Validating Models of Complex Physical Systems and Associated Uncertainty Models

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Imperfect Paths to Knowledge and Predictive Simulation

**Predictive Simulation**: the treatment of model and data uncertainties and their propagation through a computational model to produce predictions of **quantities** of interest with quantified uncertainty.
Quantities of Interest

Simulations have a purpose: to inform a decision-making process

- Quantities are predicted to inform the decision
- These are the Quantities of Interest (QoI’s)
- Models are not (evaluated as) scientific theories

Acceptance of a model is conditional on:

- its purpose
- the QoI’s to be predicted
- the required accuracy
What are Predictions?

Prediction

Purpose of predictive simulation is to predict QoI’s for which measurements are **not** available (otherwise predictions not needed)

Measurements may be unavailable because:

- instruments unavailable
- scenarios of interest inaccessible
- system not yet built
- ethical or legal restrictions
- it’s the future

How can we have confidence in the predictions?
Traditional Validation and Predictive Simulation

- Does not address the reliability/accuracy of the QoI’s
- Validation for predictive simulation requires additional analysis
Posing a Validation Process

Validation of physical models, uncertainty models & their calibration

- Challenge the model with validation data (generally not of QoI’s)
  - First opportunity is the calibration data
  - Use observations that challenge modeling assumptions
  - Use observations that are informative for the QoI’s
- Are discrepancies between model & data significant?
- There is no “one size fits all” solution
The Art of Predictive Simulation

Process of Predictive Simulation

- Identify QoI’s: reflects the purpose of the simulations
- Calibration: determine model parameters to match observations
- Validation: assess legitimacy of models for predicting QoI’s
- Prediction: computing the QoI’s with quantified uncertainty

Validation expectations are model dependent

- Interpolation “models”: simple fit to data
- Physics-based models: formulated from theory – extrapolatable
Validation for Complex Systems

Observables and Scenario Parameters

Validation is hierarchical
## Uncertainty

### Need to Treat Uncertainty in these Processes

- Mathematical representation of uncertainty (Bayesian probability)
- Uncertainty models (e.g. data, model inadequacy)
- Probabilistic calibration & validation processes (Bayesian inference)
  - Validation in the context of the QoI’s
  - Probabilistic QoI’s & validation criteria

### Uncertainty considerations can inform modeling

- How does the data inform the models?
- What new/better data are needed?
- What are the nature & consequences of model inadequacies?
The “Philosophy” of Validation

A model (theory) can never be fully validated

A model (theory) must be judged by its probability

Popper

Bayes

A validation process builds (or destroys) confidence in a model’s ability to predict QoI’s by confronting it with data

- Don’t validate or invalidate: gain or lose confidence
- May decide to reject or use a model based on our confidence

Pose validation as a Bayesian update of confidence...
Aleatoric and Epistemic Uncertainties

- Uncertainties are generally of two types:
  - Aleatoric: uncontrolled variability (e.g. as built geometric variations, random inputs)
  - Epistemic: lack of knowledge (e.g. of model parameters, of the model errors)
- Bayesian approach represents both uncertainties with probability
  - For epistemic uncertainty, probability represents subjective confidence in some proposition
  - Distinction between aleatoric and epistemic is one of interpretation
  - Distinction has consequences for validation inference
Validation and Bayesian Hypothesis Testing

Specify a validation requirement \( H \) in terms of the QoI, \( q \)

- Depends on purpose of predictions. Examples:
  - for a failure event \( f(q) \): \( H = \{ P_m(f(q)) \geq P_{true}(f(q)) \} \)
  - for point estimation \( H = \{|E_m(q) - q_{true}| < \epsilon\} \)

Test Hypothesis \( H \)

- Bayesian update of probability (\( \pi \)) of \( H \) given new data \( d \)

\[
\frac{\pi(H|d)}{\pi(H)} = \frac{\pi(d|H)}{\pi(d)}
\]

or

\[
\frac{\pi(H|d)}{\pi(H)} = \left( \pi(H) + (1 - \pi(H)) \frac{\pi(d| \sim H)}{\pi(d|H)} \right)^{-1}
\]

