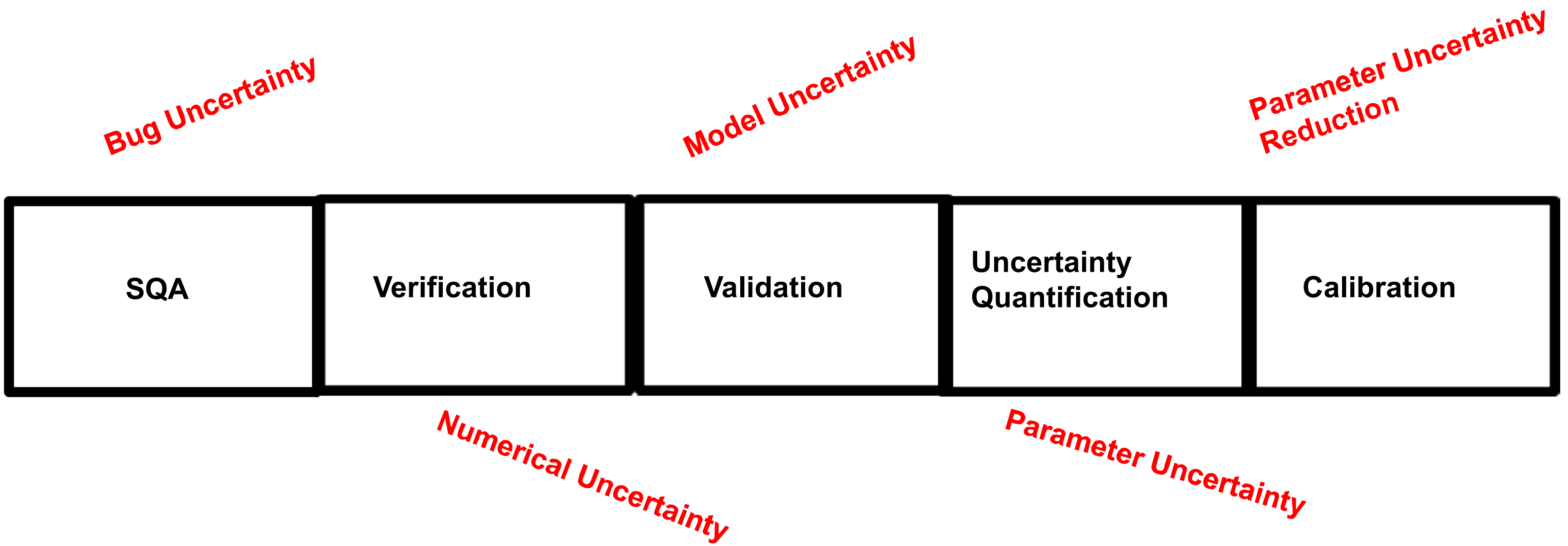
PCMM



- **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.**

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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.

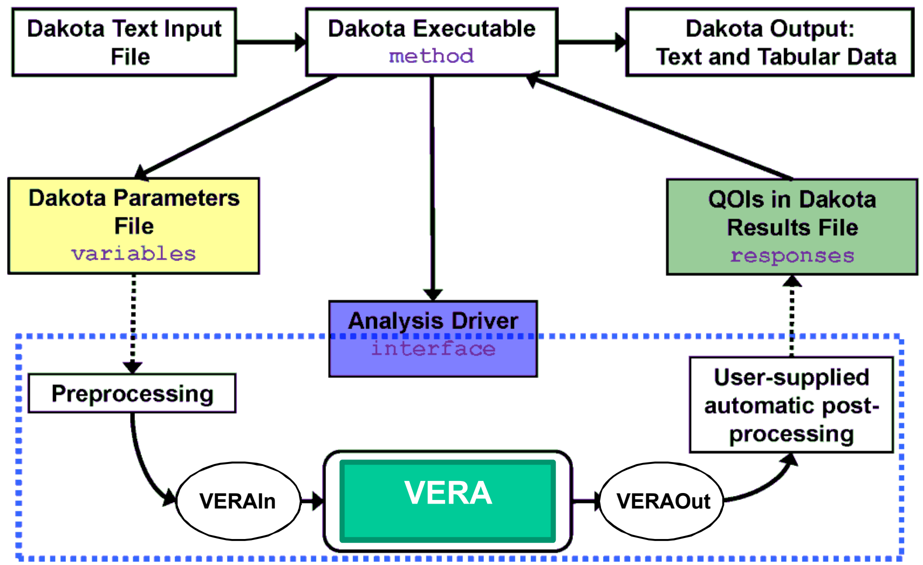
General Strategy

- 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 MVA2 re 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

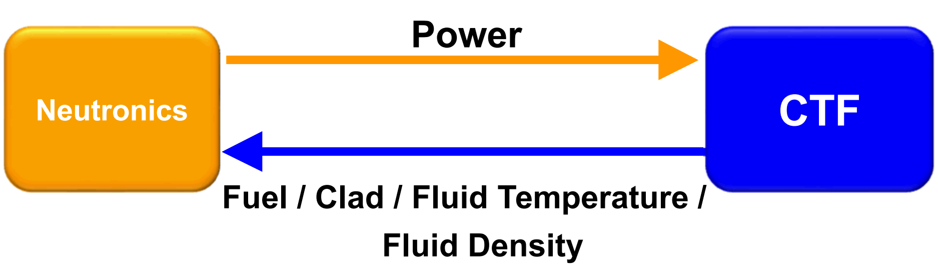
MVA1 changed so to and
Mousseau, Vincent Andrew, 5/23/2016

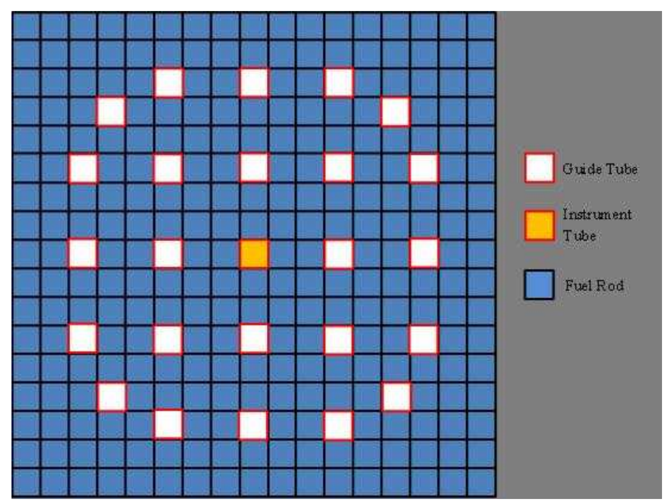
MVA2 Shoud we replace code input with "VERAIN" and code output with "VERAOUT"?
Mousseau, Vincent Andrew, 5/23/2016

