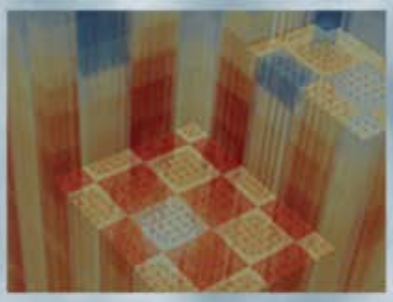
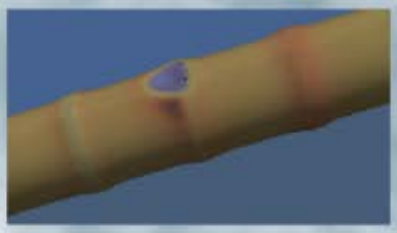
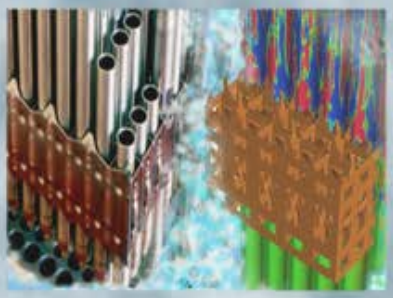
CASL-U-2015-0244-000

An Information Theoretical Approach to Use High-Fidelity Codes to Calibrate Low-Fidelity Codes







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July 7, 2015

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

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An Information Theoretic Approach to Calibrating Low-Fidelity Codes Using High-Fidelity Codes

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This research was supported by the Consortium for Advanced Simulation of Lightwater Reactors (http://www.casl.gov), an Energy Innovation Hub (http://www.energy.gov/hubs) for Modeling and Simulation of Nuclear Reactors under U.S. Department of Energy Contract No. DE-AC05-00OR22725.

Motivation

- Use validated high-fidelity codes to calibrate low-fidelity codes
  - CASL Example:
    - High-Fidelity: HYDRA
    - Low-Fidelity: COBRA-TF
- Goal: Use mutual information to calibrate parameters of low-fidelity code using minimal number of high-fidelity evaluations.

Statistical Model

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

Notation:

d_ℓ : low-fidelity model

θ : low-fidelity model parameters

ξ_n : design conditions

$\delta(\xi_n)$: model discrepancy term

$\varepsilon_n(\xi_n)$: measurement or discretization errors

Design Algorithm

Existing data: $[(\xi_1, \tilde{d}_1), (\xi_2, \tilde{d}_2), ..., \xi_r, \tilde{d}_r)]$

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

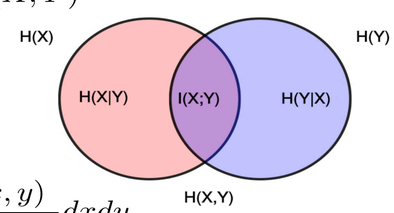
Evaluate high-fidelity model at ξ_n: $\tilde{d}_n = d_h(\xi_n) + \tilde{\varepsilon}_n(\xi_n)$

Mutual Information

- Measure of variable's mutual dependence
- I(X;Y) quantifies reduction in uncertainty in X that knowing Y provides

Shannon Entropy: $H(X) = -\int_{\mathcal{X}} p(x) \log p(x) dx$

$$I(X;Y) = H(X) + H(Y) - H(X,Y)$$
$$= H(X) - H(X|Y)$$
$$= H(Y) - H(Y|X)$$



$$I(X;Y) = \int_{\mathcal{X},\mathcal{Y}} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} dxdy$$
$$= \int_{\mathcal{X},\mathcal{Y}} p(x)p(y|x) \log p(y|x) dxdy$$
$$- \int_{\mathcal{X},\mathcal{Y}} p(x,y) \log p(y) dxdy$$

Utility Function

Mutual Information (cont.)

Utility Function:

$$U(d_n, \xi_n) = \int_\Omega p(\theta|d_n, D_{n-1}) \log p(\theta|d_n, D_{n-1}) d\theta - \int_\Omega p(\theta|D_{n-1}) \log p(\theta|D_{n-1}) d\theta$$

Mutual Information:

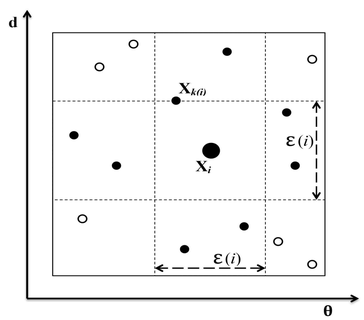
$$I(\theta; d_n|D_{n-1}, \xi_n) = \int_{\mathcal{D}} U(d_n, \xi_n) p(d_n|D_{n-1}, \xi_n) ddn$$

Choice of Design Condition: $\xi_n^* = \arg\max_{\xi_n \in \Xi} I(\theta; d_n|D_{n-1}, \xi_n)$

k^{th}-Nearest Neighbor Method

- Estimate of mutual information proposed by Kraskov et.al (2004)

$$I(\theta; d_n|D_{n-1}, \xi_n) \approx \psi(k) - \mathbb{E}\left[\psi(n_\theta + 1) + \psi(n_d + 1)\right] + \psi(N)$$



Notation:

$\psi(\cdot)$: digamma function

n_θ , n_d : number of points in each marginal space within $\epsilon(i)/2$ of $X_i = (\theta^i, d_n^i(\xi_n))$

$k = 1$, $n_\theta(i) = 3$, $n_d(i) = 4$

DRAM

- Improvement on the basic metropolis algorithm proposed by Haario et.al (2006)
  - **Delayed Rejection**: If a candidate is rejected, an alternate candidate is constructed to induce greater mixing
  - **Adaptation**: The covariance matrix for the parameters is continuously updated using accepted candidates

Neutron Diffusion Model

High Fidelity Model: 1-D kinetic neutron diffusion

$$\frac{1}{\nu_{th}} \frac{\partial \phi}{\partial t} - \frac{1}{3\Sigma_{sc}} \frac{\partial^2 \phi}{\partial x^2} = \Sigma_f \phi n_f - \Sigma_a \phi n_a, \text{ BC, IC}$$

Low Fidelity Model: Point kinetic equation

$$\frac{dn}{dt} = \frac{(r-1)}{\beta} n(t) \quad \text{for } \theta = [r, \beta] \text{ , where}$$

r : reactivity, β : mean lifetime of neutron, n : neutrons/m³

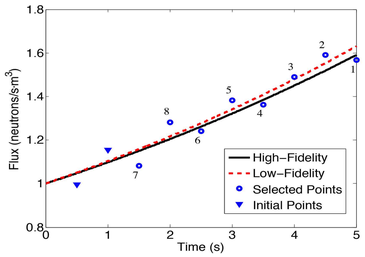
Design Conditions: Assume pre-existing data at $t = 0.5$, $t = 1.0$

Design #	1	2	3	4	5	6	7	8
Time (s)	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0

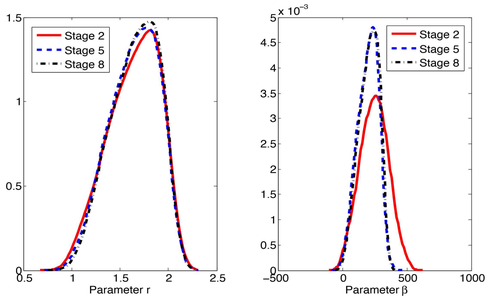
Neutron Diffusion (cont.)

Mutual Information: Point selection at each step

Time	Step 1	Step 2	Step 3	Step 4	Step 5	Step 6	Step 7	Step 8
1.5	0.971	0.053	0.021	0.013	0.001	0.001	**0.005**	
2.0	1.211	0.116	0.027	0.001	0.002	0.001	0.004	**0.001**
2.5	1.443	0.206	0.044	0.001	0.013	**0.015**		
3.0	1.555	0.289	0.080	0.019	**0.022**			
3.5	1.711	0.361	0.097	**0.048**				
4.0	1.839	0.441	**0.135**					
4.5	1.866	**0.550**						
5.0	**1.949**							



Evolution of Parameter Distributions:



Calibration Results:

$r = 1.6721$, $\beta = 178.01$

Thermal-Hydraulics Model

Regime: Laminar flow in a pipe

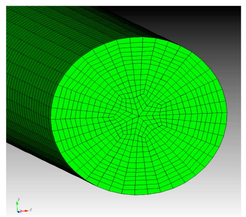
- Poiseuille flow permits verification of HYDRA & calibration procedure.

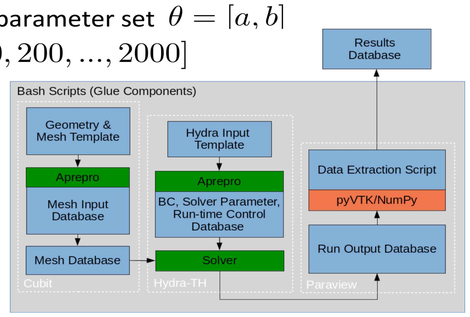
$$\frac{dp}{dz} = -\frac{V^2}{2}\frac{\rho}{D} f \quad \text{where } V = \frac{\text{Re} \cdot \mu}{\rho D} \text{ and } f = \frac{64}{\text{Re}}$$

High-Fidelity: Validated HYDRA Code

Low-Fidelity: $f = a\text{Re}^b$ for parameter set $\theta = [a, b]$

Design conditions: $\text{Re} \in [100, 200, ..., 2000]$





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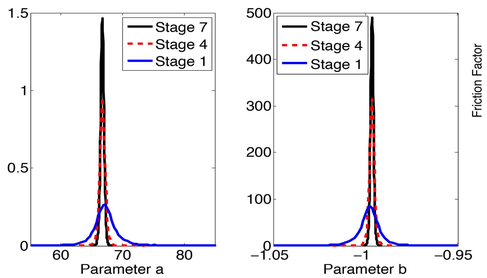

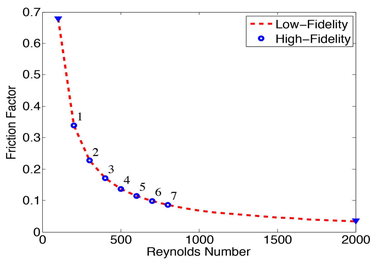

Calibration Results:

$a = 66.717$, $b = -0.997$

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