A Prime on Uncertainty Quantification

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Uncertainty Quantification (UQ)

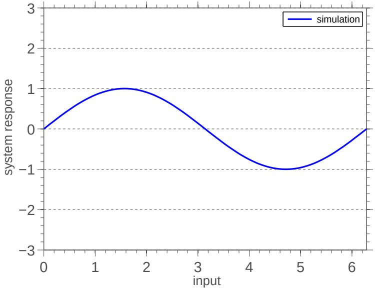
What is Uncertainty Quantification?

Uncertainty quantification (UQ) is multidisciplinar area involving engineering, mathematics, and computer science. It deals with quantitative characterization and reduction of uncertainties in applications.

Why Uncertainty Quantification?

- Decision Making
  Some kind of certification is essential for high-risk decisions
- Model Validation
  Verify model limitations is necessary for accurate predictions
- Robust Design/Optimization
  Devices with low sensitivity to variations are often required

In a simplistic way UQ aims to:



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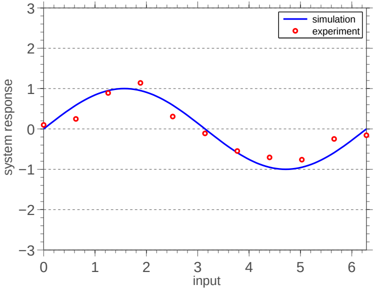

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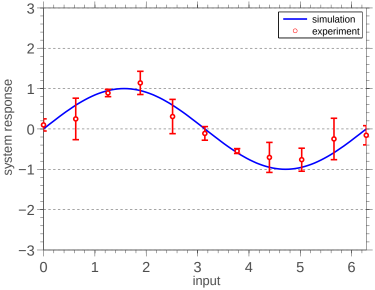

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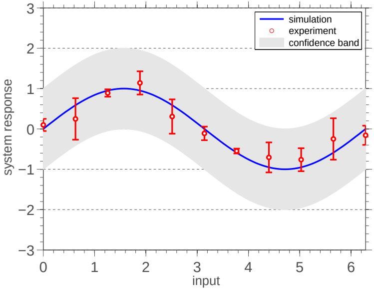
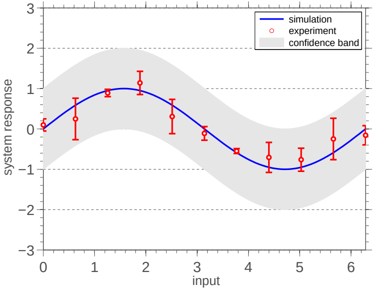


In a simplistic way UQ aims to:

(i) add error bars to simulations



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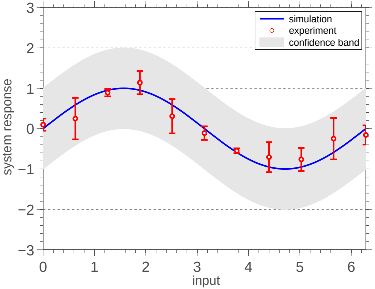

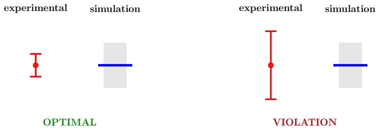

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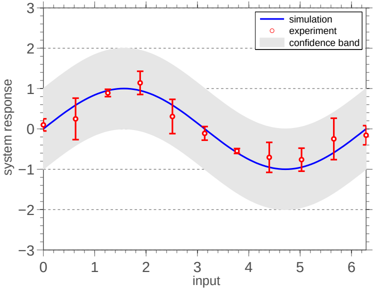
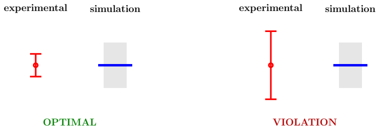


(ii) define a precise notion of validated model



UQ Vocabulary

Errors vs Uncertainties

errors and uncertainties in UQ

$$\neq$$

errors and uncertainties in metrology

- Uncertainties: associated to variabilities intrinsic to the system of interest and potential lack of knowledge about the physics (aleatory or epistemic)
- Errors: associated to the translation of a mathematical model into a computational model/code (discretization, round-off, computer bugs)

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Uncertainties: physical nature

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Uncertainties: physical nature

Errors: mathematical nature

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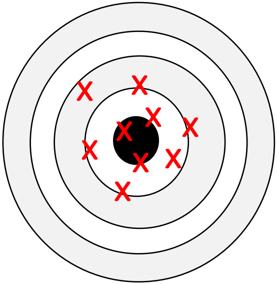
Aleatory Uncertainties (data uncertainties)

Characteristics:

- induced by variabilities in the real system/environment
- arises naturally from observations (noise)
- impossible to be eliminated/reduced (irreducible)

