Credible Simulation, Emphasizing, Sensitivity, Uncertainty, and Calibration

Brian Adams and Vince Mousseau
Sandia National Laboratory

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Credible Simulation, Emphasizing Sensitivity, Uncertainty, and Calibration

Brian Adams  Vince Mousseau

CASL Summer Student Workshop
June 19, 2015
Goals

• Reflect on components of simulation credibility

• Understand benefits of automated parametric analysis: sensitivity analysis, uncertainty quantification, and model calibration

• See concrete examples with CASL progression problem 6, modeled with VERA Core Simulator:
  – Sensitivity: determine most influential parameters
  – Calibration: tune closure models to experimental data
  – Uncertainty: determine effect of parametric uncertainty
Scenario: CASL Progression Problem 6

- Single PWR assembly, hot full power, 1300 ppm boron
- Decision maker requests predictions, with error bars, for steady-state quantities of interest (QOI):
  - reactivity
  - maximum pin power
  - maximum fuel temperature
- Analyst assesses relevant phenomena; simulates with CASL’s VERA CS, coupling:
  - Insilico (later MPACT) for neutronics
  - COBRA-TF for thermal-hydraulics and fuel (later Peregrine for fuel)

- Is the simulation is sufficiently accurate to inform decisions?
- If not, where should resources be invested?
- How can sensitivity, calibration, and uncertainty analysis help?
Expectations of the accuracy of scientific simulations vary. 

Who are you trying to convince?

- Code developers
- Analysts
- The customer
- The public

Expectations of Quality

- My job
- My employer’s reputation
- My paycheck
- Your paycheck

- I’d bet X on the result; X=…
- Uncertainty Quantification
- Error bars on simulation results
- Result converges with refinement
- Mesh refinement
- Eyeball norm
- Trends are reasonable
- Result is plausible
- Result is not ridiculous
- Code returns a result
Simulation relies on a modeling process:

- Reality (observed or postulated)
- Theory or explanation
- Conclusions
- Data
- Computation model
- Model solution
- Software implementation
- Discretization/solution scheme
- Code
- Direct analysis
- Compare/interpret
- Run simulation
- Update understanding
- Simplifying assumptions
- Abstract/quantify
- Computational analysis
Prediction with a simulation code is easy, right?

- **Limited** physical data (observational or experimental)
- **Limited** simulations (high computational demands…)
- **Imperfect** computational models (missing physics, etc.)
- **Under-resolved** approximations or numerics
- **Unknown** model parameters and boundary conditions
- **Imperfect** humans
- We want to *extrapolate* to conditions beyond validation regime…

Do you acknowledge strengths and weaknesses of your computational results?
Effective Use of Simulations

- Intended use should dictate simulation quality (PCMM)
- Account for and represent myriad uncertainty sources

Initial predictive capability maturity assessment for COBRA-TF

PDF Error
Prediction Error

PDF Error
Numerical Method Error

PDF Error
Parameter Variability

PDF Error
Modeling Error

Credit: François Hemez

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Systematic Way to Address These Challenges

- **Software quality**: must be engineered in from the start: requirements, revision control, testing, documentation

- **Code verification**: does the implementation of an algorithm exhibit the properties expected from numerical analysis, e.g., conserves mass, converges second order?

- **Solution verification**: is computed solution correct for the problem of interest? Convergence to correct answer, at correct rate (order), as model is refined.
Systematic Way to Address These Challenges

• **Validation**: Are the model and equations right for the intended application? If not, what needs improvement?

Validation is ultimately a quantitative comparison with data, accounting for uncertainty.
Dakota: Software Delivery Vehicle for CASL VUQ Algorithms

- Apply sensitivity analysis, UQ, optimization, and calibration to computational models
- Facilitate design trade-offs, V&V, QMU, risk-based decision making

- Extensive algorithm toolbox
- Non-intrusive iterative systems analysis
- Parallel computing: desktop to HPC
- Simulation management

Included with VERA, or download from http://dakota.sandia.gov/
Parametric Analysis

- Automated sensitivity, calibration, or uncertainty analyses can be helpful at various stages of code maturity.
- However, some level of software quality, verification, and validation is required: otherwise iterative analysis can hide bugs, insufficient numerical methods, etc.
- To use Dakota, need a “run-ready” model:
  - Parameters must be accessible for programmatic adjustment; may not be appropriate to expose in user input.
  - Analysis workflow must be automated and robust to parameter variations.
  - Quantities of interest must be accessible.
- For a few key CASL cases, this work has been done.
What is a “Parameter”?