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



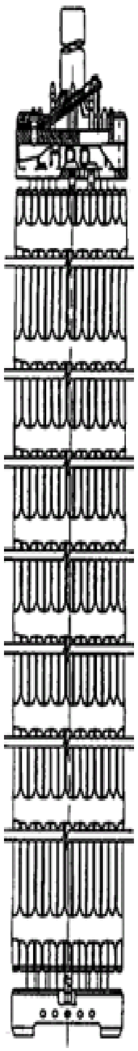


Slide 9

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

Cobra-TF Solution Verification

CTF-only: With Spacer Grids*



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

Spacer Grid Challenge

$$E_{(f=1.0)} = 0.0066$$

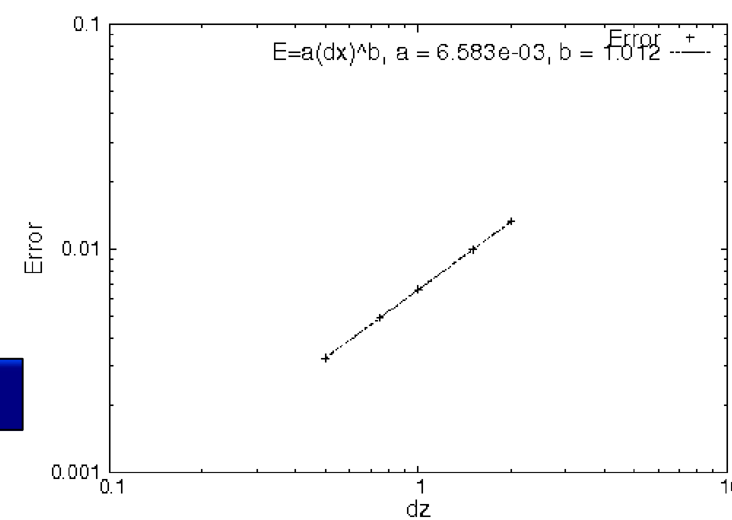
Mesh factor, f	Δz (cm)	#Axial elements	Tot. Press. (bar)
0.5	4.036	72	1.16843
0.75	6.054	48	1.1701
1.0	8.072	36	1.17176
1.5	12.108	24	1.17508
2.0	16.144	18	1.17845

Error Model:

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

$$b = 1.012$$

Very good agreement with theoretical 1.0



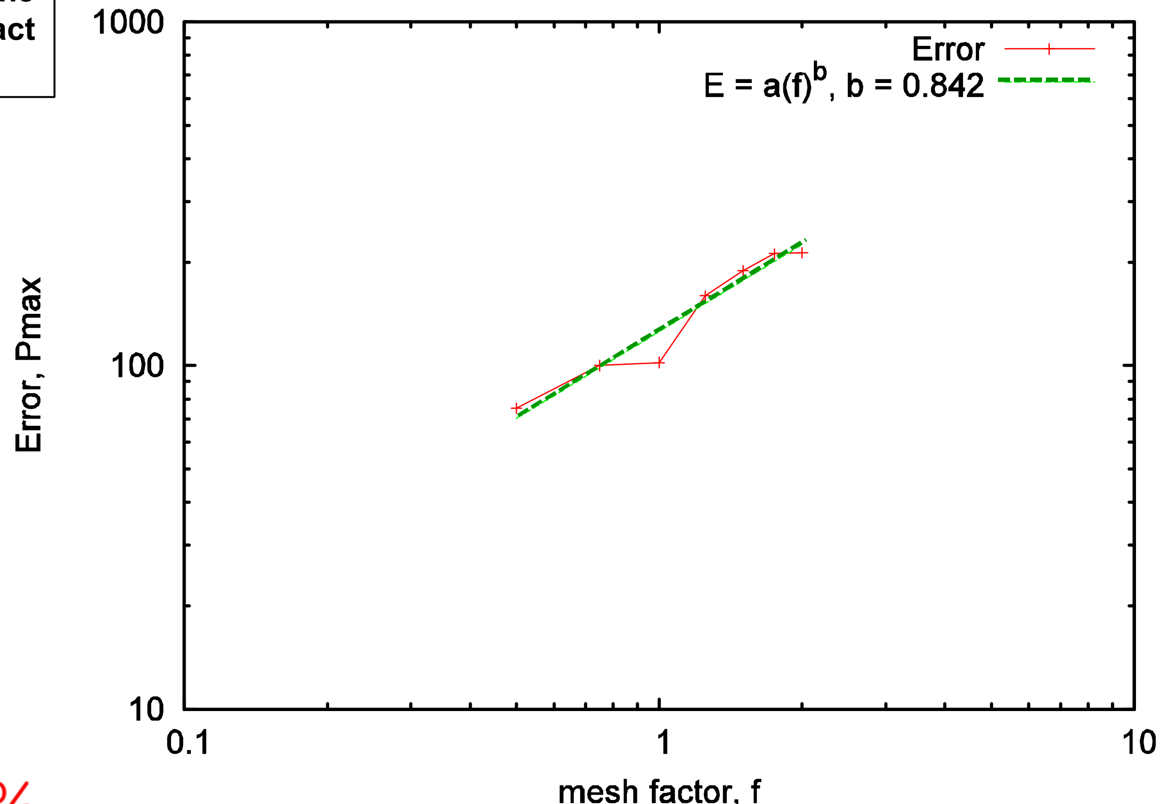
MVA5 MVA6

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.

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

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



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

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

$$b = 0.842$$

Degraded order-of-convergence but still usable.