Examples:

- geometric dimensions
- material properties
- measurement noise
- etc



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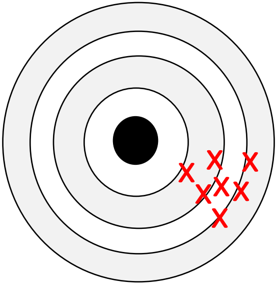
Epistemic Uncertainties (model uncertainties)

Characteristics:

- induced by lack of knowledge / ignorance
- arises from modeling hypotheses (bias)
- can be reduced/eliminated (reducible)

Examples:

- geometric form
- boundary conditions
- constitutive equations
- surrogate models
- etc



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Verification and Validation (V&V)

- Verification
  Are we solving the equation *right*?

- Validation
  Are we solving the *right* equation?

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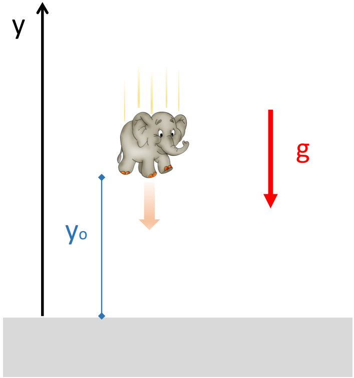
An example in V&V



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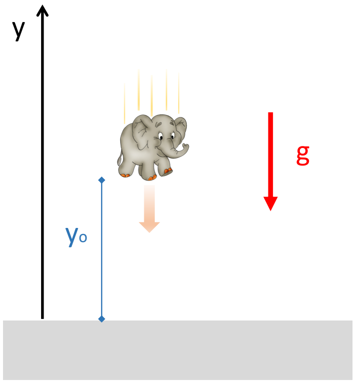

Mathematical model:

$$m\,\ddot{y}(t) = -m\,g$$
$$\dot{y}(0) = v_0$$
$$y(0) = y_0$$

Verification of the equation solution

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$$+ \text{ initial conditions}$$

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- Numerical (Runge-Kutta)

$$y_{n+1} = y_n + \frac{h_n}{6}(k_1 + 2\,k_2 + 2\,k_3 + k_4)$$

$$t_{n+1} = t_n + h_n$$

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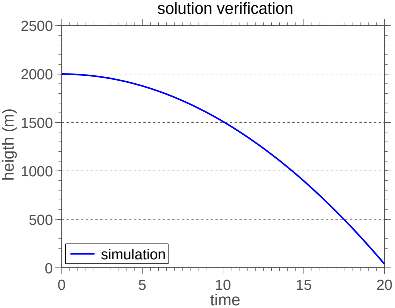

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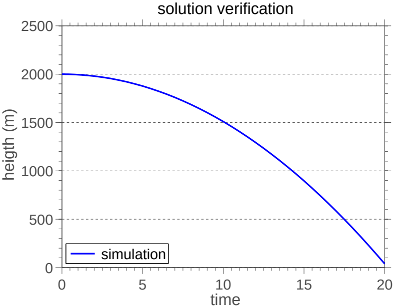
- Reference (analytical)

$$y(t) = -\frac{1}{2} g\,t^2 + v_0\,t + y_0$$



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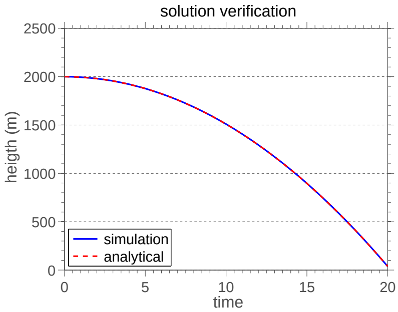

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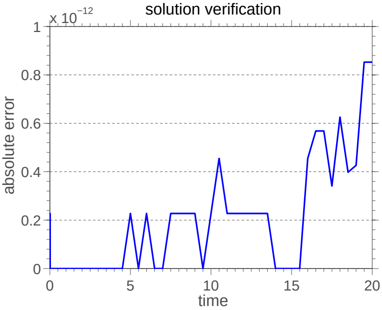

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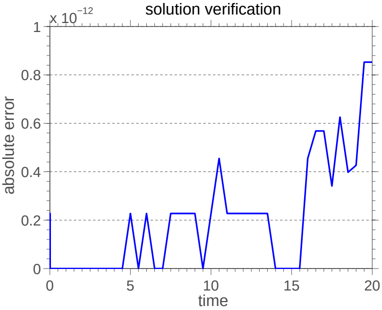
The model equation is well solved



Validation of the model

Toy model:

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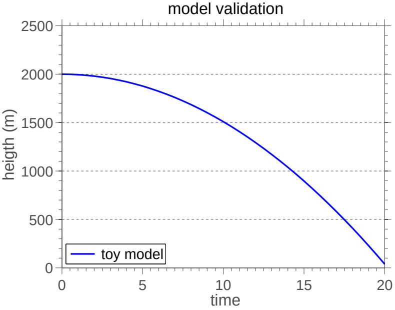

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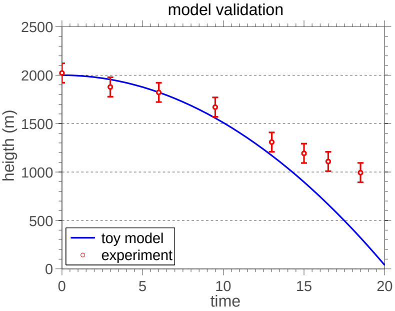

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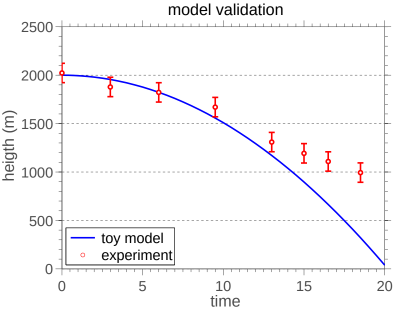

The mathematical model is not representative

Validation of the model

Improved model:

$$m\,\ddot{y}(t) = -m\,g + \frac{1}{2}\rho\,A\,C_D\,\left(\dot{y}(t)\right)^2$$

$$\dot{y}(0) = v_0$$

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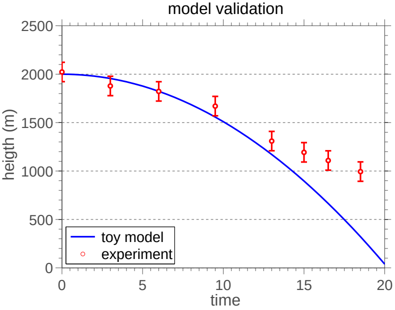

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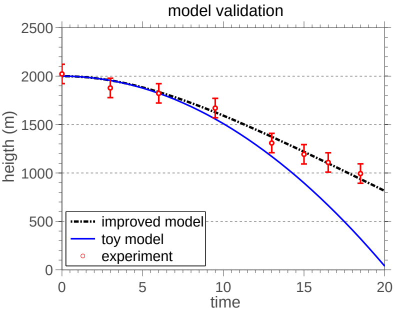

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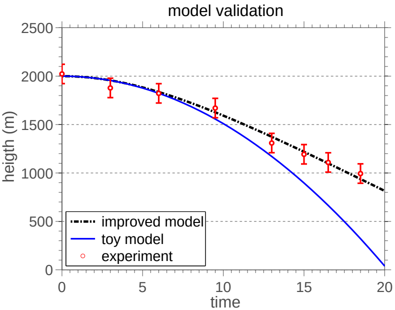
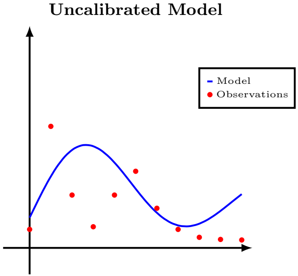
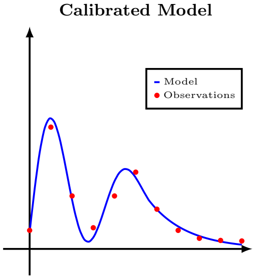
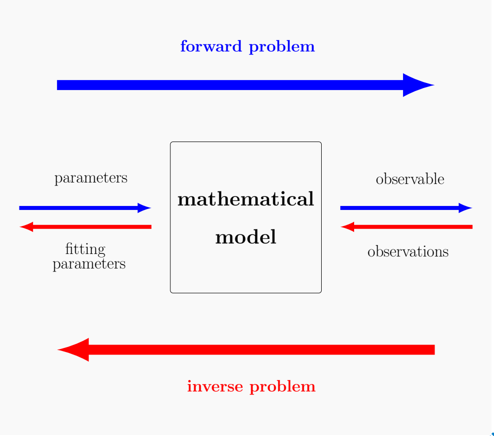


An improved model enhance the predictions

Calibration of the model

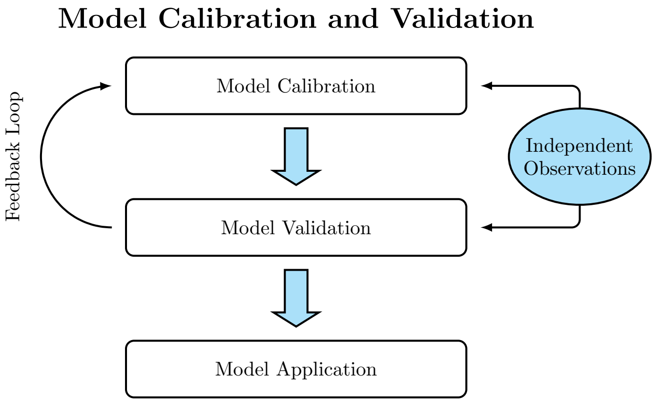






* Left pictures prepared by Michel Tosin.