- How to estimate \( \pi(d| \sim H) \), \( \pi(d|H) \)?
- Start by determining the consequences of \( d \) on the QoI.
Traditional Validation

Stage 1: Maps Calibration Data to Validation Observables

Model with unknown parameter(s) → Calibration Data → Calibration Process → Calibrated Parameter(s) → Model Evaluation → Observables → Challenge

Experimental Validation Data
Experimentally Inaccessible QoI

Stage 1: Maps Calibration Data to QoI
- Calibration Data
  - Calibration Process
  - Calibrated Parameter(s)
  - Model Evaluation
  - Quantity of Interest

Stage 2: Maps Validation Data to QoI - Traditional Validation is Embedded
- Model Evaluation
  - Challenge
  - Validation Data
  - Model Evaluation
  - Quantity of Interest

Decision
Bayesian Inference (Calibration)

Nomenclature

- $x$ – observable
- $d$ – observed values of $x$ (data)
- $m(q, x|\theta)$ – theoretical model
- $\theta$ – model parameters
- $q$ – QoI’s
- $P(\cdot)$ – prior probabilities
- $\pi(\cdot)$ – posterior probabilities
- $P_m(d|\theta) = \int_x P(d|x)m(x|\theta) \, dx$ – probability of model producing $d$

- Bayesian inference of $\theta$
  \[ \pi(\theta|d) \propto P_m(d|\theta)P(\theta) \]

- Posterior QoI
  \[ \pi(q|d) = \int_\theta m(q|\theta)\pi(\theta|d) \, d\theta \]
Consequences of Validation Observations on the QoI’s

Two examples:

Model parameters represent calibration & validation data

- Calibration observations $d_c$

  $\pi(\theta_c|d_c) \propto P_m(d_c|\theta)P(\theta)$
  \[
  \pi(q|d_c) = \int_{\theta_c} m(q|\theta_c)\pi(\theta_c|d_c)\,d\theta_c
  \]

- Validation observations $d_v$

  $\pi(\theta_v|d_v) \propto P_m(d_v|\theta)P(\theta)$
  \[
  \pi(q|d_v) = \int_{\theta_v} m(q|\theta_v)\pi(\theta_v|d_v)\,d\theta_v
  \]

- Inconsistency between $\pi(q|d_c)$ and $\pi(q|d_v)$ is a problem, but how to infer $\pi(H|d_v)$

- Consider $P(H(\pi(q|d_c)) & H(\pi(q|d_v)))$

Multiple Stochastic Model Classes

- Consider a set $M$ of stochastic models $m_i$
- Calibrate using observations $d$

$$\pi(\theta_i | d, m_i, M) \propto P_m(d | \theta_i, m_i, M) P(\theta_i)$$

- Bayes’ theorem again

$$\pi(m_i | d, M) \propto P(d | m_i, M) P(m_i | M)$$

where the “evidence” $P(d | m_i, M)$ is

$$P(d | m_i, M) = \int_{\theta_i} P_m(d | \theta_i, m_i, M) P(\theta_i) \, d\theta_i$$

- Low probability $m_i$ are problematic, but need to estimate $\pi(H | d, m_i, M)$—approximate by evaluating $H$ relative to high probability $m$. 
Validation & UQ in a Multiphysics Application

At PECOS, UQ developments pursued in the context of atmospheric reentry vehicles

- Make V&V-UQ developments concrete
  - Conceptual issues: multi-physics coupling, model uncertainty and limited data (cost)
  - Data issues: reliability of real data
  - Algorithmic issues: high dimensional probability spaces and expensive models
Atmospheric Reentry

- RV problems present physical modeling challenges at multiple scales
- Models involve numerous uncertain parameters
- Models are not always reliable (e.g. turbulence)
We Simulate

- Earth reentry vehicle with ablative TPS
- ISS and Lunar return trajectories
- The thermal environment
  - Radiative
  - Convective
  - Chemical
- The heat loads on the vehicle
- The consumption of ablative TPS
- During the peak heating regime

