MODELING AND SIMULATION, UNCERTAINTY QUANTIFICATION AND THE INTEGRATION OF DIVERSE INFORMATION SOURCES

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DoD/NASA Statistical Engineering Leadership Webinar, May 2017

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BACKGROUND
CURRENT COLLABORATIONS

Los Alamos National Laboratory
EST. 1943

NASA

P&G
“Given inevitable flaws and uncertainties, how should computational results be viewed by those who wish to act on them? The appropriate level of confidence in the results must stem from an understanding of a model’s limitations and the uncertainties inherent in its predictions.”

— National Academy Report, 2012
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Modern testing: “do more with less”

A pressing issue: most statistical, mathematical, and engineering programs do not provide sufficient training to tackle these difficult issues.
- Commonly encountered data sources (not meant to be exhaustive!)

- Developmental testing (lab testing)
- Operational testing (field testing)
- Modeling and simulation (computer experiments)
- Engineering judgement

- Commonly encountered data types
  - Continuous
  - Discrete
  - Functional
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DEFINITION OF TERMS
Modeling and Simulation
“A ROSE BY ANY OTHER NAME ...” (SHAKESPEARE)

- Modeling and Simulation
  - Computer Experiments
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  · Examples: CFD, FEA, etc.
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- Modeling and Simulation
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- Uncertainty Quantification
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  - Examples: CFD, FEA, etc.
- Uncertainty Quantification
  - Model Validation
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· Uncertainty Quantification
  · Model Validation
  · Model Calibration
· Modeling and Simulation
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  · Examples: CFD, FEA, etc.

· Uncertainty Quantification
  · Model Validation
  · Model Calibration
  · Design of Experiments
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- Uncertainty Quantification
  - Model Validation
  - Model Calibration
  - Design of Experiments
  - Sensitivity Analysis
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  - Model Validation
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  - Sensitivity Analysis
  - Propagation of Uncertainty
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- Integrated Analysis of Physical and Computer Experiments
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- Integrated Analysis of Physical and Computer Experiments
  - Data Assimilation
Modeling and Simulation
- Computer Experiments
- Examples: CFD, FEA, etc.

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Integrated Analysis of Physical and Computer Experiments
- Data Assimilation
- Resource Allocation Decisions
MODELING AND SIMULATION (M&S)
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MODELING AND SIMULATION

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  - Biomechanics

Often functional output rather than \( y_c(x) \) vs. \( y_c(t; x(t)) \).

Ultimate codification and integration of expert opinion, physical theory, and computer model “tuning” parameters.

May be less expensive than field data.

Tradeoff: inherent bias or discrepancy.
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WHY COMPUTER EXPERIMENTS?

· Benefits
  · Resource savings
    1. Financial
  · Potential for exploration of expanded “settings” (covariates)
· Disadvantages
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    3. Testing resources
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Why computer experiments?

- **Benefits**
  - Resource savings
    1. Financial
    2. Time
    3. Testing resources
  - Potential for exploration of expanded “settings” (covariates)

- **Disadvantages**
  - Require *different* resources
  - May be biased (we use the term *discrepancy*)
  - Difficult/impossible to validate without physical data
Treat computer experiments as data!

- $x$: predictor variables (observed)
- $\theta$: computer model parameters
- $\eta(x, \theta)$: computer model estimate for $y$ given $x$ and $\theta$.
- $y$: actual outcome at $x$
- $\epsilon$: statistical error

Assume: $y = \eta(x, \theta) + \epsilon \theta$ unknown.
Bayes’ Rule

\[
\pi(\theta|y) \propto L(y|\theta) \times \pi(\theta)
\]

- Goal is to understand \( \theta \) to “tune” computer model
- Bayesian approach provides very general approach for inference
- Required element: prior pdf for \( \theta \) is required (perhaps noninformative)
- Issue 1: normalizing \( \pi(\theta|y) \) is generally difficult, but rarely necessary
- Issue 2: high dimensional \( \theta \) can lead to computational challenges
UNCERTAINTY QUANTIFICATION
- Field experiments (physical experiments)
  - Traditionally “real” data
  - Measured without bias/discrepancy
  - Univariate, $y(x)$, multivariate, $y(x)$, or functional, $y(t; x)$
  - Hereafter, $y(x)$. 
\( y(x) = \zeta(x) + \epsilon(x) \)

