A crash course on

Uncertainty Quantification

UPPSALA UNIVERSITET

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THE UNIVERSITY of NEW MEXICO

Fall 2018

Course webpage: *http://math.unm.edu/~motamed/UQ2018/uq.html*

Prerequisites: Basic knowledge on

- Calculus
- Differential Equations (ODEs and PDEs)
- Probability
- Numerics & Programming (e.g. MATLAB)

Grading:

Homework 5 hp

Final Project 2.5 hp (??)

Homework (5 hp)

- In total 3-4 homework sets (HWs) will be assigned. You will need to do at least 3 HWs to receive full credit.
- Each HW may consist of a number of theoretical problems and computer assignments:
- You are **strongly** encouraged to **work in pairs** and hand in a **single report**.
- Groups of more than 2 students are not allowed.
- You need to hand in a hard copy of your reports in class on due date.
- Do not send your reports by email.
- If you are going to miss a deadline, talk to me in advance.

HW Reports

- First page of your report must be a **cover page**, which should look like this:

HW 1
UQ

Student's full name 1
Student's full name 2

DATE

- **Organize** your report according to the order of questions.
  (2nd page must start with question # 1 in HW and continue with questions #2, #3, ...)
- **No Appendix**! Do not put any appendix in your report.

Suggestions:

- The following strategy is recommended when writing answer to a question (if applicable):
  1- What: write briefly what the question is (what you are asked to do)
  2- How: write how you solve the question, and show your results (figures, tables, numbers, etc)
  3- Why: discuss your results
- Try to use an editing program/document processor (Microsoft Word, Latex, *etc.*).
  If you write by hand, make sure it is readable.

Final Project (2.5 hp)

- A final project MAY be assigned to you by the end of the course (October 25th).

- I may propose several topics and help you choose one that matches your interests and goals. You are also welcome to propose a project that is of your interest.

- In the end of the semester (by December 24th), you will need to send me a written report by email. You will have 2 months to do the project. I will be available to help as much as I can from distance.

- You are strongly encouraged to work on the projects in **groups of two** and hand in a **single report**.

Lectures (tentative)

1. Introduction to UQ
2. Probability theory + Karhunen-Loeve expansion
3. Stochastic ODEs/PDEs
4. Monte Carlo (MC) sampling with cost-error analysis
5. Multi-level MC sampling
6. Multi-order MC sampling
7. Orthogonal Polynomials + Stochastic collocation
8. Sparse computations + Stochastic Galerkin

Other potential topics:

* Bayesian inversion
* Markov chain Monte Carlo sampling
* Gibbs and Metropolis-Hastings sampling

Office hours:

Mondays 10.00 - 12.00 @ *place will be announced later*

If you cannot make it, you are welcome to email me and make an appointment.

Exceptionally on *Monday Sep. 10th* I will hold office hours @ Rum 2348

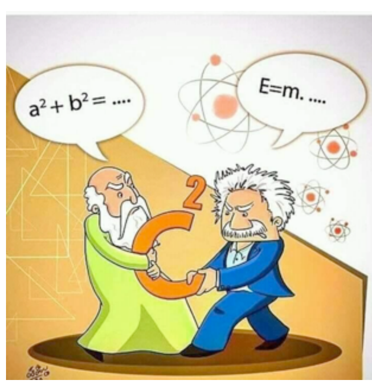
Email policy:

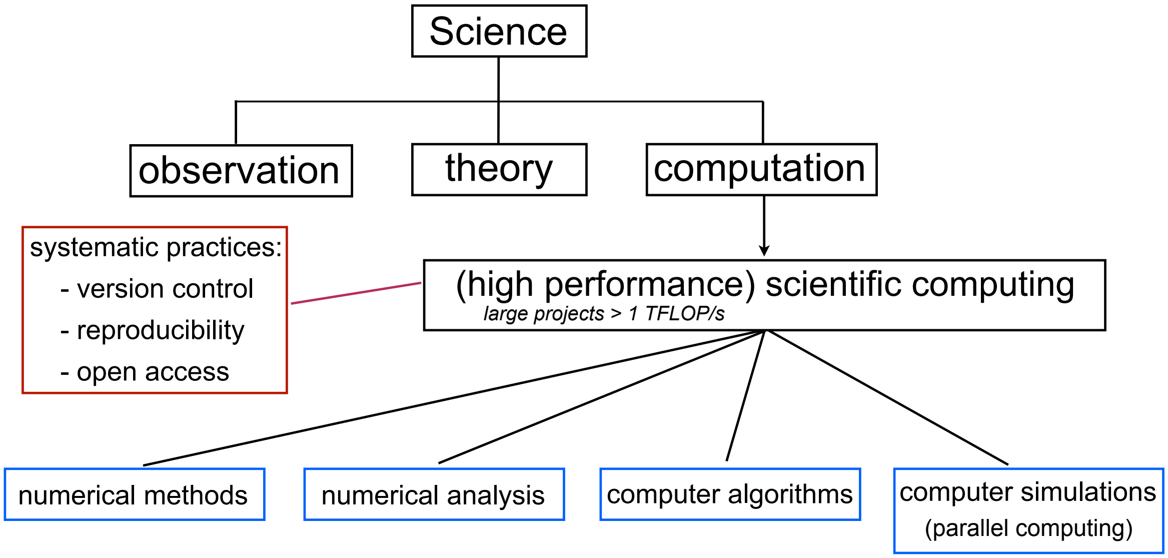
Please do not email me for scientific questions. I will not be able to answer your scientific questions through email.

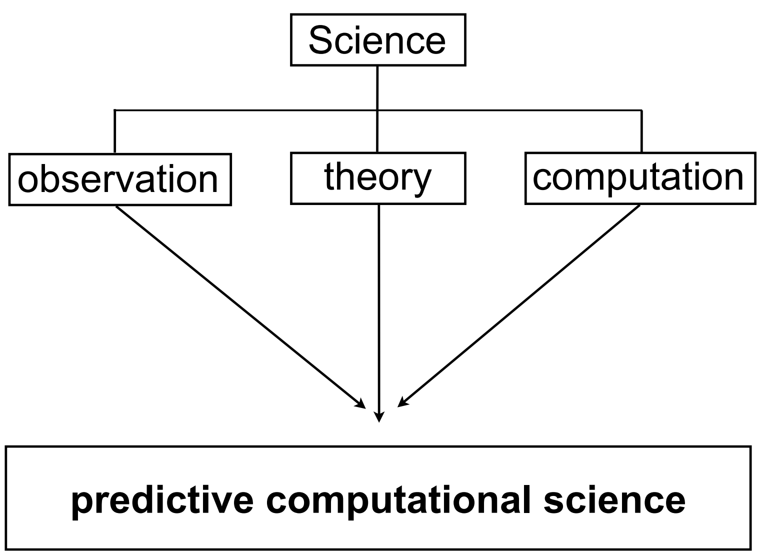
Email me only if you have a general, non-scientific question related to the course, e.g. to make an appointment with me, or to let me know that you will be missing a lecture, etc.

As the title of your email, please write **UQ** so that I easily distinguish it among many other emails that I receive.

Now let's talk science ...



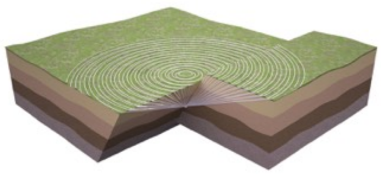




An emerging, interdisciplinary field concerned with assessing the *predictability* of mathematical and computational tools.

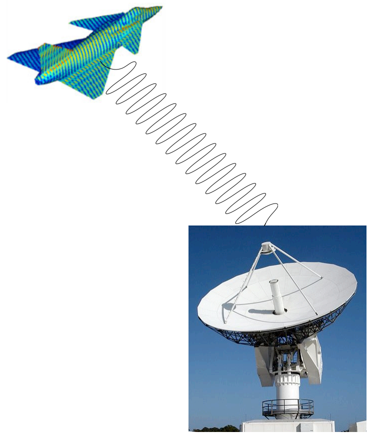
It is based on a *systematic incorporation* of all three pillars of the scientific method.