What might we want to parameterize in a model?

• physics/science parameters; closure laws, rate constants
• statistical variation, inherent randomness
• model forms / accuracy
• material properties (fluids, solids)
• manufacturing quality / tolerances
• operating environment, interference, e.g., reactor operating conditions
• initial, boundary conditions; forcing
• geometry / structure / connectivity
• Input data, e.g., cross section libraries, chemical reactions DBs
• numerical accuracy (mesh, solvers); approximation error
Decomposing QoI Yields Parameters Per Phenomenon

Validation Pyramid

3-D Fuel Temperature

- Fuel temp.
- Gap cond.
- Heat removal
- Subcooled boiling
- Moderator density
- Fission heat

Density
- Heat capacity
- Conduction

Specific heat
- Convection
- Radiation

Cross flow
- Single phase heat trans.
- Spacer loss coeff.
- Latent sensible heat
- Surface effects
- Bubble drag

Boron density
- Energy per fission

Decompose QoI into its component pieces
Why Perform Sensitivity Analysis?

• What? Understand code output variations as input factors vary

• Why? Identify most important variables and their interactions
  – Ranking/screening: Identity the most important variables, down-select for further UQ or optimization analysis
  – Provide a focus for resources
    • Data gathering and model development
    • Code development
    • Uncertainty characterization
  – Identify key model characteristics: smoothness, nonlinear trends, robustness

• Secondarily:
  – Identify code and model issues (robustness)
  – Reuse designs to construct surrogate models
Selected Approaches to Global Sensitivity Analysis

- Local derivatives or sensitivities
- Univariate or joint parameter studies
- **Global methods: sample designs spanning input space**
  - Sampling: Monte Carlo, Latin hypercube, Quasi-MC, CVT
  - DOE/DACE: factorial, orthogonal arrays, Box-Behnken, CCD
  - Morris one-at-a-time
- **Typical analysis results for responses**
  - Simple and partial (including rank) correlation coefficients
  - Regression and resulting coefficients
  - Variance-based decomposition
  - Importance factors
  - Scatter plots
Sensitivity Studies with VERA CS

• Mousseau, Hooper, Belcourt “top-down” approach with Insilico/COBRA-TF to identify most important parameters for UQ, possibly later model improvements

• Based on QOI, identified key equations and related closure laws, e.g., gap conductivity, fuel temperature models, and added factors A, B:

\[ A \times F_w(Re) + B(x, t) \]

• Typical for these studies: \( A \in [0.95, 1.05] \) \( B(x, t) = 0 \), but can also use \( B(x,t) \) to perform numerical verification

• Also included cross sections, axial mesh spacing

• Basic centered parameter study: each parameter at nominal, positive increment, negative increment

• Sometimes for initial studies, a coarse down-select suffices
## Reactivity Sensitivity

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<th>Variable Description</th>
<th>Multiplier</th>
<th>Percent Difference</th>
<th>Physics</th>
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Fuel and Coupling are “important”
# Max Pin Power Sensitivity

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## Max Fuel Temp Sensitivity

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Model Calibration

- **Calibration**: use data to improve characterization of input parameter values, by maximizing agreement between simulation and experiment (inverse modeling)
  - Tune models to match specific scenarios
  - Make them more robust to predict a range of outcomes
- **Deterministic calibration**: seek a single set of parameter values that best match the data, typically in the two-norm

\[ SSE(\theta) = \sum_{i=1}^{n} [(y_i - s_i(\theta))^2 = \sum_{i=1}^{n} [r_i(\theta)]^2 \]

  - Initial iterate \( \theta_0 \), nonlinear optimization, updated values \( \theta \)
- **Bayesian calibration**: combine prior parameter distributions with data to update the statistical characterization of the parameters

  - Prior, statistical inference (MCMC), posterior
- **Calibration is not validation**! Separate data must be used to assess whether a calibrated model is valid.
Bayesian Calibration to Heat Transfer Closure Law

- Use data to refine predictions with COBRA-TF
- Nusselt number ($Nu$): ratio of convective to conductive heat transfer normal the boundary
- Instead of fixed closure law coefficients in Dittus-Boelter, make them variable parameters $\theta$ (for expert users only):

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

- In a typical sensitivity or uncertainty study, might use expert opinion to say

$$\theta_1 \in [0.0, 0.046] \quad \theta_2 \in [0.0, 1.6] \quad \theta_3 \in [0.0, 0.8]$$

- 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.
- Used delayed rejection adaptive metropolis for Bayesian calibration with this data
Updated Parameter Distributions