- \( x \): known system inputs
- \( y(x) \): experimental data
- \( \zeta(x) \): unobs. system response
- \( \epsilon(x) \): statistical error
\[ \zeta(x) = \eta(x, \theta) + \delta(x) \]

- \( \zeta(x) \): unknown calibration inputs
- \( \eta(x, \theta) \): computer model
- \( \delta(x) \): model discrepancy
Discrepancy = 0 \rightarrow \text{Agreement!}

- feedback to modelers
- difference “surface” (data - model)
- 95/5 uncertainty bounds
predicted $\zeta(x)$
- 95/5 uncertainty bounds
- predicted $\zeta(x)$
- unobserved “truth”
- Discrepancy adjusted!
Background
Definition of Terms
Modeling and Simulation (M&S)

Uncertainty Quantification
  Integrated Analysis of Computer and Physical Experiments

Model Validation
Model Calibration
Design of Experiments/Resource Allocation
Sensitivity Analysis
Examples

Summary
Questions and Answers
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· Ambiguous definition: oft discussed, seldom resolved!
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  3. Physical experiment is a noisy (statistical error) version of reality.
MODEL CALIBRATION

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- Requires:
  1. True input/output relationship
  2. Computer experiment is a biased version of reality.
  3. Physical experiment is a noisy (statistical error) version of reality.
  4. Built in to most COTS/publicly available software.
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SENSITIVITY ANALYSIS

- Assess the sensitivity of output to individual variables ("main effects") or combinations of variables ("interactions").
- ANOVA-type decomposition gives variability attribution.
- Useful in determination of important variables/combination of variables.
- Active area of research.
- Built in to most COTS/publically available software
EXAMPLE 1: MICROENCAPSULATION FOOD COATING

- Goal: Model uniformity of foot coating application, find “best” computer model.
- Physical Experiment: actual food coating process as use 28 runs of food coating line with different (operational testing) settings of temperature, air pressure, density of coating material, etc.
- Computational Models: 3 different models with different “physics” at each of the exact same settings.
- Unique aspects:
  - Possible to run computer experiments at all physical experiments
  - Multiple teams competing to build more accurate experiment
  - All models perfectly “tuned” (almost never happens!)
EXAMPLE 1 (OUTPUT)

Discrepancy = 0 → Agreement!
- Computer model 3 is best
- $\delta$ (data - model)
- Full distribution for each $\delta$

$\leftarrow$ constant $\delta(x) \equiv \delta$
EXAMPLE 2: STOCKPILE STEWARDSHIP

- Goal: Assess safety, security and effectiveness of the stockpile
- Physical Experiments: underground tests (operational-ish), non nuclear tests
  - Operational physical experiments are desired by nobody.
  - Lab tests expensive, only partially representative
- Computer Experiments: complex computer codes
  - Months of CPU time on world’s fastest supercomputers.
  - Specialized computing equipment required.
  - Computational experiments almost as costly as physical experiments.
Example 3: NASA Slosh Estimation

- Goal: Model effect of damping on fluid slosh in booster tanks
- Physical Experiment: Shaker table (lab testing)
  - Operational physical experiments costly.
  - Computational experiments are as costly.
- Computer Experiments: Computational Fluid Dynamics (CFD)
  - Expensive, difficult to obtain
  - Computational experiments are perhaps more costly to run (at least in terms of time)
  - Viewed by some as higher fidelity than physical experiments
Fill Height: 12.6 in
All Wave Heights

← predicted $\zeta(x)$
- 95/5 uncertainty bounds
- Impressive agreement
- unobserved “truth”
- Discrepancy adjusted!
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- Each situation has unique elements that make integrated analysis difficult to create and use COTS solutions.
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- Resources are available and research continues to pour out of both statistics and applied math (see below).
REFERENCES


· LANL Gaussian Spatial Process (GaSP) Code:
RESOURCES FOR COMPUTATION

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  - MATLAB based

SmartUQ
- COTS solution
- Fee based
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  ![Image of conference and journal covers]