Some applications of Predictive Computational Science

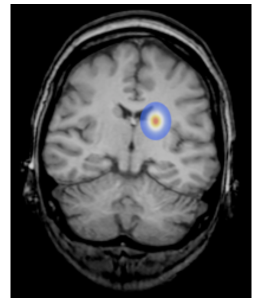


earthquake engineering

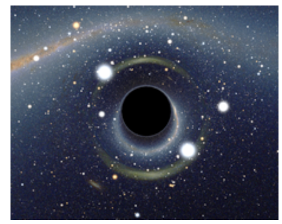
aerospace industry



radar technology



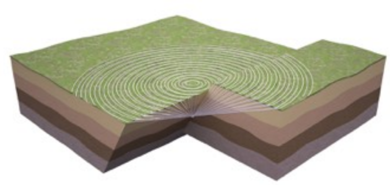
tumor growth



astronomy

Predictive Computational Science

- Goal: to model/solve/design systems in science & engineering fields
- ***Example***: Earth science / Earthquake engineering



Observation (experiments)
Theory (mathematics & physics)

Is the model well-posed?
(*existence* & *uniqueness*)

Mathematical Model (ODE's/PDE's)

Computational Science
- Numerical Methods
- Numerical Analysis
- Computer Algorithms
- Computer Simulation

Solution of Mathematical Model

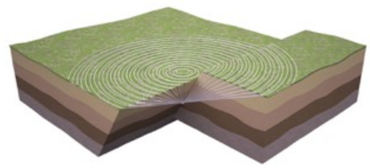
Use the solution:
- to design/build things
- to make decisions

Physical systems are often modeled by deterministic equations.

Input parameters (PDE coefficients & data) → Mathematical Model (*PDEs*) → Output quantities of interest

Θ $\qquad$ $\mathcal{M}$ $\qquad$ $\mathcal{Q}$

$$\mathcal{M}(\Theta) = \mathcal{Q}$$



$\mathcal{M}$: acoustic/elastic wave equ's + IC's + BC's

Θ : PDE coefficients (density & wave speed in each layer, location of layers)
Location of hypocenter (source term)

$\mathcal{Q}$: displacement, spectral acceleration, Arias intensity, energy, etc.

$$\mathcal{M}(\Theta) = \mathcal{Q} \quad \xrightarrow{\text{numerical simulation}} \quad \tilde{\mathcal{M}}(\Theta) = \tilde{\mathcal{Q}}$$

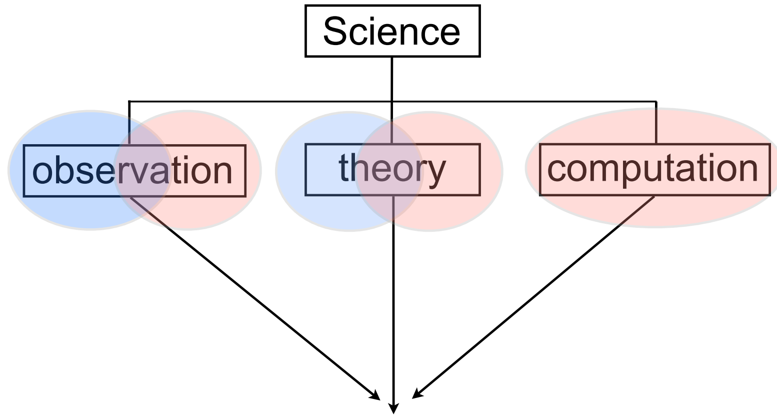
- Steps of numerical simulation task:

  1- specify input parameters
  2- discretize the PDE (select discretization approach & discretization parameters)
  3- visualize & post-process the computed solution to obtain QoIs

- ***Assumptions***:

  (i) for the input parameters fixed, the PDE has a unique solution
  (ii) the discrete model has a unique solution converging to the model solution
  (iii) sufficiently small discretization errors can be achieved

- ***Note:*** The above methodology reflects an idealized situation that may not be always achieved in practice. In many cases, the input parameters may not be completely specified or known.



predictive computational science

An emerging, interdisciplinary field concerned with assessing the *predictability* of mathematical and computational tools, particularly in the presence of inevitable **uncertainty** and **error**.