- Lead coefficient $\theta_1$ now lower: 0.004 from 0.023.
- Reynolds exponent $\theta_2$ now larger: 0.99 from 0.8
- Prandtl exponent $\theta_3$ slightly larger: 0.41 from 0.4.
- This only used 1 of 13 data sets informing Dittus Bolter
Joint Samples for the Parameters

- Uncertainty range is similar
- Bayesian analysis indicates correlations among parameters
- If lead coefficient increases, Reynold’s exponent must decrease
- Defines a 3-D surface indicating combinations of parameters that best match the data
Effect on Predicted Maximum Fuel Temperature

- Predicted maximum fuel temperature with COBRA-TF (power from neutronics held constant)

- Uniform ("expert" opinion) and Bayes Marginal have different shape but roughly same 95% uncertainty range.

- Bayes Joint shows the impact of recognizing correlation between the parameters

- The final uncertainty is roughly 5 degrees versus 40 degrees

- Bayesian methods give a way to continually make better use of available data to inform models.
Calibration for Dittus-Boelter

- Improved process, based on experimental data, to compute parameter distributions.
- More defensible than expert opinion.
- New experimental data can be easily incorporated to improve the accuracy of the new calibrated correlation.
Uncertainty Quantification

- **What?** Determine variability, distributions, statistics of code outputs, given uncertainty in input factors (“error bars” or impact due to parameter uncertainty)

- **Why?** Assess likelihood of typical or extreme outcomes. Given input uncertainty…
  - Determine mean or median performance of a system
  - Assess variability in model response
  - Find probability of reaching failure/success criteria (reliability metrics)
  - Assess range/intervals of possible outcomes

- **V&V, QMU:** assess how close uncertainty-endowed code predictions are to
  - Experimental data (validation, is model sufficient for the intended application?)
  - Performance expectations or limits (quantification of margins and uncertainties; QMU)
Prevalent UQ Method: Random Sampling

- Assume distributions on each of the $n$ uncertain input variables
- Sample from each distribution and pair into $N$ samples
- Run the simulation model for each of the $N$ samples
- Use results ensemble to build up a distribution for each of the $m$ outputs

- **sample mean**
  \[ \overline{T} = \frac{1}{N} \sum_{i=1}^{N} T(u^i) \]

- **sample variance**
  \[ T^{\sigma^2} = \frac{1}{N} \sum_{i=1}^{N} \left[ T(u^i) - \overline{T} \right]^2 \]
Selected UQ Approaches

- **Sampling**: robust, understandable, can require many samples (Monte Carlo, LHS, importance)
- **Reliability methods**: efficient optimization search to find behaviors or failure modes (mean value, MPP, FORM, SORM)
- **Stochastic expansions**: highly efficient on smooth responses (tailored surrogates: polynomial chaos, stochastic collocation)
- **Other**: interval estimation, evidence theory, mixed aleatory/epistemic
- **All can be adaptive, surrogate-enhanced to be efficient on costly simulation models**

\[
\begin{align*}
\mu_T &= T(\mu_u) \\
\sigma_T &= \sum_i \sum_j \text{Cov}_u(i, j) \frac{dg}{du_i}(\mu_u) \frac{dg}{du_j}(\mu_u)
\end{align*}
\]

\[
\text{minimize } u^T u \\
\text{subject to } T(u) = T_{\text{critical}}
\]

\[
R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi)
\]
Coupled Code UQ Study

- Conducted sampling-based UQ study with coupled Insilico/COBRA-TF
- Used down-selected parameters from earlier sensitivity study:
  1. Beta - turbulent mixing in CTF
  2. D.B. – Dittus Boelter single phase wall heat transfer
  3. MCA – McAdams wall friction
  4. Gridloss – Pressure loss coefficient for the grid spacers
  5. Xsec – cross sections
  6. Kcond – fuel thermal conductivity
  7. Hgap – Gap conductivity model
Cross section uncertainty dominates
UQ: Maximum Pin Power

Gap Conductivity dominates
UQ: Maximum Fuel Temperature

Gap conductivity dominates

Note gap conductivity is not Gaussian; care in assuming

Gap conductivity dominates
Making simulation credible

• Ask critical questions of theory, experiments, simulation to understand simulation credibility

• Use processes and tools that ensure quality and rigor: software quality, verification, validation

• Dakota parametric studies can help with model development and analysis:
  – Sensitivity: screen for model development or UQ
  – Calibration: help accurate characterize input parameters
  – Uncertainty quantification: understand total variability in outputs
  – Other: optimization, verification, validation

• Enable scientific discovery, engineering and policy decisions