CCSI™

Carbon Capture Simulation Initiative

Calibration of Computational Models with Categorical Parameters and Correlated Outputs via Bayesian Smoothing Spline ANOVA

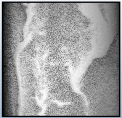
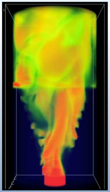
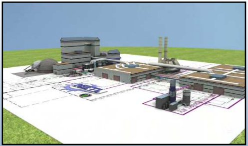
Curtis Storlie
Los Alamos National Laboratory

June 7, 2013

U.S. DEPARTMENT OF ENERGY

CCSI For Accelerating Technology Development

Carbon Capture Simulation Initiative

Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

National Labs

Berkeley Lab
Pacific Northwest National Laboratory
NETL
Los Alamos National Laboratory EST. 1943
Lawrence Livermore National Laboratory

Academia

Carnegie Mellon
Princeton University
West Virginia University
Boston University
The University of Texas at Austin
Institute for Clean and Secure Energy, The University of Utah

Industry

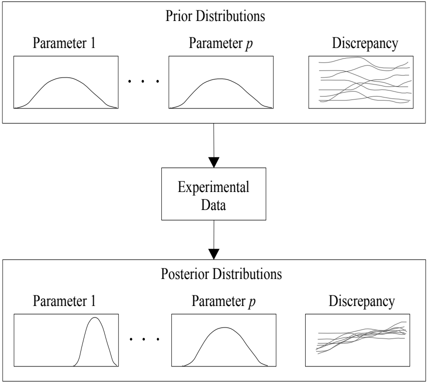
ADA Environmental Solutions
ALSTOM
B&W the babcock & wilcox company
GE
EPRI Electric Power Research Institute
FLUOR
Southern Company
Phillips 66
AEP American Electric Power
Chevron
Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
ExxonMobil
URS
Air Products
Eastman
ANSYS
aspentech
invensys
PSE

CCSI™ Carbon Capture Simulation Initiative
NETL
Berkeley Lab
Lawrence Livermore National Laboratory
Los Alamos National Laboratory EST. 1943
Pacific Northwest National Laboratory
U.S. Department of Energy

What is Computer Model Calibration?

- Find a plausible set of model parameter values ($\boldsymbol{\theta}$) that best produce the reality of experimental (or field) data.
- In the Bayesian paradigm, this entails putting a prior distribution on $\boldsymbol{\theta}$ and conditioning on the expirimental data to refine this prior distribution.
- There can also be a model form discrepancy function which admits the possibility of model bias.

Bayesian Calibration



"Traditional" (Kennedy & O'Hagan 2001) Calibration

- Represent the output of the physical system producing the experimental data as

$$y_n = \eta(\mathbf{x}_n, \boldsymbol{\theta}) + \delta(\mathbf{x}_n) + \varepsilon_n, \quad n = 1, \ldots, N.$$

  (i) $\eta(\mathbf{x}_n, \mathbf{t})$ is a simulator of the physical system.

  (ii) $\delta(\mathbf{x})$ is a discrepancy function to alow for model bias.

  (iii) $\varepsilon_n \overset{iid}{\sim} \mathcal{N}(\mathbf{0}, \sigma^2)$ are observational measurement errors.

  (iv) $\mathbf{t} = [t_1, \ldots, t_Q]$ is a vector of model parameters. If fixed at an appropriate (unknown) value of $\mathbf{t} = \boldsymbol{\theta}$, then $\eta(\mathbf{x}, \boldsymbol{\theta})$ will best approximate the physical system.

