A Prime on Uncertainty Quantification

Prof. Americo Cunha Jr

americocunha.org

@AmericoCunhaJr

@AmericoCunhaJr @AmericoCunhaJr

Uncertainty Quantification (UQ)

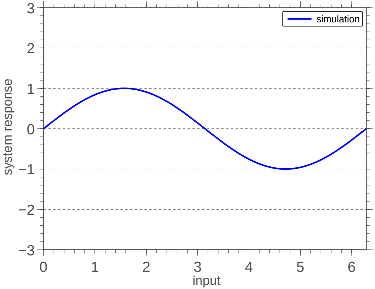
What is Uncertainty Quantification?

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

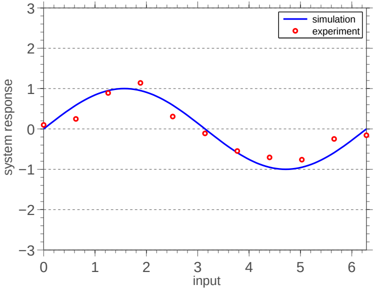
Why Uncertainty Quantification?

- 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

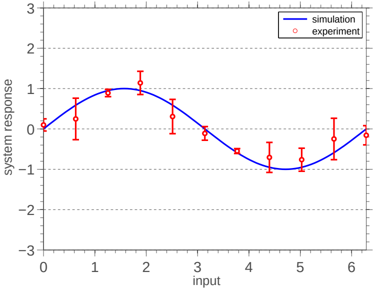
In a simplistic way UQ aims to:



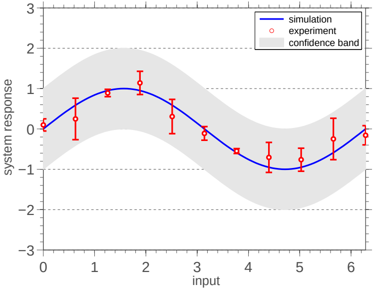
In a simplistic way UQ aims to:



In a simplistic way UQ aims to:

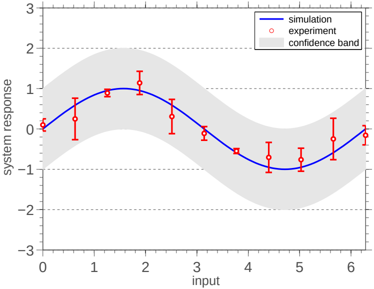


In a simplistic way UQ aims to:



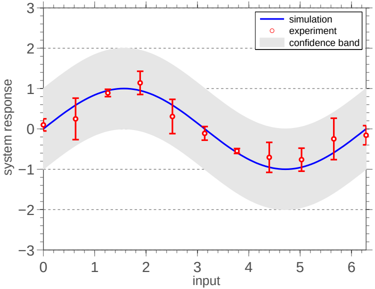
In a simplistic way UQ aims to:

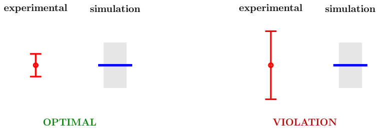
(i) add error bars to simulations



In a simplistic way UQ aims to:

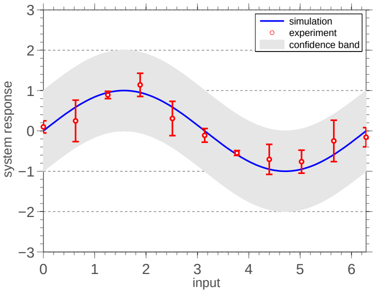
(i) add error bars to simulations



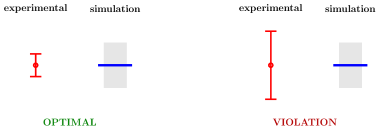


In a simplistic way UQ aims to:

(i) add error bars to simulations



(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)

G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*,

VKI Lecture Series, Stanford University, 2008

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)

Uncertainties: physical nature

G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*,

VKI Lecture Series, Stanford University, 2008

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)

Uncertainties: physical nature

Errors: mathematical nature

G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*, **VKI Lecture Series**, Stanford University, 2008

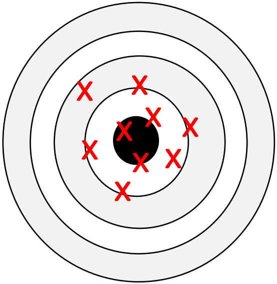
Aleatory Uncertainties (data uncertainties)