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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

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

Dittus Boelter Uncertainty Quantification

$$Nu = 0.023\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.4} = \theta_1\,\mathrm{Re}^{\theta_2}\,\mathrm{Pr}^{\theta_3}$$

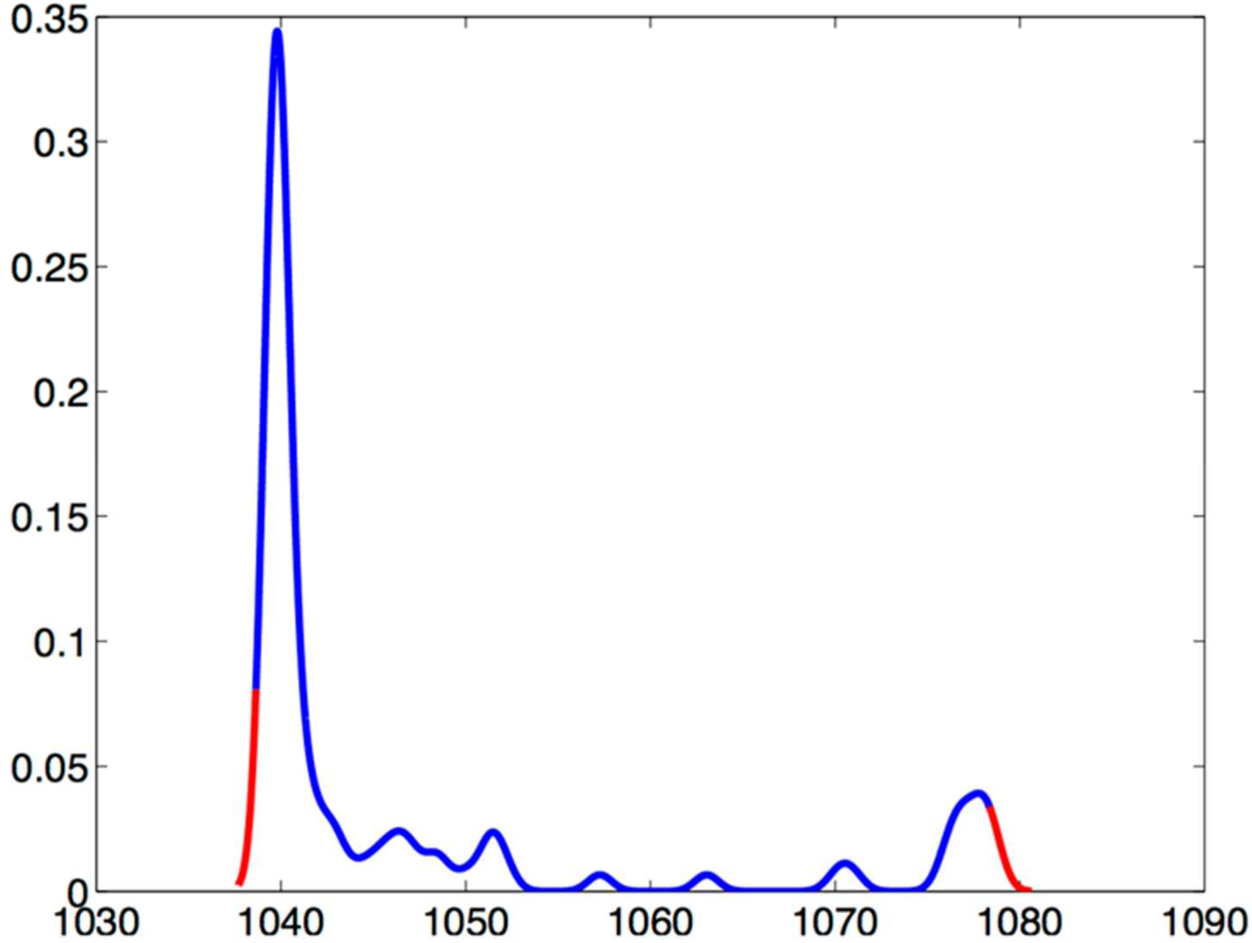
- We have three parameters, lead coefficient, θ_1, Reynolds exponent, θ_2, Prandlt exponent, θ_3 .
- The challenge is to determine the parameter distribution for these three parameters.
- We will initially use "expert opinion" to say

  $\theta_1 \in [0.0, 0.046]$

  $\theta_2 \in [0.0, 1.6]$

  $\theta_3 \in [0.0, 0.8]$
- We then assume a uniform distribution and do 93 samples to get a 95%-95% confidence interval from Wilks Formula.

Initial Results



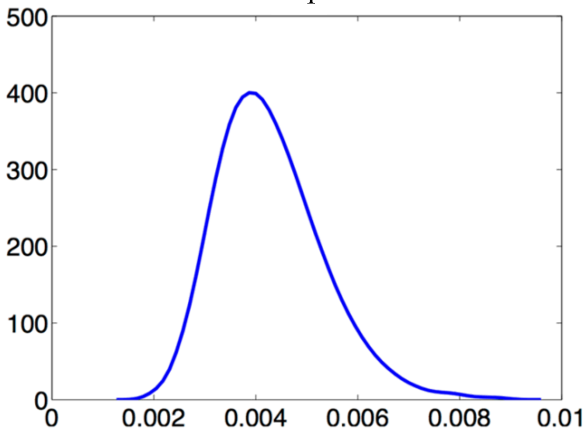
Max Fuel T, (C)

Second Attempt

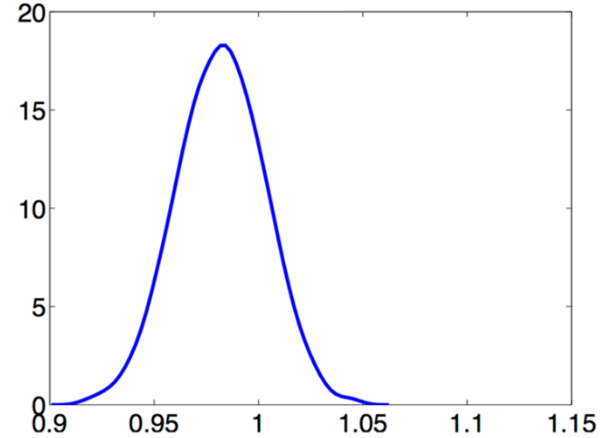
- Dittus Boelter was based on 13 data sets, this analysis is based on one, Morris and Whitman, "Heat Transfer for Oils and Water in Pipes," *Industrial and Engineering Chemistry*, **Vol. 20, No. 3**, pp.234-240, 1928.
- From this data set we can build the following parameter distributions.
- We use the Delayed Rejection Adaptive Metroplis (DRAM) algorithm.
- Given the experimental data, and the correlation, the following parameter distributions can be constructed by Bayesian analysis.