Our QoI: rate of consumption of the TPS
Our Current Modeling Capabilities (DPLR++)

- Simplest physics models in common use
  - Algebraic turbulence model
  - Thermochemical non-equilibrium using two-temperature model
  - Gray gas, 1-D (slab) thermal radiation
  - CMA-type solid phase ablation

- All models coupled into hypersonics code, including:
  - Thermal radiation
  - Ablation (gas-phase treated in flow code)

- DPLR (from M. Wright, NASA-Ames) is currently used for reentry vehicle simulation
  - Radiation & ablation models developed in-house
  - Radiation & ablation models coupled to DPLR using loose-coupling scheme

- Basic numerical formulations
  - Line relaxation solves
  - Structured grids
Developing a New RV Simulator — FIN-S

- Chemistry Modeling
  - Thermochemical non-equilibrium using two-temperature model

- Turbulence Modeling
  - One-equation - Spalart-Allmaras complete
  - Two-equation - k-epsilon in development

- Ablation Modeling
  - Loose coupling to transient Chaleur simulations
  - Fully coupled quasi-steady CMA-type in development

- Advanced numerical formulations
  - Preconditioned Krylov solvers
  - Unstructured, adaptive grids
  - Goal-oriented adaptivity
  - A posteriori error estimation
  - Adjoint-based sensitivities
  - Support advanced UQ algorithms
Full System and UQ

Full System Simulation

- All Relevant Physics
  - Flow
  - Transport
  - Reacting Chemistry
  - Surface Reaction, Ablation
  - Radiation, Reradiation

- Forward Uncertainty Propagation
  - Calibrated Input Parameter Probability Density Function (PDF)
  - Output Quantity of Interest (QoI) Statistics
Uncertain Parameters

Submodel Uncertainties

- Hypersonic Flow
  - Chemical reaction rates
  - Diffusive flux model coefficients
  - Turbulent mixing inadequacy
- Radiation
  - Absorptivity/Model Error
- Ablation
  - Virgin, char densities
  - Reaction rate, equilibrium constants

\[ \sim 300 \text{ independent parameters} \]
Latin Hypercube Sampling

Algorithm
- Form quantile bins in each parameter
- Permute samples to bins
  - Reducing correlations
- Randomly place each sample within its bin

Uses
- Reduce variance from additive response components
- $O\left(N^{-3/2}\right)$ convergence for separable functions
Results: Outputs

Accuracy

- $\sim 2$ significant figures on mean
- $\sim 1$ significant figure on standard deviation
- Higher order statistics: worse
- $\sim 0.5$ million CPU-hours on Hera
Results: Parameter Sensitivities

- (In)sensitivities consistent with deterministic perturbation results
  - Perturbations subject to nonlinearity, multiparameter “cross terms”
  - Sampling correlations subject to Monte Carlo error

- Top uncertainties
  - Turbulent transport augmentation
  - Nitridation reaction rate

- Data mining: analysis of surrogate QoI choices
Results: Submodel Sensitivities

Submodel Updates
- Enlarged nitridation prior
- Chemistry/radiation coupling

Top Priorities
- Nitridation validation
- Turbulence model validation
Example Applications Calibration & Validation Processes

- Multiple model class
- Information gain to design experiments
- Characterizing data uncertainty
# Incompressible Turbulent Flow Example

## Motivation

Explore turbulence model validation in a simpler, but relevant, flow regime

Explore uncertainties from model inadequacy

## Calibration/Validation Process Overview

1. **QoI**: Wall shear stress ($\tau_w$) in favorable pressure gradient (FPG) turbulent boundary layer (TBL) flow.