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



G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*, **VKI Lecture Series**, Stanford University, 2008

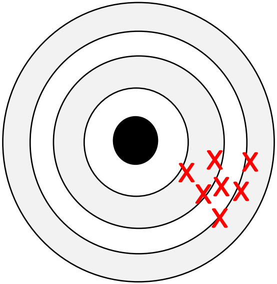
Epistemic Uncertainties (model uncertainties)

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



G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*, **VKI Lecture Series**, Stanford University, 2008

Verification and Validation (V&V)

- Verification
  Are we solving the equation *right*?

- Validation
  Are we solving the *right* equation?

G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*,
VKI Lecture Series, Stanford University, 2008

Verification and Validation (V&V)

- Verification
  Are we solving the equation *right*?
  It is an exercise in *mathematics*.

- Validation
  Are we solving the *right* equation?

G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*,

VKI Lecture Series, Stanford University, 2008

Verification and Validation (V&V)

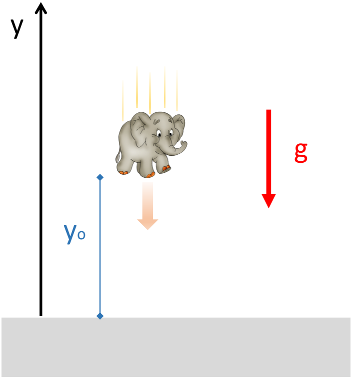
- Verification
  Are we solving the equation *right*?
  It is an exercise in *mathematics*.

- Validation
  Are we solving the *right* equation?
  It is an exercise in *physics*.

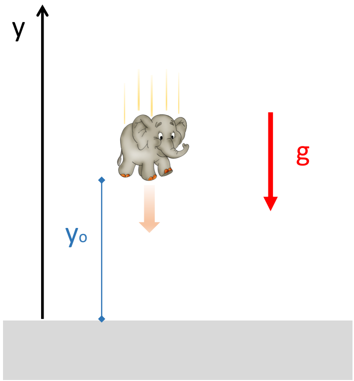
G. Iaccarino *Quantification of Uncertainty in Flow Simulations Using Probabilistic Methods*,

VKI Lecture Series, Stanford University, 2008

An example in V&V



An example in V&V



Mathematical model:

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

Verification of the equation solution

- Mathematical model

$$m\,\ddot{y}(t) = -m\,g$$

$+$ initial conditions

Verification of the equation solution

- Mathematical model

$$m\,\ddot{y}(t) = -m\,g$$

$$+ \text{ initial conditions}$$

- Numerical (Runge-Kutta)

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

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

Verification of the equation solution

- Mathematical model

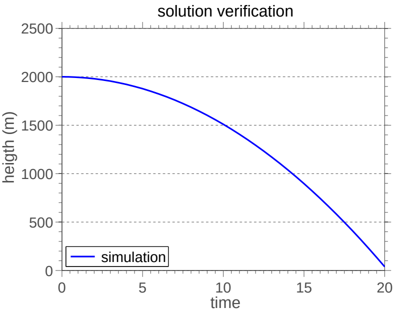
$$m\,\ddot{y}(t) = -m\,g$$

$$+ \text{ initial conditions}$$

- Numerical (Runge-Kutta)

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

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



Verification of the equation solution

- Mathematical model

$$m\,\ddot{y}(t) = -m\,g$$

$$+ \text{ initial conditions}$$

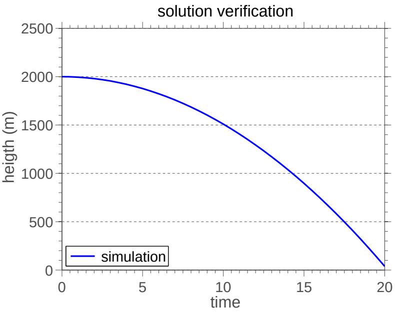
- Numerical (Runge-Kutta)

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

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

- Reference (analytical)