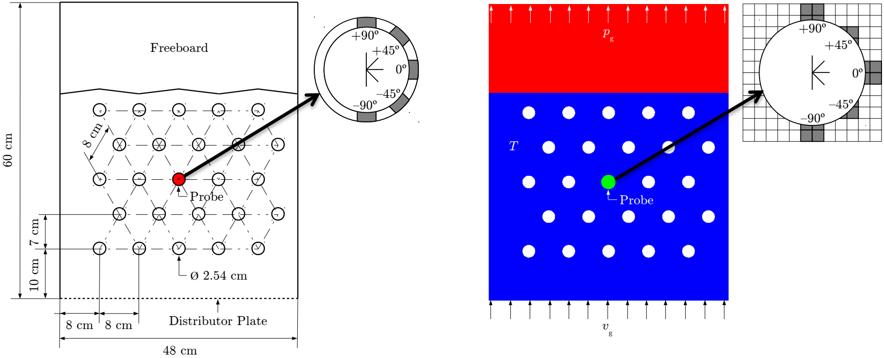
- Typically it is assumed that δ is a Gaussian Process (GP)
- If simulator runs are expensive, then a sample (e.g., LHS) of runs is obtained and η is modeled as a GP as well.
- Estimation of $\boldsymbol{\theta}$, η, and δ is done within a Bayesian framework (Higdon, Kennedy, Cavendish, Cafeo & Ryne 2004).

Bubbling Fluidized Bed Example

Goal: Calibration of a computational fluid dynamics (CFD) model as a first step toward upscaling to a large CO_2 capture system.

Experimental Setup

CFD simulation Setup



(a) (b)

Bubbling Fluidized Bed Example

- Experimental Outputs $\mathbf{y}$:

  y_1 : Bubble Frequency (measured in Hertz)

  - observed at angles $\{-90, -45, 0, 45, 90\}^\circ$ and velocities $\{5.5, 7.0, 11.0, 12.6\}$ cm/sec.

  y_2 : Phase Fraction (proportion of time a bubble is present)

  - observed at angles $\{-90, -45, 0, 45, 90\}^\circ$ and velocity 12.6 cm/sec).

- Experimental Inputs $\mathbf{x}$:

  x_1 : Gas Velocity, $[5.5, 16.1]$

  x_2 : Angular Location on Tube, $[-90, 90]$

- Model Parameters $\mathbf{t}$:

  t_1 : Coefficient of restitution, particle-particle $\in [0.8, 0.997]$

  t_2 : Coefficient of restitution, particle-wall $\in [0.8, 0.997]$

  t_3 : Friction angle, particle-particle $\in [25.0, 45.0]$

  t_4 : Friction angle, particle-wall $\in [25.0, 45.0]$

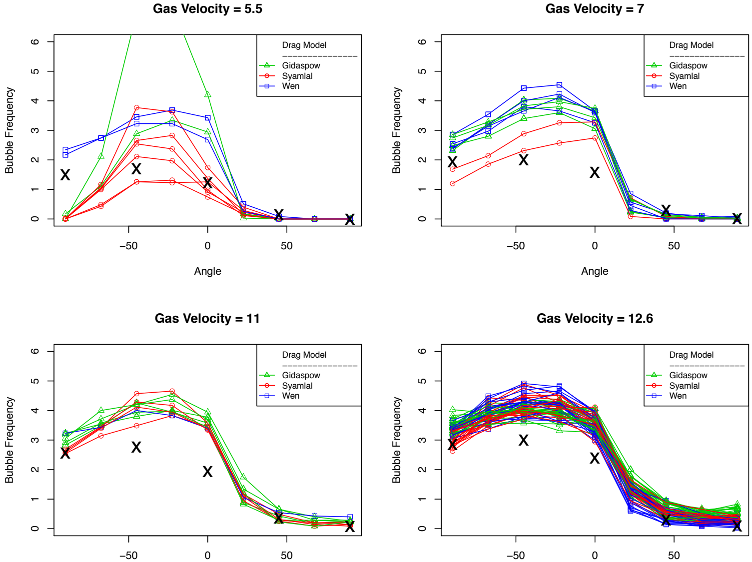
  t_5 : Packed bed void fraction $\in [0.3, 0.4]$