It is based on a *systematic incorporation* of all three pillars of the scientific method.

Uncertainty (absence of certainty)

Aleatory (or *random*)

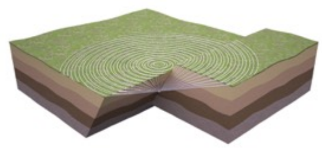
- Inherent variations and randomness in a system
  - earthquake hypocenters (location and intensity of the source)
  - variability between patients in biomedical applications

Epistemic (or *non-random*)

- Lack of information
  - limited experimental observations (scarce data)
  - limited information about the mathematical model (PDEs)
- Variability of observational data
  - data are extracted from different sources or standards/handbooks
  - material come from different manufacturers and hence have different qualities
- Conflicting beliefs/opinions
- Partial truth (or ambiguity)

Many real-world problems exhibit a mixture of aleatoric and epistemic uncertainties.

Example: Earthquake motion



$\mathcal{M}$: acoustic/elastic wave equ's + IC's + BC's

Θ : PDE coefficients (density & wave speed in each layer, location of layers)
Location of hypocenter (source term)

$\mathcal{Q}$: displacement, spectral acceleration, Arias intensity, energy, etc.

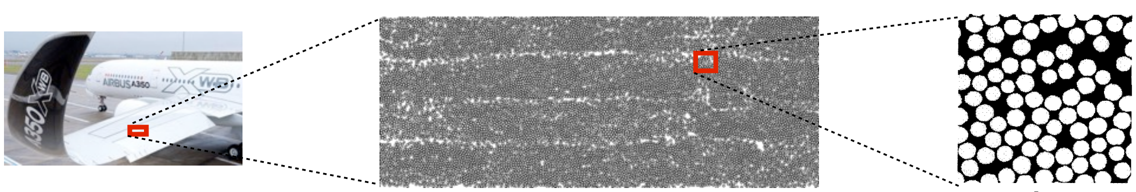
- **Question:** is the location of hypocenter deterministic or random?
  - It is random due to the nature of earthquakes (intrinsic variability in the system)

- **Question:** is the wave speed in each layer deterministic? YES!
  do we perfectly know the wave speed in layers or the position of layers? NO!
  - Speed is uncertain due to the lack of knowledge

◉ ***Note:*** Uncertainties may have different origins.

Many real-world problems exhibit a mixture of aleatoric and epistemic uncertainties.

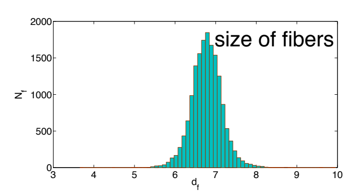
Example: *Materials with hierarchical microstructure*, e.g carbon fiber polymers

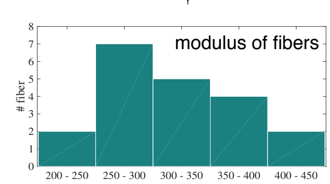


macro	meso	micro
composite plate (~1 m)	ply thickness (~10^{-3} m)	fiber diameter (~10^{-5} m)

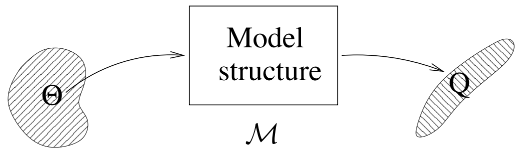
Sources of uncertainty:

- Randomness in size & spatial distribution of fibers (*aleatoric*)
- Variability in material properties, e.g. modulus of elasticity (*aleatoric*)
- Random noise in experimental devices (*aleatoric*)
- Scarcity in observational data (*epistemic*)
- Experimental and literature-based variations (*epistemic*)





- In many real applications, parameters in the model are affected by uncertainty, either because they are not perfectly known or because they are intrinsically variable.
- Input parameters Θ are uncertain.
- Need to include and treat uncertainty in the PDE model



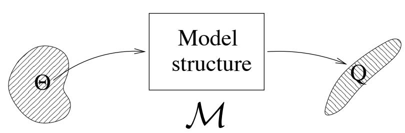
Instead of a single predicted value, we obtain information about the range of values that Q may have in light of uncertainty

- Need to include and treat uncertainty in the PDE model
- **Uncertainty Quantification** is a process that enables us to **identify** and **characterize** uncertainty in systems and **propagate** it through the model to obtain output predictions.