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



Verification of the equation solution

- Mathematical model

$$m\,\ddot{y}(t) = -m\,g$$

$$+ \text{ initial conditions}$$

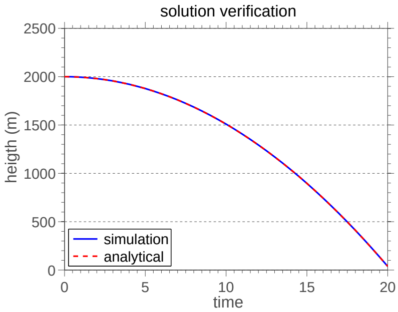
- Numerical (Runge-Kutta)

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

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

- Reference (analytical)

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



Verification of the equation solution

- Mathematical model

$$m\,\ddot{y}(t) = -m\,g$$

$$+ \text{ initial conditions}$$

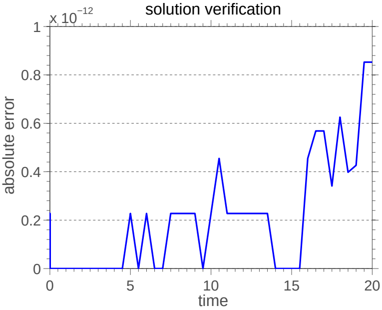
- Numerical (Runge-Kutta)

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

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

- Reference (analytical)

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



Verification of the equation solution

- Mathematical model

$$m\,\ddot{y}(t) = -m\,g$$

$$+ \text{ initial conditions}$$

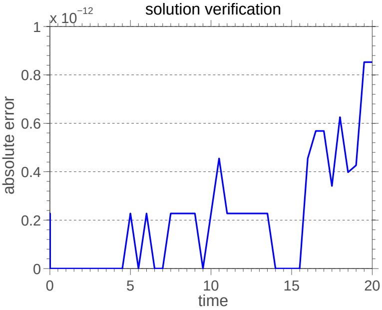
- Numerical (Runge-Kutta)

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

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

- Reference (analytical)

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

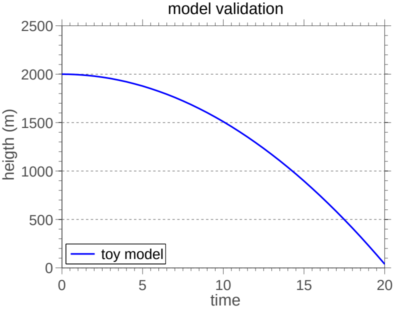


The model equation is well solved

Validation of the model

Toy model:

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



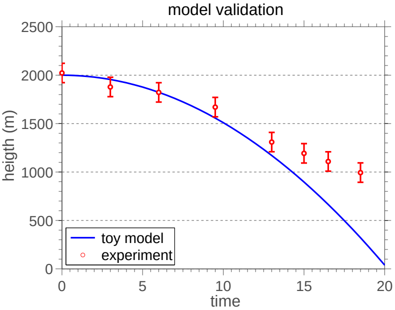
Validation of the model

Toy model:

$$m\,\ddot{y}(t) = -m\,g$$

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

$$y(0) = y_0$$



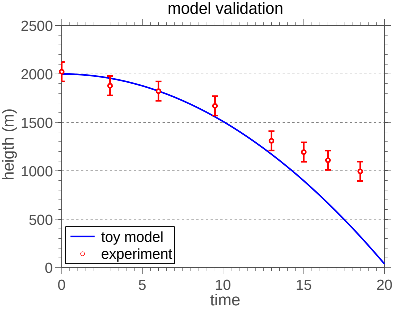
Validation of the model

Toy model:

$$m\,\ddot{y}(t) = -m\,g$$

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

$$y(0) = y_0$$



The mathematical model is not representative

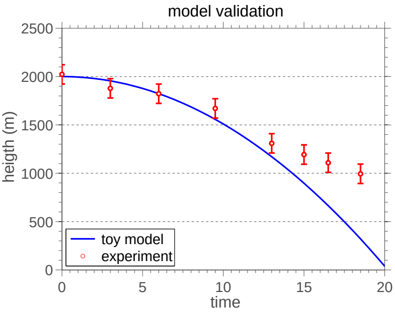
Validation of the model

Improved model:

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

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

$$y(0) = y_0$$



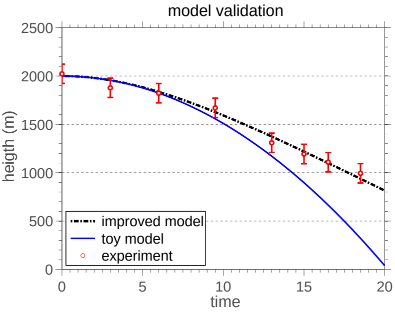
Validation of the model

Improved model:

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

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

$$y(0) = y_0$$



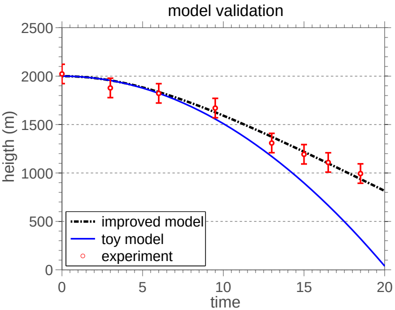
Validation of the model

Improved model:

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

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

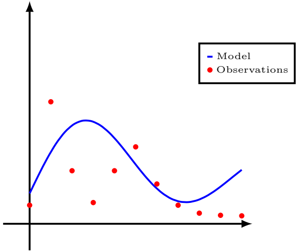
$$y(0) = y_0$$



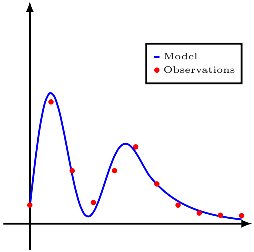
An improved model enhance the predictions

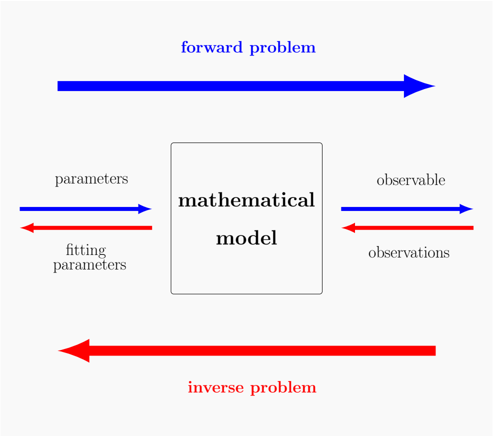
Calibration of the model

Uncalibrated Model



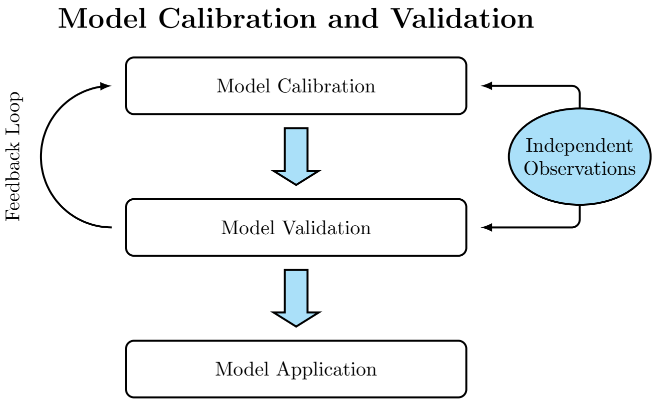
Calibrated Model





* Left pictures prepared by Michel Tosin.

Calibration vs Validation



* Picture prepared by Michel Tosin.

Sensitivity Analysis $\neq$ Uncertainty Quantification

- Sensitivity Analysis (SA)

  Goal: Identify which inputs most influence the outputs

  - May be based on derivatives (local SA)
  - May be based on variance decomposition (global SA)
  - Characterization of input variability is optional
  - **Important:** Large sensitivity $\not\Rightarrow$ large uncertainty

- Uncertainty Quantification (UQ)

  Goal: Quantify the impact of uncertain inputs on model outputs

  - Involves propagation of uncertainties through the model
  - Characterization of input uncertainty is mandatory (typically probabilistic)
  - Provides statistical descriptors for model response: mean, variance, confidence intervals, etc.

Surrogate model (a.k.a metamodel)

A **surrogate model** is a fast, approximate representation of a computationally expensive simulation model.

Why use surrogates in UQ?

- UQ requires many evaluations of the computational model
- High-fidelity models are often too costly
  (prohibitive for stochastic simulations)
- Surrogates allow fast propagation of uncertainty

Common surrogate techniques:

- Polynomial Chaos Expansion (PCE)
- Gaussian Process Regression (GPR) / Kriging
- Neural Networks (NN), especially physics-informed (PINNs)

Digital Twin

A **Digital Twin** is a live, virtual representation of a physical system that is continuously updated using real-time data and simulation.