Calibration vs Validation



* Picture prepared by Michel Tosin.

Sensitivity Analysis $\neq$ UQ

- Sensitivity Analysis:
  - based on derivatives $\partial u_i / \partial \xi_j$
  - measure response sensitivity to changes on a certain input
  - characterization of input variabilities is not required (deterministic method)
  - valid only for a fixed (nominal) set of parameters in general (local analysis)
  - large sensibility $\not\Longrightarrow$ large uncertainties
- Uncertainty Quantification:
  - based on propagation of uncertainties
  - identify overall output uncertainty
  - characterization of input variabilities is required (stochastic method)

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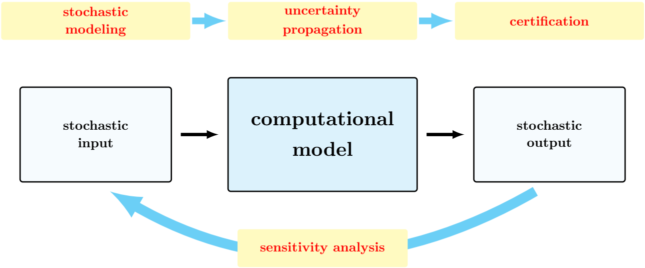
Computers & Uncertainties

General framework for uncertainty quantification (UQ)



1. Stochastic Modeling: characterize inputs uncertainties
2. Uncertainty Propagation: quantify output uncertainties
3. Certification: establish acceptable levels of uncertainty
4. Sensitivity Analysis: explain the output variability

B. Sudret *A short review of computational methods for uncertainty quantification in engineering*, 2013.

Stochastic Modeling

How to model/characterize uncertainties?

- Probabilistic approaches:
  - Parametric probabilistic approach
  - Nonparametric probabilistic approach
- Nonprobabilistic approaches:
  - Interval analysis
  - Evidency theory
  - Fuzzy logic

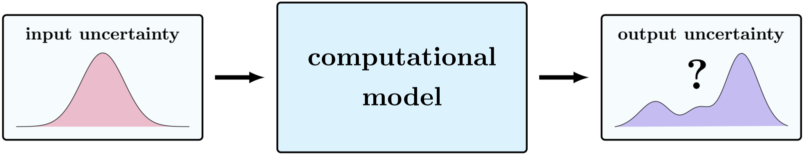
Uncertainty characterization must be based on available information

- experimental data
- theoretical arguments
- etc

Uncertainty Propagation

Given: **computational model** and **input uncertainty**

Find: **output uncertainty**

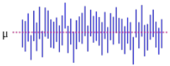


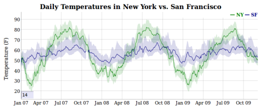
- The most complex and computationally intensive step
- Propagation technique depends on representation approach

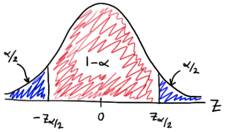
Certification

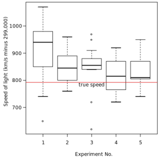
Specify levels of reliability for predictions:

- confidence interval/band
- probability of events of interest
- boxplot
- etc





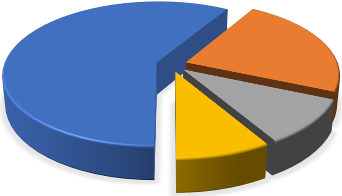




Sensitivity Analysis

Determine how input uncertainty explains output variability:

- model structure decomposition
- detection of nonlinearities
- screening / feature setting
- ranking
- exploration



Variance decomposition-based global sensitivity analysis:

- Morris method
- Sobol indices (ANOVA)
- etc

Key points about UQ

- UQ is essential for applied tasks such as
  decision making, model validation, and robust design
- UQ is a new discipline with much theory to be developed
- Until today there is no consensus on UQ basic vocabulary
- Certification for numerical simulations is a worldwide trend

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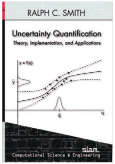

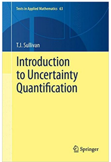

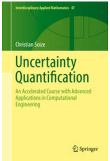

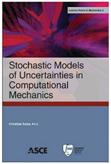

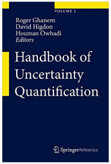

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