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NEAMS VU Overview

Jim Stewart, SNL

NEAMS PI Meeting
October 20, 2010

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NEAMS VU FY11 Work Package Overview

- **Overall Strategy**
  - Direct IPSC partnering and support
  - Partnering with NGNP and LWRS (R7)
  - Strategic methods development (Bayesian calibration, predictive maturity)
- **Participants**
  - Ralph Nelson (VU Lead)
  - SNL (Jim Stewart, VU Deputy Lead)
  - LANL (Brian Williams)
  - INL (Gilles Youinou)

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VU FY11 Tasks

SNL	PCMM-based VU Assessment (with Waste IPSC)
	Bayesian Multiple Model Inference (with LANL)
	Reactors V&V Plan Support (with Reactors IPSC)
LANL	LIFE-IV Calibration/Validation (with ANL, Fuels IPSC)
	AMP Verification/Validation Support (with Fuels IPSC)
	Bayesian Multiple Model Inference (with SNL)
	Predictive Maturity Development
	Safeguards/Separations V&V Plan Support (with Safe/Seps IPSC)
INL	NGNP UQ Methods
	R7 VU-Assessment

VU FY11 Tasks

IPSC Partnering

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Methods

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Partnering (other)

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Some FY10 Accomplishments

(*Including some things you won't otherwise hear about today…)*

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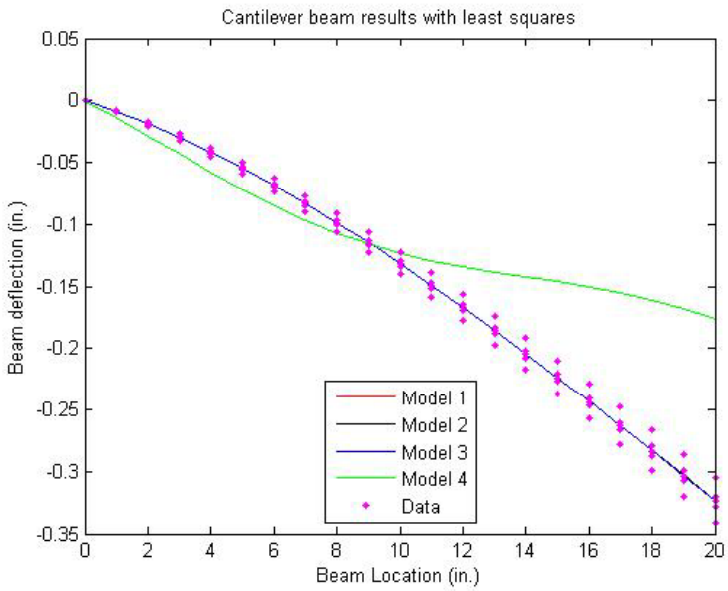
Multiple Model Inference With Application to Uncertainty Quantification for Complex Codes

- **Given multiple models, how do we select the "best" one or use all of them to make model predictions?**
  - Joint project between LANL and SNL
  - Combines both model calibration (parameter estimation) and forward UQ
  - Investigate tradeoff between model accuracy and model parsimony (don't want to overfit to a particular dataset)
  - Initial report and demonstration on a beam deflection problem completed