Bayesian Based Parameter Distributions

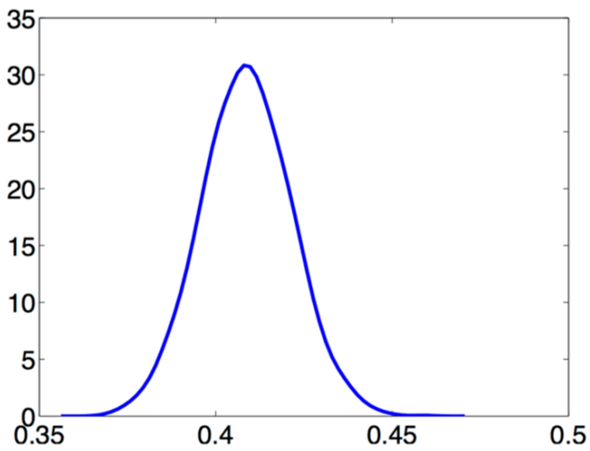
θ_1



θ_2



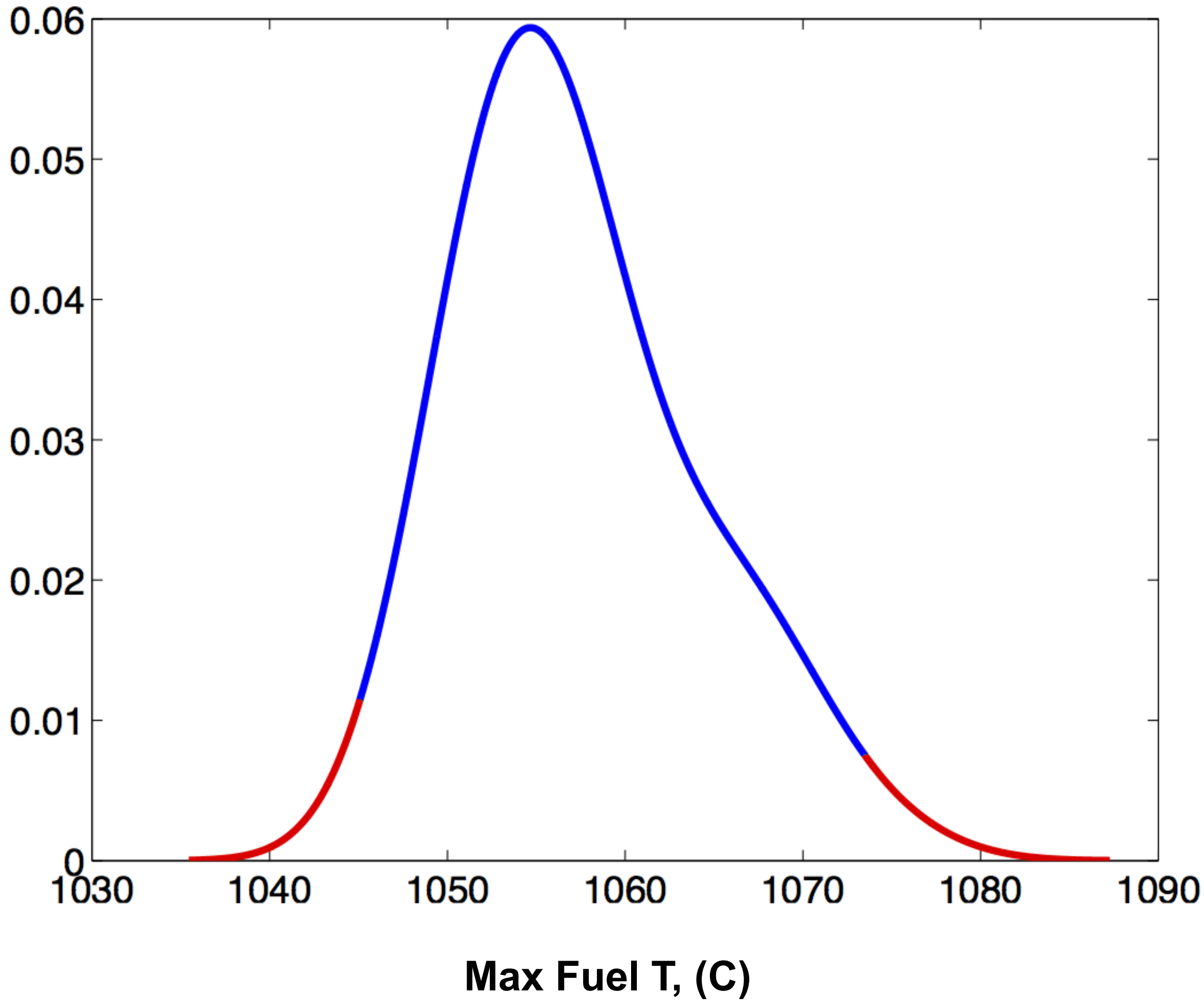
θ_3



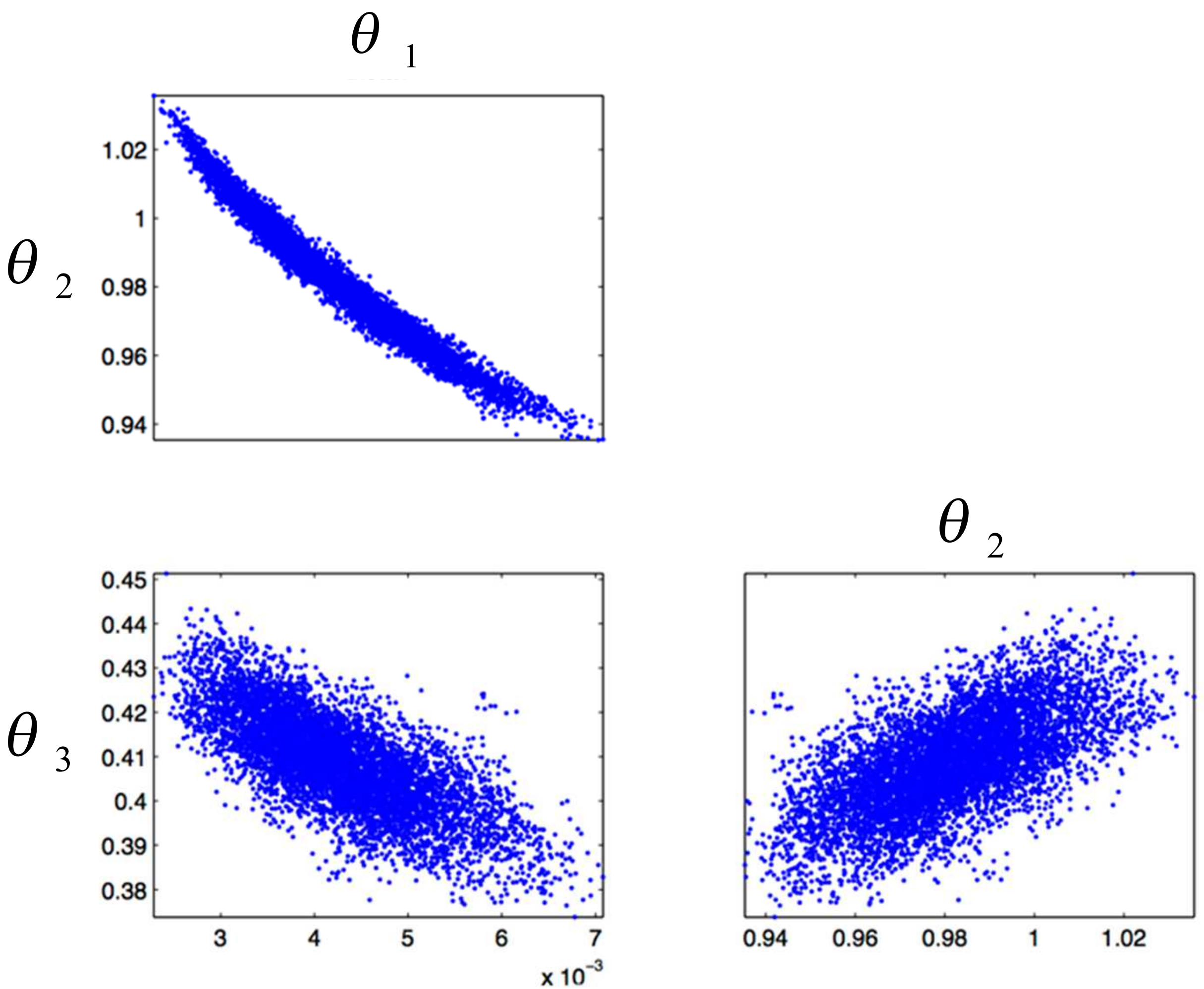
Dittus Boelter

- We note that the maximum probability for the lead coefficient (labeled θ_1) is now lower 0.004 from 0.023.
- The Reynolds exponent (labeled θ_2) is now larger 0.99 from 0.8
- The Prandlt exponent (labeled θ_3)is only slightly larger 0.41 from 0.4.
- These differences are because we only used 1 of the 13 data sets employed to build Dittus Boelter.
- We can then take 93 random samples from these distributions and get the following maximum fuel temperature distribution.