  t_6 : Drag model $\in$ {Syamlal-OBrien, Wen-Yu, Gidaspow}

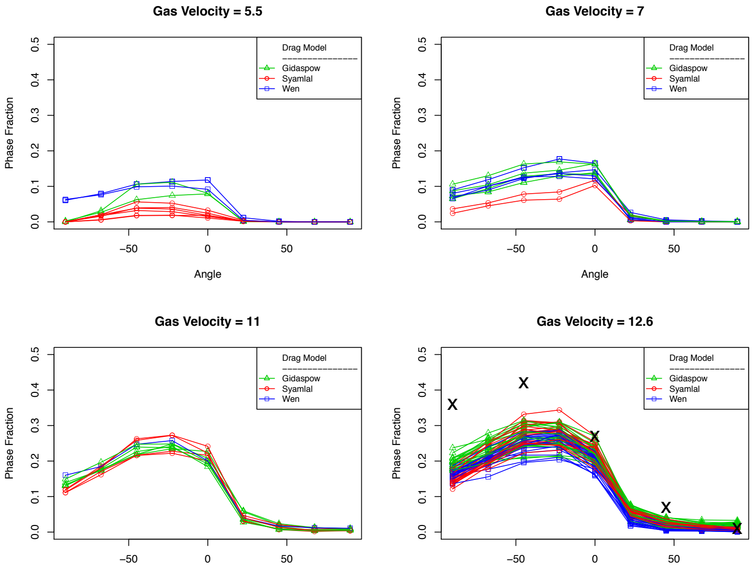
Bubbling Fluidized Bed Example

- Latin Hypercube Sample (LHS) of 90 runs was used to make CFD model runs.
- Each run produced (after post-processing) the y_1 and y_2 values at angles $x_2 = \{-90.0, -67.5, -45.0, -22.5, 0.0, 22.5, 45.0, 67.5, 90.0\}$.
- Seven free "parameters" to choose values for are then $(x_1, t_1, t_2, \ldots, t_6)$.
- x_1 was restricted to values where there were experimental data $x_1 \in \{5.5, 7.0, 11.0, 12.6\}$ cm/sec.
- So all in all there are:
  - experimental observations for y_1 at 4 velocities (each at 5 angles)
  - experimental observations for y_2 at 1 velocity (each at 5 angles)
  - 90 CFD runs total covering four distinct velocites (each run provides output at 9 distinct angles)

Bubbling Fluidized Bed Example



Bubbling Fluidized Bed Example



Common Complications in Computer Model Calibration

1. There are multiple correlated outputs (e.g., Bubble Frequency and Void Fraction) so the observations ($\mathbf{y}_n$) are really vectors.
2. There are categorical model parameters (e.g., which Drag model is used inside the CFD model).
3. There may be multiple possible models η (e.g., a coarse approximation that runs much faster than a more accurate high resolution model. Not in the bubbling bed example, however.)
4. There may be some missing experimental observations for some of the outputs. (e.g., not all outputs were measured in all trials, or data is combined from multiple sources).

Calibration w/ Multiple Outputs & Categorical Parameters

A multivariate output of the physical system $\mathbf{y} = [y_1, \ldots, y_M]^T$ is now a vector of simulator outputs plus a multivariate discrepancy function δ, plus the measurement error vector, ε, i.e.,

$$\mathbf{y}_n = \eta(\mathbf{x}_n, \boldsymbol{\theta}) + \delta(\mathbf{x}_n) + \varepsilon_n, \quad n = 1, \ldots, N.$$

- e.g., $\eta(\mathbf{x}_n, \boldsymbol{\theta}) = [\eta_1(\mathbf{x}_n, \boldsymbol{\theta}), \ldots, \eta_M(\mathbf{x}_n, \boldsymbol{\theta})]^T$
- η, δ and ε_n need a multivariate representation to appropriately account for correlation among the multiple outputs.
- The emulator also needs to account for categorical parameters (e.g., which drag model to use).
- These will be accomplished within the Bayesian Smoothing Spline (BSS-)ANOVA GP (Reich, Storlie & Bondell 2009, Storlie, Fugate, Higdon, Huzurbazar, Francois & McHugh 2012).