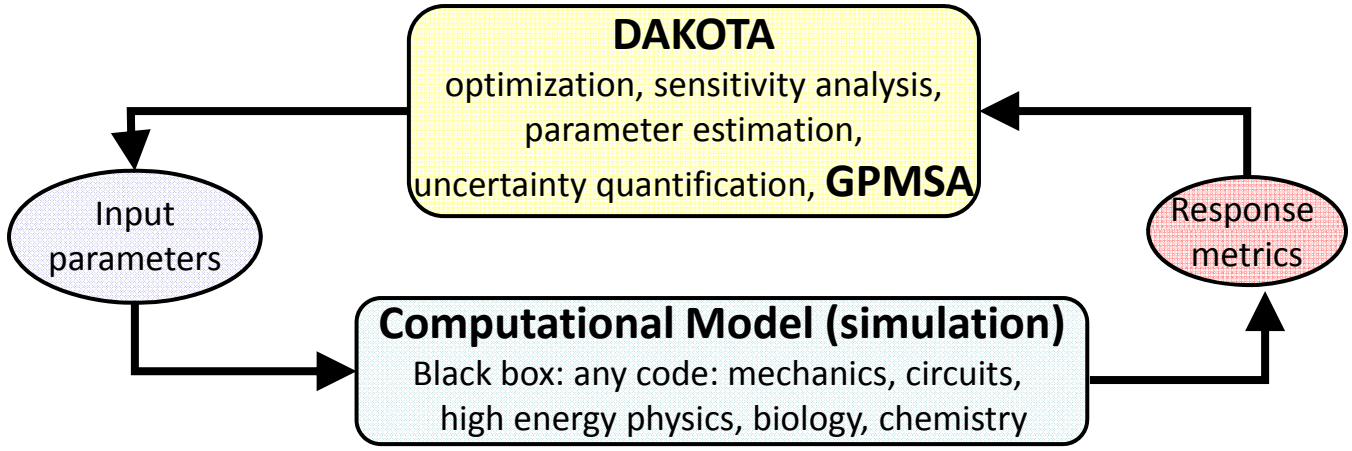


	Model 1	Model 2	Model 3	Model 4
AIC	**-245.4**	-243.4	-243.4	-186.1
AICC	**-244.8**	-242.2	-242.2	-185.6
BIC	**-242.9**	-239.7	-239.7	-183.7
Wolpert	0.44	**0.48**	0.08	7.E-06
Harmonic	0.24	0.34	**0.42**	1.E-04
RJMCMC	**0.35**	0.34	0.31	0.00

Blue = Information Criteria (likelihood-based)
Green = Bayesian Posterior Model Probabilities

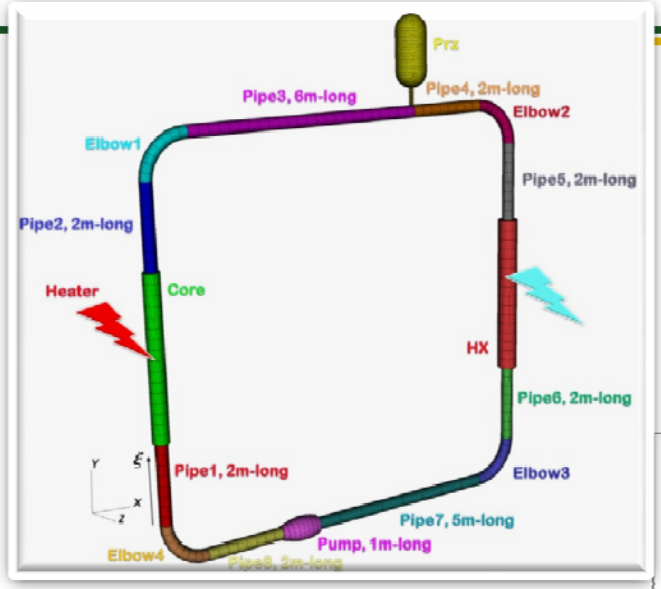
In FY10, GPMSA was integrated in DAKOTA to provide a Bayesian calibration capability

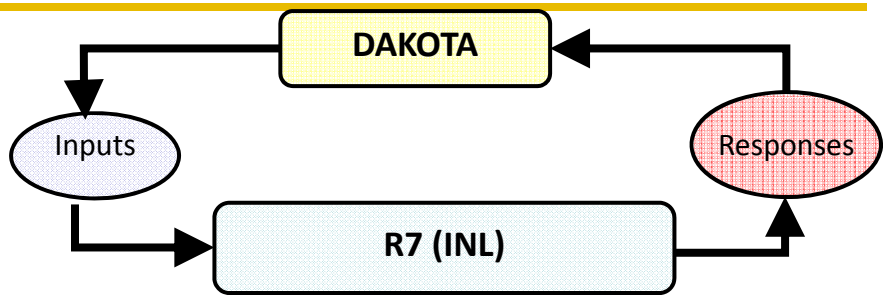
- **DAKOTA (SNL): Design Analysis Kit for Optimization and Terascale Applications**