2. **Prediction tolerance**: Need QoI prediction to 5%

3. **Modeling**: RANS + Spalart-Allmaras turbulence model + multiple uncertainty models

4. **Prior**: SA common choice for TBL with mild pressure gradient; plenty of literature

5. **Experimental data**: Three flat plate TBL experiments with varying pressure gradient conditions
Example: Models of Interest

Physical Model

- Reynolds-averaged Navier-Stokes (RANS) equations
- Boussinesq approximation: \[-u'_i u'_j = 2\nu_t \bar{s}_{ij} - \frac{2}{3} k \delta_{ij}\]
- Spalart-Allmaras turbulence model: \[\nu_t = \nu_{sa} f_v\]

\[
\frac{\partial \nu_{sa}}{\partial t} + \bar{u}_j \frac{\partial \nu_{sa}}{\partial x_j} = c_{b1} S_{sa} \nu_{sa} - c_{w1} f_w \left( \frac{\nu_{sa}}{d} \right)^2 + \frac{1}{\sigma} \frac{\partial}{\partial x_j} \left[ (\nu + \nu_{sa}) \frac{\partial \nu_{sa}}{\partial x_j} \right] + \frac{c_{b2}}{\sigma} \frac{\partial \nu_{sa}}{\partial x_j} \frac{\partial \nu_{sa}}{\partial x_j}
\]

Structural Uncertainty Models

RANS-SA is known to be imperfect. Evaluate three uncertainty models.

- \(M_1\): SA model is perfect \(\rightarrow\) no uncertainty
- \(M_2\): Independent, Gaussian uncertainty in observables
  \[y_i = \eta_i f_i(\theta), \quad \eta \sim N(1, \sigma^2 I)\]
- \(M_3\): Correlated, Gaussian uncertainty in velocity field
  \[U(x; \theta; \alpha) = A(x; \alpha) u_{sa}(x, \theta), \quad A \sim \mathcal{N}(1, k(x, x'; \alpha))\]
Example: Experimental Data

Three experimental data sets

Mean velocity and wall shear stress measurements from

- Osterlund et al., 2000
  - ZPG
  - Max $Re_\theta \approx 2.7 \times 10^4$
- Nagib et al., 2004
  - APG and FPG
  - Max $Re_\theta \approx 5.0 \times 10^4$

Experimental Uncertainties (assumed from authors’ assessment)

- Velocity measurements: Gaussian with 2% standard deviation
- Wall shear stress: Gaussian with 5% standard deviation
Example: Parameter Posterior PDFs

Observations

- Uncertainty representation can affect parameter posterior
- $\kappa$ very well determined by the data, but is different from nominal
Example: Plausibility and Model Selection

Bayes’ Theorem

\[
P(M_i|d, M) = \frac{P(d|M_i, M)P(M_i|M)}{P(d|M)}
\]

- Bayesian process enables relative evaluation of models
- \( M_3 \) dramatically preferred by the data
- Depending on requirements, may reject \( M_1 \) (the physical model) & \( M_2 \)
- Says nothing about the validity of \( M_3 \)

| \( M_i \) | \( N \) | \( P(M_i|d, M) \) |
|---|---|---|
| \( M_1 \) | 7 | \( 1.6 \times 10^{-10} \) |
| \( M_2 \) | 8 | \( 1.4 \times 10^{-10} \) |
| \( M_3 \) | 9 | \( \approx 1 \) |
Information Theoretic Interpretation

Rearranging Bayes formula:

\[ P(d|M_1) = \frac{P(\theta|M_1) P(d|\theta, M_1)}{P(\theta|d, M_1)} = \frac{P(d|\theta, M_1)}{P(\theta|d, M_1)} \]

Log and integrating:

\[ \int \ln[P(d|M_1)] P(\theta|d, M_1) \, d\theta = \ldots \]

Then:

\[ \ln[P(d|M_1)] = \underbrace{E[\ln[P(d|\theta, M_1)]]} \quad \underbrace{\text{log evidence}} \quad \underbrace{\text{how well the model class fits the data}} \quad \underbrace{E\left[\ln \frac{P(\theta|d, M_1)}{P(\theta|M_1)}\right]} \quad \underbrace{\text{how much the model class learns with the data}} \quad \underbrace{\text{(expected information gain, EIG)}} \]
**Example Application: $HCN/O_2/Ar$ Kinetics**