BSS-ANOVA Model

- We assume the emulator for η (and the discrepancy δ with obvious changes) is a GP with the *BSS-ANOVA* covariance function.
- This GP can be conveniently written as a sum of main effects plus interaction components, i.e.,

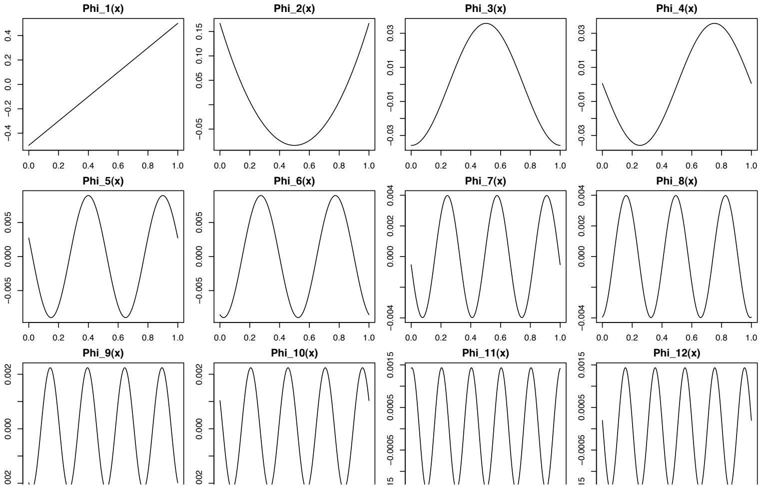
$$\eta(\mathbf{x}) = \beta_0 + \sum_{j=1}^{J} \eta_j(x_j) + \sum_{j<j'}^{J} \eta_{j,j'}(x_j, x_{j'}) + \cdots \quad (1)$$

- Each functional component in (1) can be further written as an orthogonal basis expansion via Karhunen-Loéve, e.g.,

$$\eta_j(x_j) = \sum_{p=1}^{P} \beta_{p,j}\phi_p(x_j), \ \text{with} \ \beta_{p,j} \overset{iid}{\sim} \mathcal{N}(0, \tau_j^2). \quad (2)$$

BSS-ANOVA Model: Basis Functions

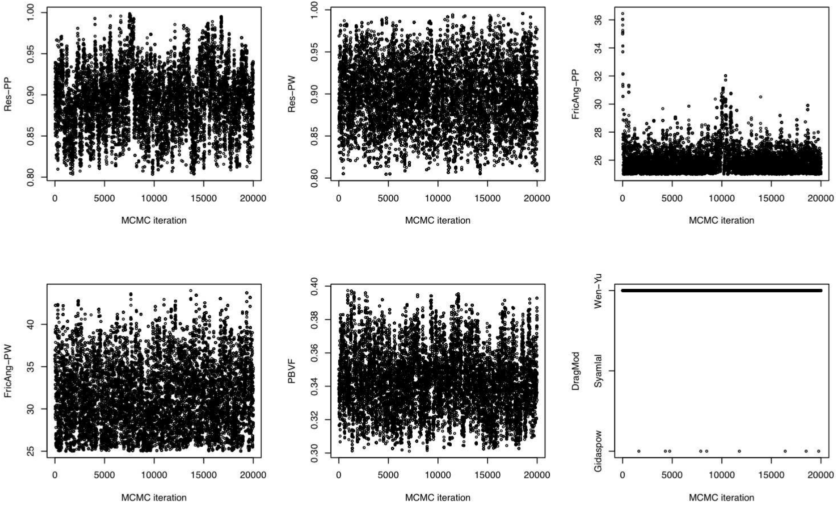
- The ϕ_p get increasingly higher frequency and have decreasingly less magnitude, so the expansion can be truncated at some value P.