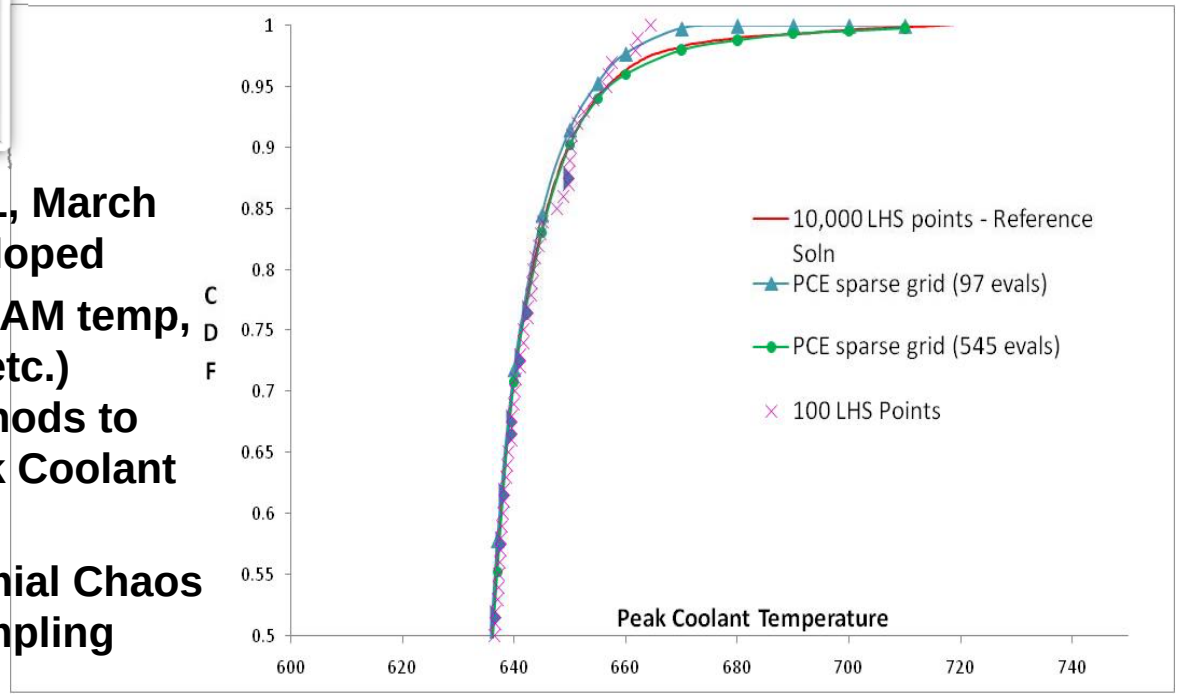
- **GPMSA (LANL): Gaussian Process Models for Simulation Analysis**
  - Bayesian calibration capability for estimation of model parameters under uncertainty
- **Motivation for integration:**
  - DAKOTA is a main delivery vehicle of UQ methods for NEAMS
  - DAKOTA manages a variety of parallel execution models on HPCs; translating GPMSA from Matlab to C++ removes license issues
- **Status**
  - Initial C++ version of GPMSA complete and integrated in DAKOTA

In FY10, R7 was integrated with DAKOTA and UQ studies were performed





- DAKOTA Training course at INL, March 2010, Dakota-R7 interface developed
- Multiple input parameters (SCRAM temp, pump power, pump stop time, etc.) examined with various UQ methods to understand distribution of Peak Coolant Temp.
- Promising results with Polynomial Chaos Expansion as alternative to sampling



Manufactured Solutions for Code Verification

- **Manufactured solution development for Waste IPCS (Knupp, Arguello (SNL)):** *[2D Reaction-Transport Equation]*

$$\frac{\partial}{\partial t}(\phi\, s\, R\, c) + \nabla\cdot(\phi\, s\, D\, \nabla c + V\, c) + \phi\, s\, R\, \lambda\, c = \Psi$$