$HCN/O_2$ chemistry with 11 species ($O$, $N$, $H$, $Ar$, $O_2$, $OH$, $CN$, $CO$, $NO$, $HCN$, and $NCO$) and 6 reactions:

- $R_1: HCN + Ar \rightarrow H + CN + Ar$
- $R_2: O_2 + H \rightarrow OH + O$
- $R_3: O_2 + CN \rightarrow NCO + O$
- $R_4: HCN + O \rightarrow NCO + H$
- $R_5: NCO + Ar \rightarrow CO + N + Ar$
- $R_6: O_2 + N \rightarrow NO + O$

- Related to the problems of interest in this project
- Experimental data ([O] and [N]) for 22 different initial conditions from (Thielen and Roth 1987) are available.
Maximize EIG from Data (Experimental Design)

Choosing experimental scenario parameters that give large information gain will reduce the number of experiments needed to calibrate the model.
Validation and Uncertainty Quantification require experimental data
Data Validation & UQ

Data reduction model requires validation

![Diagram showing the process of data validation and uncertainty quantification (UQ)].
## Calibration & Validation Cases

### Extensive experimental data

- NASA Orion Project via Space Act Agreement
  - Ames EAST
  - Langley RCS
  - Ames & JSC Arc Jets
  - AEDC T9
  - CUBRC
  - Cal Tech

- Legacy data
  - Sandia

- PECOS

### Calibration & Validation Cases Table

<table>
<thead>
<tr>
<th>Facility</th>
<th>Description</th>
<th>Flow Measure</th>
<th>Calibration</th>
<th>Validate</th>
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<tbody>
<tr>
<td>UT TGA</td>
<td>N/A</td>
<td>Mass(T)</td>
<td>Ablation</td>
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<td>EAST Shock Tube</td>
<td>Hypersonic Radiometry</td>
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<td>Langley RCS</td>
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<td>RV model w/wo roughness</td>
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<td>PICA and copper targets</td>
<td>Particles</td>
<td>Part. gen/transport</td>
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<td>ArcJet</td>
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<td>TPS condition</td>
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Data Reduction Models for Heat Flux

Thermocouple surface $T(t)$

- Radiative heating tests conducted at AEDC Heat-Flux Lab
  - Uniform radiative heating at 1, 4, 6, 8, 12 BTU/s ft$^2$
  - NIST calibrated Schmidt-Boelter
  - Multiple installation scenarios (e.g. 15-5PH and 17-4PH SS)

![Graph showing heat flux data](image)

![Experimental setup diagram](image)
1-D Heat Equation DRM

Calibrate heat equation parameters

- Two parameters: $\alpha = k/\rho C_p$, $\beta = \rho C_p k$
- Assume Gaussian distribution with 4% of the mean for standard deviation for heat flux (NIST states $\pm 4\%$ on heat flux gauge accuracy)
- Assume Gaussian distribution with $3\sigma = 3.1^\circ F$ for temperature data (Type-E spec states $\pm 1.7^\circ C$ or 0.5%, whichever is greater, over range of $0 - 900^\circ C$).
- Assume uniform priors on material parameters
Posterior Parameter Distributions

Comments

• $\alpha_0$ becomes informed at late time as analogy with self similar solution degrades

Material Parameters

Heat Flux

- Prior
- $\alpha$ Posterior
- $\beta$ Posterior

Marginal Posterior

$(qw \text{ (normalized)})$
Uncertainty in Heat Flux Guage

Comments

- \( \approx 20\% \) uncertainty in heat flux due to uncertainty in coefficients
- Uncertainty in coefficients stems from uncertainty in temperature and heat flux measurements
Some Open Issues

- Formulating uncertainty models
  - Models of prior information
  - Data uncertainty models
  - Model inadequacy
- Validation inference about the QoI’s
  - Scarce validation data
  - Coupled multi-physics problems
- Computational algorithms
Thank you!

Questions?