UQ in probabilistic framework

- Both types of uncertainty are often described in **probabilistic framework**.
- UQ major parts:

1. **Identification** (identify sources of uncertainty ---> input uncertain parameters)
2. **Characterization** (characterize input uncertainty by probability distributions)
3. **Propagation** (evolve input uncertainty through the model ---> distribution of outputs)



- **Forward UQ** (propagation of uncertainty):

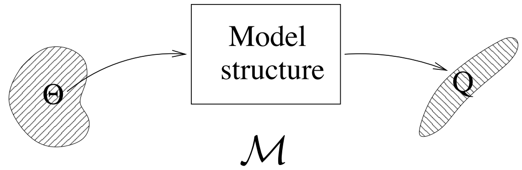
  given the probabilistic characterization of the input uncertain parameters,

  quantify the uncertainty in the output quantities of interest (QoI): $\mathcal{M}(\Theta) = \mathcal{Q}$

- **Inverse UQ** (characterization of uncertainty):

  use available measurements on observables of the system to characterize (or to improve the characterization of) uncertainty in input parameters: $\mathcal{M}^{-1}(\mathcal{Q}) = \Theta$

Forward UQ in a probabilistic framework:



(1) Identify uncertain input parameters $\Theta = \Theta(\omega)$

ω an element of a sample space with a given probability measure

(2) Characterize uncertainty in input parameters $\Theta(\omega) \approx \Theta(Y(\omega)) = \Theta(Y)$

$Y \in \mathbb{R}^N$ an N-dimensional random vector of independent variables

(3) Propagate uncertainty in input parameters through the model

$$\mathcal{Q}(Y) \approx \tilde{\mathcal{Q}}(Y) = \tilde{\mathcal{M}}(\Theta(Y))$$

- Monte Carlo Sampling (standard MC, Multi-Level MC, Multi-Order MC, ...)
- Spectral methods (Stoch. Galerkin, Stoch. Collocation, Stoch. least squares, ...)

Inverse UQ in probabilistic framework: $\mathcal{M}^{-1}(\mathcal{Q}) = \Theta$

Use Bayesian approach:

$$p(\Theta|\mathcal{Q}) \propto p(\mathcal{Q}|\Theta)\, p(\Theta)$$

posterior pdf $\propto$ likelihood $\times$ prior pdf

Problem types:

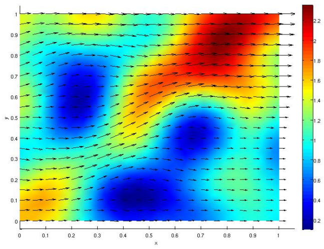
Bayesian inference (Bayesian inversion)

Bayesian experimental design

Methods:

- Markov Chain Monte Carlo method (MCMC)
  - ⋆ Gibbs sampling
  - ⋆ Metropolis-Hastings sampling

Example 1. Groundwater flow in random heterogeneous porous media



$$\left.\begin{aligned} \mathbf{u} &= -k(\mathbf{x})\,\nabla p \\ \nabla\cdot\mathbf{u} &= f \end{aligned}\right\} \quad \text{in} \quad D$$

$$+\,\text{BC's} \qquad \text{on} \quad \partial D$$

- The first equation is the Darcy's law: the pressure gradient ∇p and the fluid velocity $\mathbf{u}$ in a porous medium follow a linear relation.
- The second equation is the mass conservation relating sinks and sources of flow to the velocity field.
- In most aquifers, permeabilities $k(\mathbf{x}) > 0$ of the ground are not perfectly known.
- They can be described as a random field $k(\mathbf{x}, \omega)$:

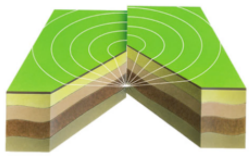
  The permeability $k(\mathbf{x}_i)$ at each point $\mathbf{x}_i \in D$ is a random variable. Taking N points $\{\mathbf{x}_i\}_{i=1}^N$ the random variables $\{k(\mathbf{x}_i)\}_{i=1}^N$ are in general correlated.
- The solution is also a random field: $\mathbf{u} = \mathbf{u}(\mathbf{x}, \omega)$

Main questions to be addressed by UQ:

1. How to characterize permeability by a random field?
2. How to guarantee positivity of the permeability random field?
3. How to numerically treat random fields?
4. How to solve the stochastic problem?