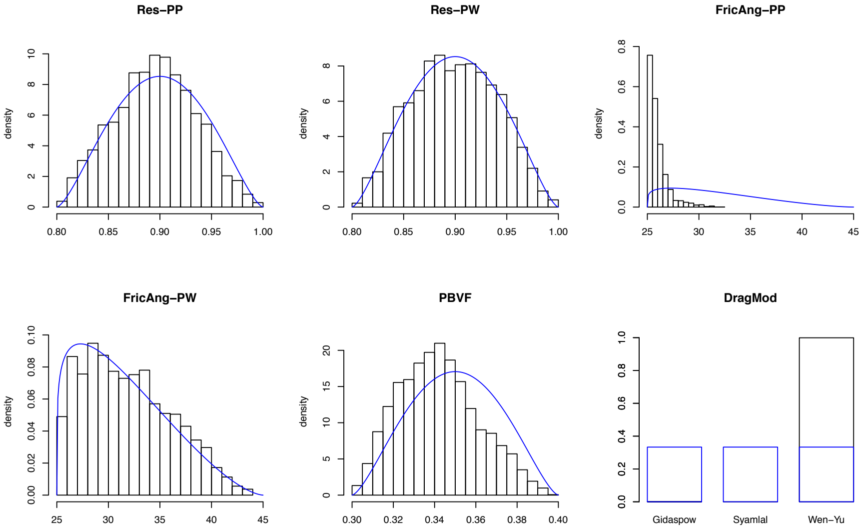
BSS-ANOVA Model Advantages

- This is just a linear model in the β's! Just need to estimate the β's and the discrepancy function is analytically specified by (1) and (2).
- Categorical parameters can be easily treated (Storlie, Reich, Helton, Swiler & Sallaberry 2013). Multiple models can be treated as levels of a categorical parameter.
- $O(J^2(N+M))$ computational efficiency for the MCMC algorithm as opposed to $O((N+M)^3)$ for the traditional squared exponential covariance GP, where $N+M$ is the total number of experimental observations plus simulator runs.
- Analytic forms are also nice for portability from one problem to the next (calibration $\rightarrow$ uncertainty propogation, or upscaling,...).
- Conjugate priors (i.e., inverse Wishart) for the variance terms (τ_j) leads to Gibbs sampling for all parameters in the model, with the exception that MH updates are needed for the elements of $\boldsymbol{\theta}$.

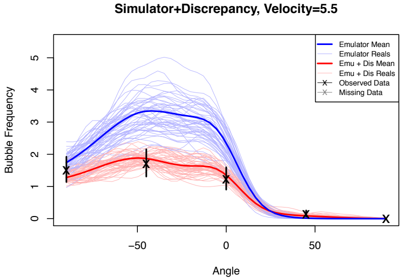
Bubbling Fluidized Bed: Theta Trace Plots

