Uncertainty quantification for numerical model validation

Introduction – Concepts - Organization

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Starting point: uncertainties everywhere in the modeling chain!

Main problem: credibility of predictions

- Physical phenomenon
- Observations
- Variables of interest
- Numerical model
- Parameters
- Input data
- Algorithm
- Simplifications
- Coding Errors
- Numerical approximation
- Model uncertainties

- Physicist
- Mathematician
- Statistician
- Computer scientist
Similar safety and uncertainty issues in CS&E and Nature sciences

- Climate Modeling: Prediction
- Nuclear industry: Conception, Maintenance, risks
- Oil, gas, CO2: Production optimization
- Car and plane: Conception
- Astrophysics: Understanding
Main stakes of uncertainty management

- **Modeling phase:**
  - Improve the model
  - Explore the best as possible different input combinations
  - Identify the predominant inputs and phenomena in order to prioritize R&D

- **Validation phase:**
  - Reduce prediction uncertainties
  - Calibrate the model parameters

- **Practical use of a model:**
  - **Safety studies:** assess a risk of failure (rare events)
  - **Conception studies:** optimize system performances and robustness
Uncertainties in simulation experiments

Two kinds of uncertainties

1. Epistemic
   aka "reducible" (with sufficient learning)

2. Stochastic (aleatoric)
   aka "irreducible" (excepted huge extra expense, ie meas. devices)

An open problem: What is the best way to model such uncertainties?

Hints:

1. Stochastic → Probability Theory
   aka "reducible" (with sufficient learning)

2. Epistemic → idem ... but many other ways:
   • Possibility Th., Evidence Th., Fuzzy Sets, Dempster-Schaffer, ...

Only Probability Th. used in the framework of this Summer School
Uncertainties in simulation experiments

\[ Y = a_1 x_1 + a_2 x_2 \]

**Ancient way**
\[ \Delta Y = a_1 \Delta x_1 + a_2 \Delta x_2 \]

**Pre-modern way**
\[ x's \ identified \ to \ R.V. \]
\[ \text{... but same algebra} \]
\[ \sigma_Y = \sqrt{a_1^2 \sigma_1^2 + a_2^2 \sigma_2^2} \]

**Still used in metrology (GUM)**

**Really Modern way**
\[ x's \ fully \ treated \ as \ R.V. \]

Can give moments, quantiles, and even pdf of Y ...
... if fair waiting time
Uncertainty management - The generic methodology

Step C: Propagation of uncertainty sources

Step B: Quantification of uncertainty sources
- Modelisation with probability distributions
- Direct methods, statistics, expertise

Step A: Problem specification
- Input variables
  - Uncertain: x
  - Fixed: u

Model (or measurement process)
- f(x, u)

Variables of interest
- Y = f(x, u)

Step C': Sensitivity analysis, Prioritization

Step B': Quantification of sources
- Inverse methods, calibration, assimilation

Feedback process

Decision criterion
- Ex: Probability < 10^{-b}

Observed variables
- Y_{obs}
Step A – Focus on the quantity of interest

Inputs: X

Output: Y

What is really interesting in our study?

Mean, median, variance, (moments) of Y

Quantiles (extrems), probability of threshold exceedence

Sometimes a cost/information compromise
Step B - Quantification of uncertainty sources

Different cases

1. A lot of data
   - Fitting of probability distributions
   - Statistical hypothesis test (often parametric tests)

2. Few data (n < 10)
   - Use of probabilistic inequalities to obtain the mean and some bounds
   - Hypothesis on parametric probability distribution
   - Non-parametric tests: less powerful, wide bounds
   - Expert judgement, then Bayesian inference

3. No data
   - Maximum entropy principle
   - Expert judgment techniques
   - Cristal Ball?

Step B’ - Calibration issues: use of indirect observations of the outputs in order to retrieve the model inputs
Step C - Uncertainty propagation: main principles

Propagate uncertainties from $X$ to $Y$, via the deterministic function $f(\cdot)$

- Conceptually simple problem, but with sometimes a complex implementation
- Choice of method strongly depends on the quantity of interest
  => importance of step A
  this quantity of interest is linked to decisional issues

Two kinds of problems:

- Central tendency (ex. mean) or dispersion (variance)
  - Metrology
- High quantile, « probability of failure »
  → justification of a safety criterion

Analytical methods sometimes applicable

Numerical methods (optimization, Monte Carlo sampling)
Step C’ - Sensitivity analysis: main objectives

• Reduction of the uncertainty of the model outputs by prioritization of the sources
  • Variables to be fixed in order to obtain the largest reduction (or a fixed reduction) of the output uncertainty
    A purely mathematical variable ordering
  • Most influent variables in a given output domain
    - if reducibles, then R&D prioritization
    - else, modification of the system
    The individual cost of the reduction may change the previous variable ordering

• Simplification of a model
  • determination of the non-influent variables, that can be fixed without consequences on the output uncertainty
  • building a simplified model, a metamodel
Uncertainties management for cpu time consuming models

A useful solution: the metamodel (model of the numerical model)

\[ p \text{ input variables} \]
\[ X = (X_1, ..., X_p) \]

Physical phenomena

Computer code

\[ y(X) \text{ Time consuming} \]

\[ \hat{Y}(X) \text{ Negligible cost} \]

Metamodel

\[ y(X) \approx \hat{Y}(X) \text{ Predicted experiences} \approx \text{simulated experiences} \approx \text{observed experiences} \]

Use of the metamodel:

- C’: Sensitivity analysis

\[ \text{Variance de } Y \]

\[ \text{Distribution of the inputs} \]

\[ \text{Metamodel} \]

\[ Y_{SR} = f_{SR}(X) \]

\[ \text{Distribution of the output} \]

- C: Uncertainty propagation (via Monte Carlo methods)

- B’: Calibration

Identification of input parameters values

Adequation between observed and simulated experiences
V&V Verification and Validation

To sum up:

**Verification**: do I solve the equations right?

**Validation**: do I solve the right equations?

*(at least for the intended application)*

Two levels for Verification:

1. **Code Verification**: some kind of *internal* correctness of the code may be assessed by formal methods from Software Engineering

2. **Calculation Verification**: concerns the calculations themselves
   - Convergence, grid adaptation, solution algorithms, ...
   - Is the solution closed to the exact one?