Key Components:

- Physical asset + sensors
- Numerical model of the asset
- Data assimilation and feedback loop

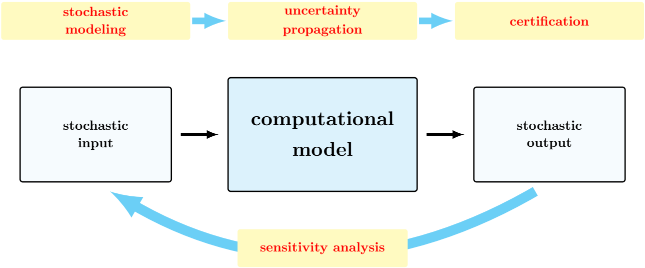
Why UQ in DT?

- Ensure reliable real-time predictions
- Quantify confidence in decision support
- Account for model bias, noise, and uncertainties

National Academies of Sciences, Engineering, and Medicine, *Foundational Research Gaps and Future Directions for Digital Twins*, 2023. https://doi.org/10.17226/26894.

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

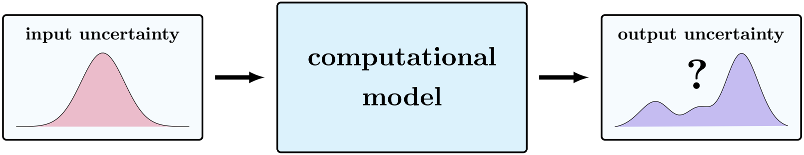
Uncertainty characterization must be based on available information

- experimental data
- theoretical arguments
- etc

Uncertainty Propagation

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

Find: **output uncertainty**

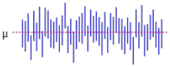


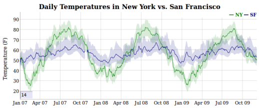
- The most complex and computationally intensive step
- Propagation technique depends on representation approach

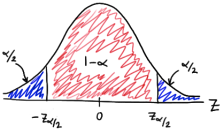
Certification

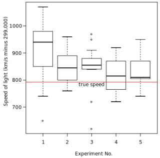
Specify levels of reliability for predictions:

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





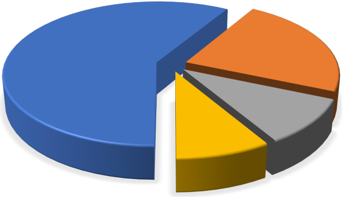




Sensitivity Analysis

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

References

A. Cunha Jr, *Modeling and quantification of physical systems uncertainties in a probabilistic framework*, In: S. Ekwaro-Osire; A. C. Gonçalves; F. M. Alemayehu (Org.), **Probabilistic Prognostics and Health Management of Energy Systems**, Springer International Publishing, p. 127-156, 2017. http://dx.doi.org/10.1007/978-3-319-55852-3_8

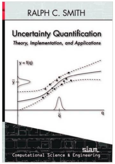
R. C. Smith, **Uncertainty Quantification: Theory, Implementation, and Applications**, SIAM, 2013.

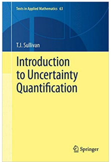
T. J. Sulivan, **Introduction to Uncertainty Quantification**, Springer International Publishing, 2015.

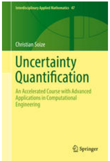
C. Soize, **Uncertainty Quantification: An Accelerated Course with Advanced Applications in Computational Engineering**, Springer International Publishing, 2017.

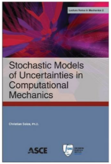
C. Soize **Stochastic Models of Uncertainties in Computational Mechanics**, Amer Society of Civil Engineers, 2012.

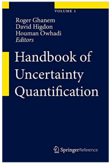
R. Ghanem, D. Higdon and H. Owhadi (Editors) **Handbook of Uncertainty Quantification**, Springer International Publishing, 2017.











How to cite this material?

A. Cunha Jr, *A Gentle Introduction to Uncertainty Quantification*, 2021.

@AmericoCunhaJr

@AmericoCunhaJr @AmericoCunhaJr

© copyrighted material

- NYC vs SF temperature:
  https://dygraphs.com
- $1-\alpha$ Gaussian:
  PennState STAT 415, https://online.stat.psu.edu/stat415/lesson/2/2.2