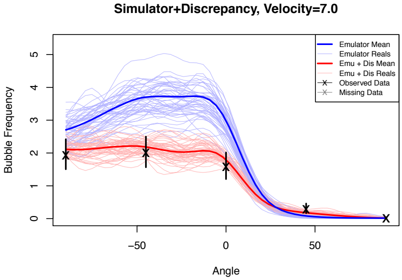


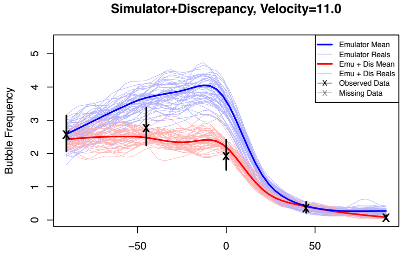
Bubbling Fluidized Bed: Theta Posterior

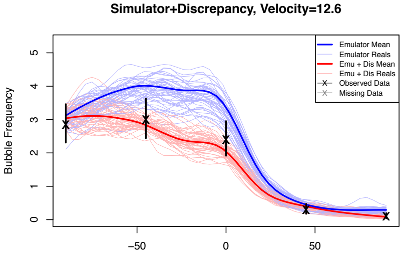


Bubble Frequency Fitted Plots

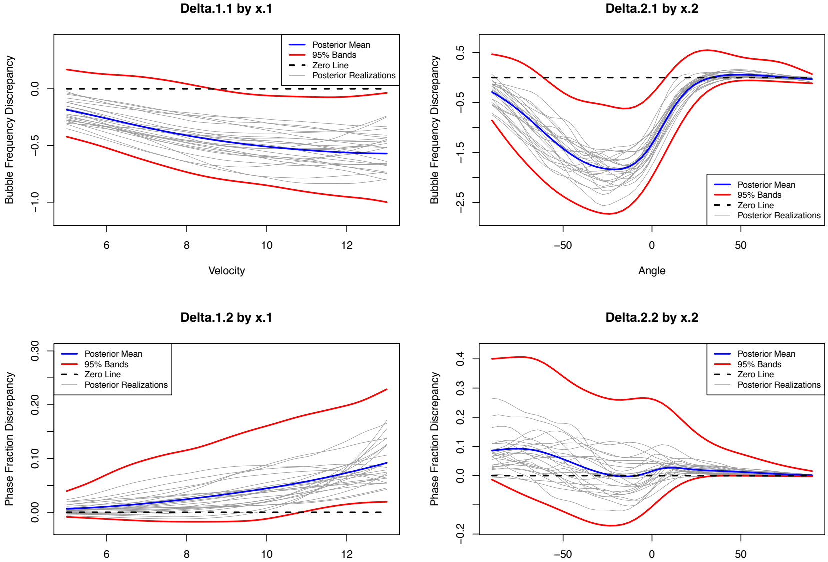




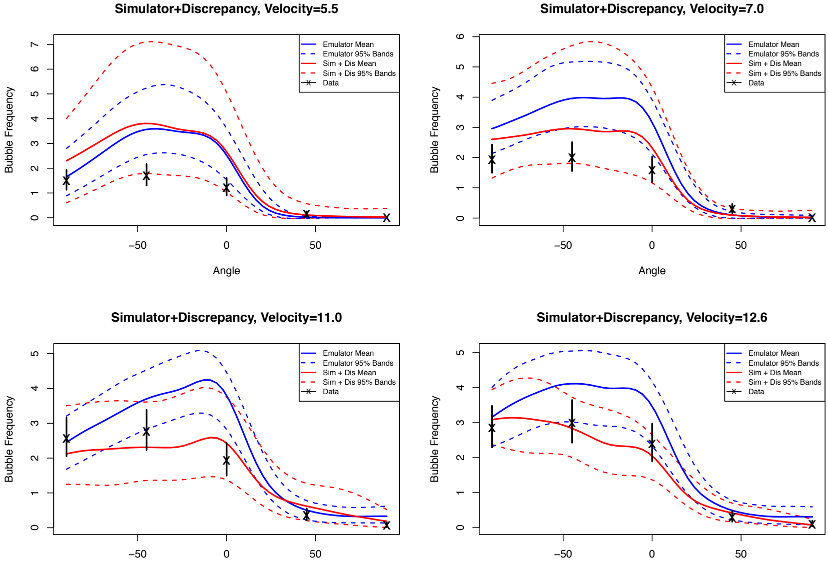




Bubbling Fluidized Bed: Discrepancy Plots



Bubbling Fluidized Bed: Cross Validation Plots



References

Higdon, D., Kennedy, M., Cavendish, J., Cafeo, J. & Ryne, R. (2004), ‘Combining field data and computer simulations for calibration and prediction’, *SIAM Journal on Scientific Computing* **26**, 448–466.

Kennedy, M. & O’Hagan, A. (2001), ‘Bayesian calibration of computer models (with discussion)’, *Journal of the Royal Statistical Society B* **63**, 425–464.

Reich, B., Storlie, C. & Bondell, H. (2009), ‘Variable selection in Bayesian smoothing spline ANOVA models: Application to deterministic computer codes’, *Technometrics* **51**, 110–120.

Storlie, C. B., Reich, B., Helton, J., Swiler, L. & Sallaberry, C. (2013), ‘Analysis of computationally demanding models with continuous and categorical inputs’, *Reliability Engineering and System Safety (in press)* **113**, 30–41.

Storlie, C., Fugate, M., Higdon, D., Huzurbazar, A., Francois, E. & McHugh, D. (2012), ‘Methods for characterizing and comparing shock wave curves’, *Technometrics (in press)* .

Thank you!

Disclaimer