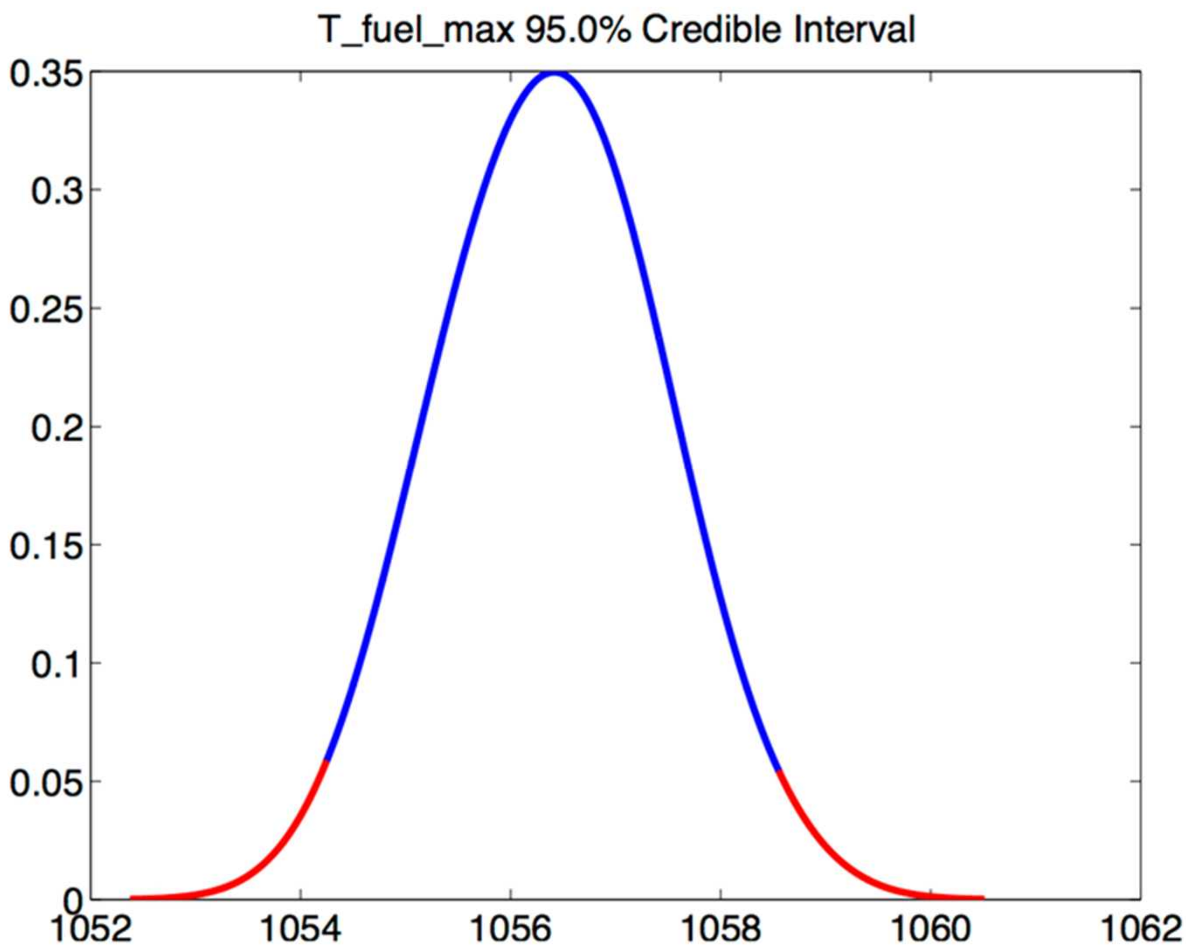
Second Uncertainty Quantification



Joint Samples for the Three Parameters



Dittus Boelter Results

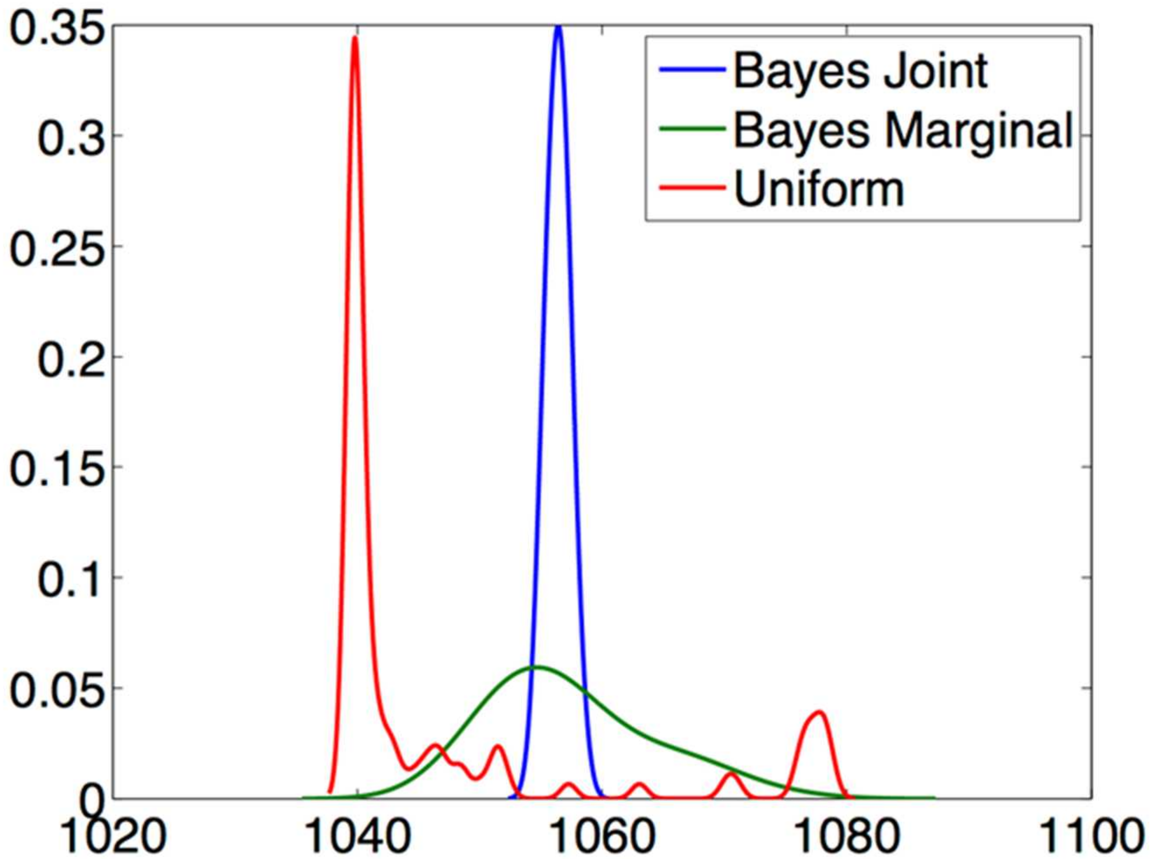


Max Fuel T, (C)

Comparing the Three Results

- On the next slide we will show all three maximum temperature distributions.
- The first two have very different shape but roughly the same 95% uncertainty range.
- The third one shows the improvement of recognizing the correlation between the parameters and building a single joint distribution.
- We continually make better use of the data we have.
- The final uncertainty is 5 degrees versus 40 degrees