⚠️ We’ll talk later on subtleties between Code and Model(s)
V&V Verification and Validation

Validation

1. Should occur AFTER Verification

2. Here the goal is to test the Code against Reality ....

   Roughly speaking: code (C) gives information I(R|C) on Reality; so does Experiment (I(R|E)); the couple (C,E) is valid if I(R|C) and I(R|E) agree (statistically)

   (need to validate also experiments !!!)

3. Must not be confused with calibration; schematically:

   1. Validation: just test for the agreement between I(R|C) and I(R|E) and then decide if (C, E) is valid or not

   2. Calibration: tune C in order to improve the agreement between I(R|C) and I(R|E)
V&V : a first step to assess the credibility of the code

Don't forget that the true objective is to gain confidence in our simulations
So ask the questions :

1. Is the code able to simulate the system/phenomena of interest ?
   that is the Accreditation (Expert-like decision) step

2. What is the strategy if $I(R|C)$ and $I(R|E)$ disagree ?

3. And if $I(R|C)$ and $I(R|E)$ agree : can I assess a confidence interval for
   future predictions ?

And always remember that

   All models are wrong but some are useful
   G.E.P. Box
Motivations for this summer school

• We are convinced that, at the present time, each simulation result should be associated with an uncertainty (as in the measurement science)

• High Performance Computing becomes accessible to many scientists

• However, statistical tools are not so easy to use; there are also some cultural barriers in the engineering world

• This subject has recently received a lot of attention (software development, interdisciplinary working groups, many research works, etc.)

For us, this summer school is an occasion to:

1. Disseminate the uncertainty culture in our research institutes and companies

2. Offer in an educational way recent advances about the topics of uncertainty quantification and simulation model validation

3. Create a strong event on this subject (in reference to the last CEA-EDF-INRIA summer school in 2005)
Organization of this summer school

Three main lectures from international experts:
1. François Hemez (Los Alamos) - Introductive course
2. Rui Paulo (Univ. Tech. Lisboa) - Bayesian view
3. Emmanuel Vazquez (SUPELEC) - Rare events evaluation
   showing the scientific diversity of the problems

Computer practical works in various programming languages:
1. Matlab
2. R

Two software demonstrations:
1. OpenTURNS (from EDF-EADS-Phimeca)
2. URANIE (from CEA/DEN)

Several seminars on connected subjects:
- Remainder of statistics
- Calibration
- Chaos polynomials
- Model validation
- Multidisciplinary and robust optimization
- High Performance Computing
First week – 27 june to 1 july

Each lecture and each practical work goes on 1h30. Morning : 8h30-12h – Afternoon : 14h-17h30

• 27 june
  – Morning (beginning 11h) : Iooss & Sancandi (45mn) – Presentation/organization of the school
  – 11h45-12h30 : Seminar 1 Part 1 (45mn) Marrel
  – Afternoon : Course 1.1 Hemez & Seminar 1’ (1h) Pasanisi
  – End of afternoon : Seminar 1 Part 2 (1h) Marrel

• 28 june
  – Morning : Course 1.2 Hemez – Course 1.3 Hemez
  – Beginning of afternoon (14h-15h30) : visit of Iter construction site
  – Afternoon : Optional TD to be chosen between TD A and TD B
  – End of afternoon : TD 1.1

• 29 june
  – Morning : Course 2.1 Paulo – Course 2.2 Paulo
  – Afternoon : TDs 1.2 et 2.1

• 30 june
  – Morning : Course 1.4 Hemez – Course 2.3 Paulo
  – Afternoon : TDs 1.3 et 2.2
  – End of afternoon : Seminar 2 (1h30) de Crécy & Couplet

• 1er july
  – Morning : Course 1.5 Hemez – Course 2.4 Paulo
  – Afternoon (end 15h30) : TD 2.3
Second week – 4 july to 8 july

Each lecture and each practical work goes on 1h30. Morning : 8h30-12h – Afternoon : 14h-17h30

• 4 july
  – Morning (beginning 11h) : Course 3.1 Vazquez
  – Afternoon : TDs C et 3.1
  – End of afternoon : Social event

• 5 july
  – Morning : Course 3.2 Vazquez – Seminar 3 (1h30) Le Riche
  – Afternoon : TD 3.2 – Seminar 4’ (45’) Blatman - ??course on sensitivity analysis?? (45’)

• 6 july
  – Morning : Course 3.3 Vazquez – Seminar 5 (1h30) Sancandi
  – Afternoon : Atelier logiciel OpenTURNS (3h)
  – End of afternoon : Seminar 4 (45’) Martinez

• 7 july
  – Morning : Course 3.4 Vazquez – Seminar 6 (1h30) Prud’homme
  – Afternoon : Atelier logiciel URANIE (3h)
  – Gala dinner

• 8 july
  – Morning : Course 3.5 Vazquez – TD 3.3 – Conclusion/Information (1h)
  – End at 13h00
The entire team wishes you a happy summer school!

Your private assistants ...

Amandine  
Vincent  
Claire  
Géraud  
Nadìa  
Mathieu

... and your major assistants

Marc  
Bertrand