We will try to address (some of) these questions in this course ...

Example 2. Seismic waves in random layered media



$$\varrho(\mathbf{x})\,\mathbf{u}_{tt} - \nabla\cdot\boldsymbol{\sigma}(\mathbf{u}) = \mathbf{f} \quad \text{in} \quad (0,T]\times D$$

$$+\,\text{IC's} \quad \text{and} \quad \text{BC's}$$

$$\boldsymbol{\sigma}(\mathbf{u}) = \lambda(\mathbf{x})\,\nabla\cdot\mathbf{u}\,I + \mu(\mathbf{x})\,(\nabla\mathbf{u} + \nabla\mathbf{u}^\top)$$

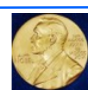
- Goal: to find the displacement of the medium $\mathbf{u}$ due to the propagation of elastic waves.
- Typically, the medium is made of N layers of different materials, whose mechanical properties $\{(\varrho_i, \lambda_i, \mu_i)\}_{i=1}^N$ are not perfectly known.
- Other parameters (position of internal interfaces, location of earthquake hypocenter) could also be uncertain.
- We therefore have a vector of at leas 3 N random variables Y.
- The solution also depends on the random vector: $\mathbf{u} = \mathbf{u}(t, \mathbf{x}, Y)$

Example 3. Option pricing with uncertain volatility

Black-Scholes model:

(Nobel prize in economics 1997)

$$\begin{cases} \dfrac{\partial f}{\partial t} + rs\dfrac{\partial f}{\partial s} + \dfrac{\sigma^2 s^2}{2}\dfrac{\partial^2 f}{\partial s^2} = rf, \quad 0 < t < T, \\ f(s,T) = \max(s-K, 0), \end{cases}$$

The Royal Swedish Academy of Sciences: 

Robert C. Merton and **Myron S. Scholes** have, in collaboration with the late **Fischer Black**, developed a pioneering formula for the valuation of stock options.

- The value of an option (a financial contract): $f : (0,T)\times(0,\infty) \to \mathbb{R}$
- The price of the stock: $s \in (0,\infty)$
- Interest rate: r
- The volatility σ (a measure for variation of price of the stock) is often uncertain. It corresponds to the standard deviation of stock's price process (in time).

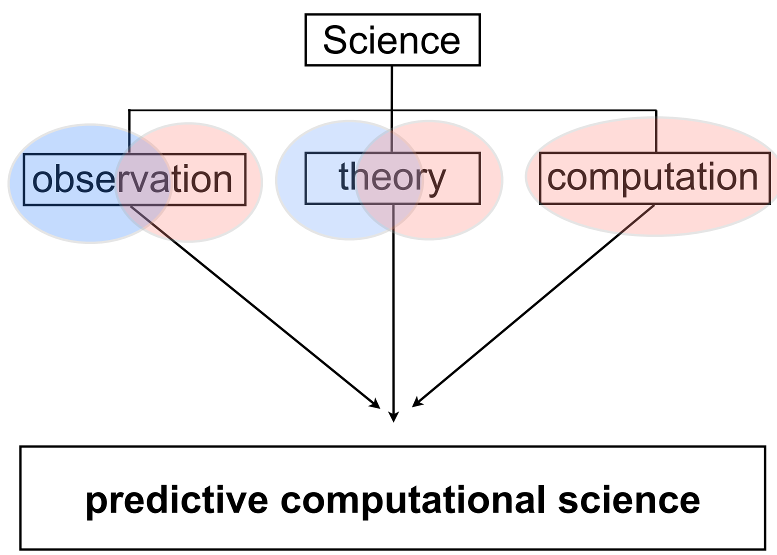
Goal: Quantify the impact of volatility uncertainty on option pricing.