Comparison of Results

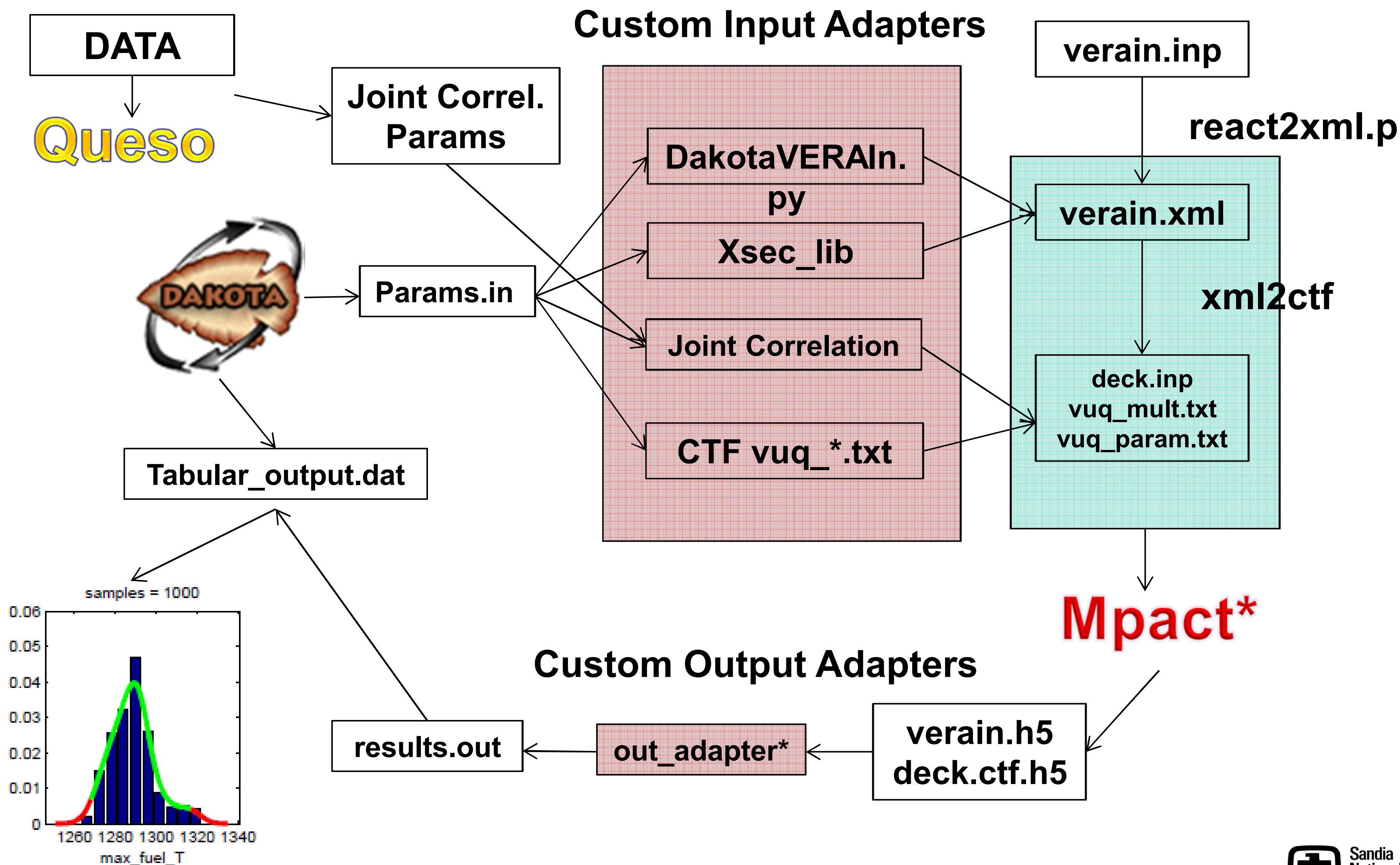


Max Fuel T, (C)

Dittus Boelter

- We now have a process to compute parameter distributions.
- The process depends on the experimental data used to produce the correlation.
- The process is easily defendable and does not rely on expert opinion.
- New experimental data can be easily incorporated to improve the accuracy of the new calibrated correlation.
- Future work will compare this uncertainty to expert opinion based parameter distributions employing Wilks formula.

The Big Picture: Automated PCMM



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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

Hi2Lo
(R. Smith et al.)

Design Algorithm

Statistical Model:

$$d_n = d_\ell(\theta, \xi_n) + \delta(\xi_n) + \varepsilon_n(\xi_n)$$

$$\tilde{d}_n = d_h(\xi_n) + \tilde{\varepsilon}_n(\xi_n)$$

$$D_{n-1} = \{\tilde{d}_1, \tilde{d}_2, \cdots, \tilde{d}_{n-1}\}$$

Existing data: $[(\xi_1, \tilde{d}_1), (\xi_2, \tilde{d}_2), \cdots, (\xi_{n-1}, \tilde{d}_{n-1})]$

↓

Calibrate parameters of low-fidelity model: $d_\ell(\theta, \xi_n)$

↓ DRAM

Choose new design ξ_n **to reduce uncertainty in** θ

↓ kNN Estimate of Mutual Information

Evaluate high-fidelity model at ξ_n**:** $\tilde{d}_n = d_h(\xi_n) + \tilde{\varepsilon}_n(\xi_n)$

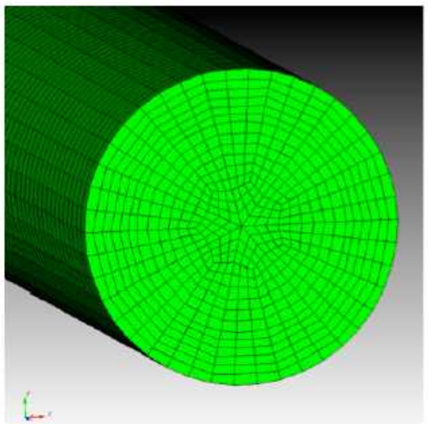
http://www.casl.gov/docs/CASL-U-2014-0197-000.pdf

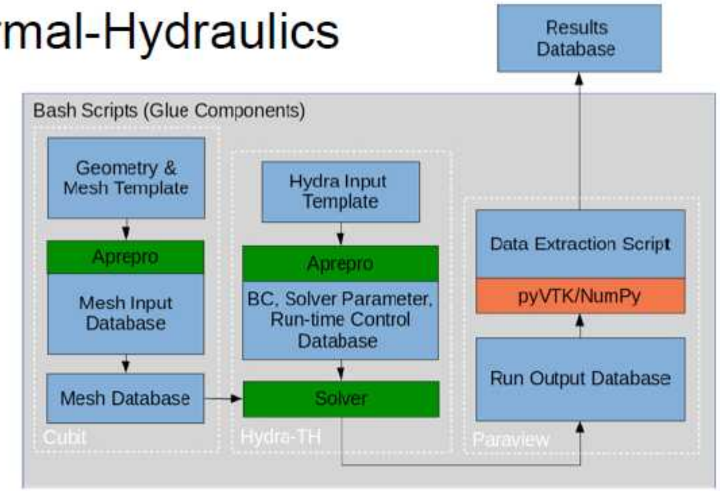
Hi2Lo

(R. Smith et al.)

Example Thermal-Hydraulics

Regime: Laminar flow in a pipe





Implementation Schematic

Poiseuille Flow: Permits verification of CFD and low-fidelity model

$$\frac{dp}{dz} = -\frac{V^2}{2}\frac{\rho}{D}f$$

where

$$V = \frac{\mathrm{Re}\cdot\mu}{\rho D}$$ Average Velocity

$$f = \frac{64}{\mathrm{Re}}$$ Friction Factor

Low-Fidelity Model:

$$f(\theta) = a \cdot \mathrm{Re}^b$$

True Parameters: $\theta = [64, -1]$

Design Value: $\xi = \mathrm{Re}$

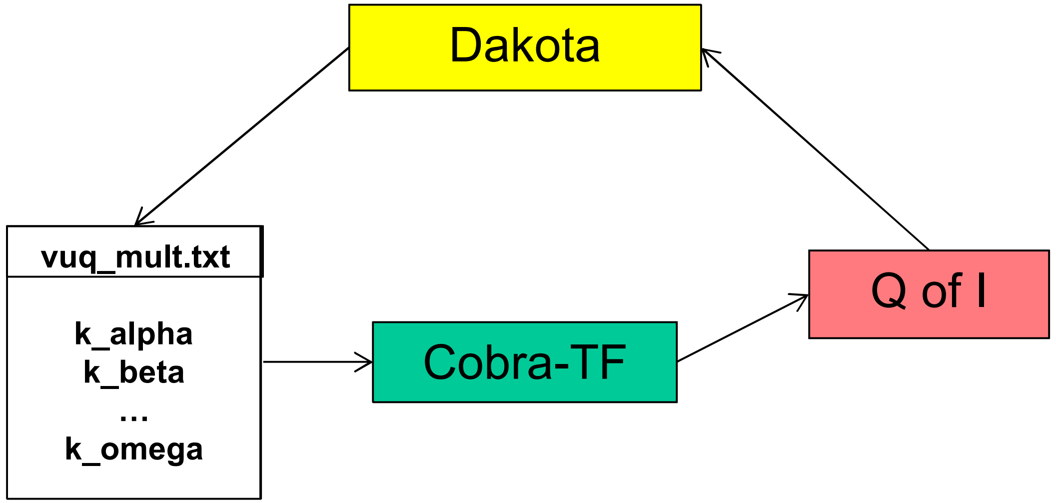
http://www.casl.gov/docs/CASL-U-2014-0197-000.pdf

Cobra-TF Parameter Exposure

with Noel Belcourt

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

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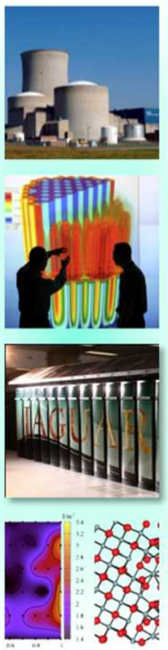
Parameter Uncertainty



- 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.

Consortium for Advanced Simulation of LWRs

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.

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Summary of Current Activities Presented at PHYSOR 2016

PHYSOR 2016, Sun Valley, ID, May 1-5, 2016

- B. Collins, R. Salko, S. Stimpson, K. T. Clarno, A. Godfrey, S. Palmtag, J. Secker, B. Kendrick, R. Montgomery, "**Simulation of CRUD-Induced Power Shift using the VERA Core Simulator and MAMBA**"
- A. Graham, T. Downar, B. Collins, R. Salko, S. Palmtag, "**Assessment of Thermal Hydraulic Feedback Models**"
- A. Godfrey, B. Collins, K.S. Kim, J. Powers, R. Salko, S. Stimpson, W. Wieselquist, K. Clarno, J. Gehin, S. Palmtag, R. Montgomery, R. Montgomery, D. Jabaay, B. Kochunas, T. Downar, N. Capps, J. Secker, "**VERA Benchmarking Results for Watts Bar Nuclear Plant Unit 1 Cycles 1-12**"
- T. Downar, B. Kochunas, B. Collins, "**Validation and Verification of the MPACT Code**"
- A. Godfrey, M. Jessee, S. Stimpson, B. Collins, T. Evans, M. Kromar, F. Franceschini, D. Salazar "**VERA Benchmarking Results for KRŠKO Nuclear Power Plant Cycle 1**"
- F. Franceschini, D. Salazar, M. Ouisloumen, A. Godfrey, S. Stimpson, B. Collins, C.Gentry, "**AP1000 PWR Cycle 1 HFP Depletion Simulations with VERA-CS**"
- S. Stimpson, B. Collins, A. Zhu, Y. Xu, **"A Hybrid Nodal P3/SP3 Axial Transport Solver for the MPACT 2D/1D Scheme"**
- S. Stimpson, J. Powers, K. Clarno, R. Pawlowski, R. Bratton, **"Assessment of Pellet-Clad Interaction Indicators in Watts Bar Unit1, Cycles 1-3 Using VERA"**
- B. Kochunas, E. Larsen, **"Fourier Analysis of Iteration Schemes for K-Eigenvalue Transport Problems with Flux-Dependent Cross Sections"**

All Papers are Available by Request

MVA7

Parameter Sensitivity → Downselect

parameter	partial correlation	simple correlation	morris main	morris interaction	CPS variation
k_eta	0.07	0.03			
k_gama	-0.03	0.04			
k_sent	-0.03	-0.02			
k_sdent	-0.07	-0.01			
k_tmasv	-0.03	0.00			
k_tmasl	0.11	0.00	6.48E-05	2.28E-05	medium
k_tmasg	-0.19	-0.01			
k_tmomv	-0.12	-0.01			
k_tmome	0.02	0.00			
k_tmoml	0.02	-0.02	2.23E-04	1.30E-04	medium
k_xk	0.08	-0.02			
k_xkes	-0.05	0.00			
k_xkge	-0.07	0.01			
k_xkl	0.04	-0.01			
k_xkle	-0.03	0.00			
k_xkvls	0.11	-0.01			
k_xkwvw	-0.10	0.01			
k_xkwlw	0.14	0.01			
k_xkwew	-0.01	0.03			
k_qvapl	-0.09	-0.01			
k_tnrgv	-0.03	0.00			
k_tnrgl	-0.01	0.03	9.00E-06	9.49E-06	low
k_rodqq	0.02	-0.01			
k_qradd	-0.02	0.00			
k_qradv	-0.01	0.00			
k_qliht	-0.01	0.00			
k_sphts	-0.05	0.03			
k_cond	-0.04	0.00			
k_xkwvx	0.03	-0.02			
k_xkwlx	1.00	0.88	1.80E-01	7.07E-03	high
k_cd	1.00	0.46	9.59E-02	7.88E-03	high
k_cdfb	-0.02	-0.01			
k_wkr	0.02	0.02			

5 Active Inputs (single phase flow):

k_cd : Pressure loss coefficient of spacer in sub-channel

k_xkwlx : Vertical liquid wall drag coefficient

k_tmasl : Loss of liquid mass due to mixing and void drift

k_tmoml : Loss of liquid momentum due to mixing and void drift

k_tnrgl : Loss of liquid enthalpy due to mixing and void drift

"User Guidelines and Best Practices for CASL UQ Analysis Using Dakota," SAND2014-2864

33 initial VUQ parameters reduced to 5 via sensitivity analysis

Slide 32

MVA7 Note single phase flow somewhere
Mousseau, Vincent Andrew, 5/23/2016

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