2. Compute (and implement) new source term

$$\Psi = c\left(\frac{\beta^2+\gamma^2}{4\,\phi\, s\, D} - \rho + \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\beta\, u + \gamma\, v}{2\,\phi\, s\, D} + \phi\, s\, R\, \lambda\right)$$

1. Choose and plug in "solution"

- **Manufactured Solutions available in AMP (Gary Dilts (with Mike Rogers), LANL):**

Geometry	Order	Dirichlet	Neumann
Unit Cube	Quadratic		X,Y,Z={0,1}
Unit Cube	Quadratic	X=0	X=1, Y,Z={0,1}
Unit Cube	Quadratic	X={0,1}	Y,Z={0,1}
Unit Cube	Cubic		X,Y,Z={0,1}
Unit Cube	Cubic	X=0	Y,Z={0,1}
Unit Cube	Cubic	X={0,1}	X,Y,Z={0,1}
Cylindrical ¼ shell	Quadratic		R={1/2,1}, ,Z={0,1}
Cylindrical ¼ shell	Cubic		R={1/2,1}, ,Z={0,1}
Cylindrical ¼ shell	Cubic Periodic		R={1/2,1}, ,Z={0,1}
Cylindrical shell	Quadratic		R={1/2,1},Z={0,1}
Cylindrical shell	Cubic		R={1/2,1}, ,Z={0,1}
Cylindrical shell	Cubic Periodic		R={1/2,1}, ,Z={0,1}
Cylindrical rod	Cubic Periodic	Z={0,1}	R=1

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Waste IPSC V&V Plan (Joint with VU)

SANDIA REPORT

SAND2010-XXXX
Unlimited Release
Printed August 2010

Nuclear Energy Advanced Modeling and Simulation Waste Integrated Performance and Safety Codes (NEAMS Waste IPSC)

Verification and Validation Plan (July 2010)

H. Carter Edwards, Jose G. Arguello Jr., Roscoe A. Bartlett, Julie F. Bouchard, Geoff Freeze, Robert Howard, Patrick Knupp, Marjorie T. McCornack, Peter A. Schultz, Angel Urbina, and Yifeng Wang

VU

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Upcoming Report Introduces VU Components and Methodology

LA-UR-10-xxxx

Approved for public release; distribution is unlimited.

Title:	Using Error and Uncertainty Quantification to Verify and Validate Modeling and Simulation Capabilities
Author(s):	Ralph Nelson, Idaho National Laboratory Cetin Unal, Los Alamos National Laboratory Jim Stewart, Sandia National Laboratories Brian Williams, Los Alamos National Laboratory
Intended for:	General reference material

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Important Remarks
(From Fall '09 PI Meeting)

- **VU is an *evidence-based* methodology**
- **In general, one takes a *graded approach***
  - Increasing formality of process
  - Increasing fidelity of underlying physics models
  - Increasing software quality and verification
  - Increasing characterization of margins and uncertainties
  - Reducing margins and uncertainties
  - Improving documentation, increasing repeatability of analysis
- **Ultimately, this leads to *increased credibility* in the results obtained using the IPSCs**

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More on "Credibility"
(From Fall '09 PI Meeting)

- **Credibility is related to *Predictive Maturity***
  - Can this be measured?
- **Elements of Predictive Maturity**
  - Geometry fidelity, Physics model and algorithm fidelity, Code verification, Solution verification, Validation coverage and discrepancy, UQ/SA, Documentation, others?
- **Some Attempts to Quantify**
  - Predictive Capability Maturity Model (PCMM), *SNL*
  - Predictive Maturity Index (PMI), *LANL*
  - Credibility Assessment Scale (CAS), *NASA*

Can we apply this concept to the NEAMS IPSCs?

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Today's VU Presentations

- ***Risk Informed Safety Margin Characterization***

  Robert Nourgaliev, INL

- ***Advanced Licensing Using VU Concepts***

  Cetin Unal, LANL

- ***Predictive Capability Maturity Model***

  Angel Urbina, SNL