UQ is not the whole story!

There are still many **Grand challenges** facing humankind:

- prediction of **climate** change
- the effects of various **medical therapies**
- performance of **energy** systems (energy development)
- prediction of **economic crises**
- dynamic response of modern/smart **materials**

UQ is not enough to deal with such challenges.

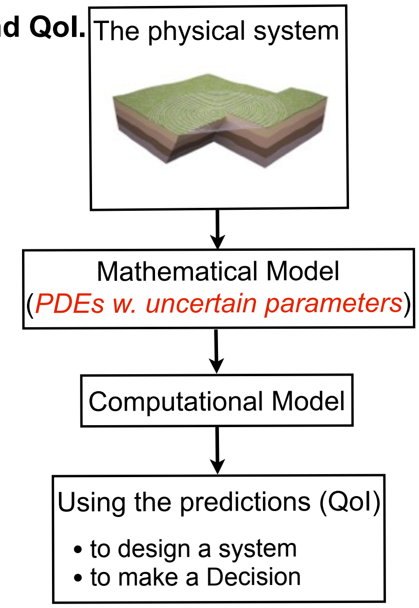


Both **uncertainty** and **error** are present.

Need a **systematic incorporation** of all three pillars of the scientific method.

Need UQ + Validation + Verification (UQVV) in a systematic way.

Suppose we include uncertainty and employ UQ to find QoI.



A main question:

- How reliable are the computational predictions (QoI)? Can they be trusted for decision-making or designing a crucial system?

Errors typically arise from:

- the choice of the PDE model (***Model error***)
- the discretization schemes (***Numerical error***)

In addition to **UQ**, we need two related processes:

- **Validation**: are we solving the correct model?
- **Verification**: are we solving the model correctly?

◉ To account for both **uncertainties** and **errors**, we need to rely on both **UQ** and **VV**.

Verification:

The goal of verification is to estimate and control the error in each QoI.

◉ Solution verification is defined only in terms of specified QoI. Different QoI will be affected differently by numerical errors.

- use a posteriori error estimates (numerical error estimates for specified QoI)
- perform self-convergence studies (QoIs are computed at different levels of refinement)

◉ Code verification: exploit the hierarchical composition of codes and mathematical models, with verification performed first on the lowest-level building blocks and then on successively more complex levels.

Validation:

Validation is defined only in terms of specified QoI. Different QoI will be affected differently by errors.

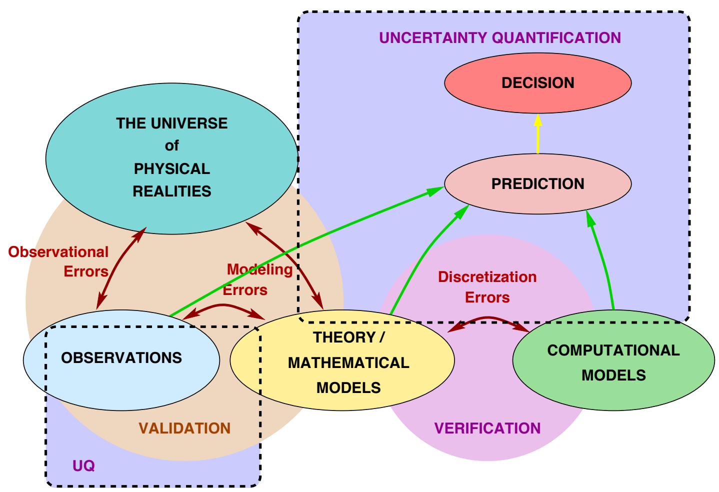
A validation assessment provides information about model accuracy only in the domain of physical observations (experimental/measured data).

Experimental data must be acquired and **integrated** into computer codes. They are used for two main purposes:

- to identify and characterize values of unknown model parameters (calibration)
- to determine whether the model can correctly predict the QoI (validation)

◉ **Note:** Measured data are often scarce and uncertain. This must be taken into account.

A conceptual diagram for UQVV:



- A systematic UQVV approach to science would bring not only confidence in the decisions one needs to make about physical systems but also deeper knowledge about our physical world.
- UQVV processes have been recently the subject of considerable research activities in CSE
- Predictive modeling of physical phenomena based on UQVV is a truly challenging problem.

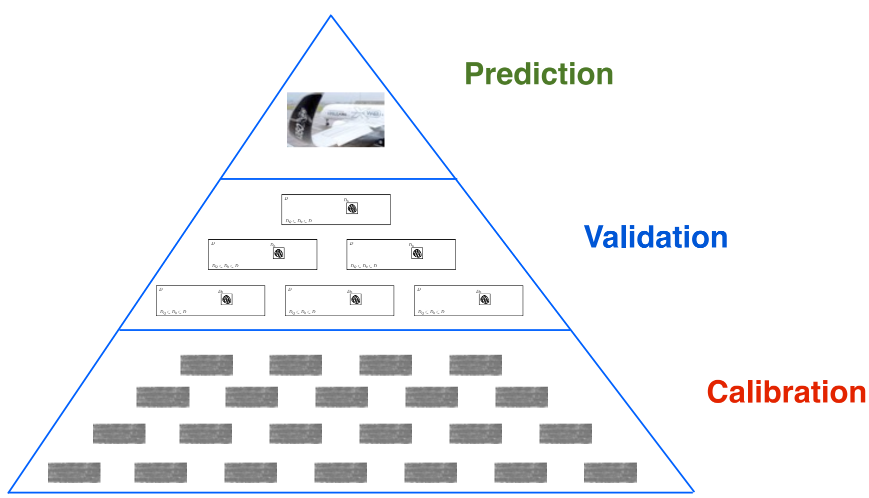
UQVV principals

✓ UQVV processes must focus on a set of specified QoIs rather than on the full solution of the model.

✓ UQVV tasks are interrelated.

✓ Verification should come before Validation.

Calibration-Validation-Prediction pyramid/hierarchy



- *Calibration* involves the characterization (and reduction) of uncertainty in the model parameters.
- *Validation* determines if the model is capable of predicting the QoI with sufficient accuracy.
- *Ultimate prediction* uses the valid model to predict the target QoI.

Finally, is a probabilistic framework enough?

1. Can we represent epistemic uncertainty (lack of knowledge) by a precise probability distribution (with known moments)?

Maybe not! We may need other frameworks: intervals, fuzzy sets, evidence theory

2. There is often no clear-cut distinction between aleatoric and epistemic uncertainty in real-world problems. There may be a random quantity whose parameters are partially known, or there may be an epistemically uncertain quantity for which some values are more likely to occur than others. Consequently, it may not be possible to simply model aleatoric uncertainty by probability distributions and epistemic one by intervals or fuzzy sets.

We may need hybrid frameworks obtained by the synthesis of two models rather than simply adding them: interval probability, fuzzy probability

A simple intuitive example

Consider rolling a die

Let us see the difference between

- *precise probability*
- *imprecise probability*

36

Precise probability

Random event: E = *rolling a six on a fair die*

Probability: P(E) = 1/6 ~ 16.67%

Interpretation: we are willing to place 16.67 cents as the fair price for a bet that returns $1 if we get a six, and nothing if we do not get a six.

37

Imprecise probability

Random event: E = *rolling a six on an unfair die*

Probability: P(E) = ? we do not know how unfair the die is (*lack of knowledge*)

We ask a few (say 10) experts with possibly different opinions:

P1(E) = 10%, P2(E) = 12%, P3(E) = 15%, …. P10(E) = 20%

We have no information on how each expert obtained his/her value (*lack of knowledge*)

For ex. each expert may run several (many or a few) experiments and use a different approach (Bayesian, classic, etc.)

Probability: P(E) $\in$ [10%, 20%] is given by an interval (taking min and max)
The true probability will lie in the interval

Interpretation: we are willing to bet $1 and get something between $5-$10 if we get a six, and nothing if we do not get a six.

38

A few good books