Uncertainty Quantification in Physical and Biological Applications

Lecture 1

Mitchel J. Colebank

MATH 728 - Spring 2025
University of South Carolina
Department of Mathematics

January 2025

Uncertainty Quantification

What is *uncertainty quantification* (UQ) ?

Uncertainty Quantification

What is *uncertainty quantification* (UQ) ?

- "... the science of quantitative characterization and estimation of uncertainties in both computational and real world applications. It tries to determine how likely certain outcomes are if some aspects of the system are not exactly known." [1]

Uncertainty Quantification

What is *uncertainty quantification* (UQ) ?

- "... the science of quantitative characterization and estimation of uncertainties in both computational and real world applications. It tries to determine how likely certain outcomes are if some aspects of the system are not exactly known." [1]

A more digestible definition (from NIST) :

- "... measurement uncertainty expresses incomplete knowledge about the measurand, and that a probability distribution over the set of possible values for the measurand is used to represent the corresponding state of knowledge about it." [2]

Motivating examples : Weather Prediction

$$\frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}$$

Conservation Relations:

Mass $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

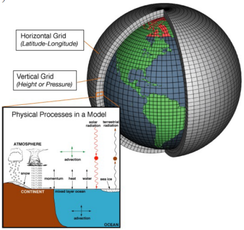
Momentum $$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

Energy $$\rho c_V \frac{\partial T}{\partial t} + p\nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k\nabla T) + \rho \dot{q}(T, p, \rho)$$

$$p = \rho R T$$

Water $$\frac{\partial m_j}{\partial t} = -v \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho) \ , \ j = 1, 2, 3,$$

Aerosol $$\frac{\partial \chi_j}{\partial t} = -v \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho) \ , \ j = 1, \cdots, J,$$



Constitutive Closure Relations: e.g.,

$$S_{m_2} = S_1 + S_2 + S_3 - S_4$$

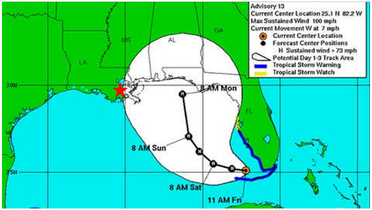
where

$$S_1 = \bar{\rho}(m_2 - m_2^*)^2 \left[1.2 \times 10^{-4} + \left(1.569 \times 10^{-12} \frac{n_r}{d_0(m_2 - m_2^*)} \right) \right]^{-1}$$

[3]

Motivating examples : Weather Prediction

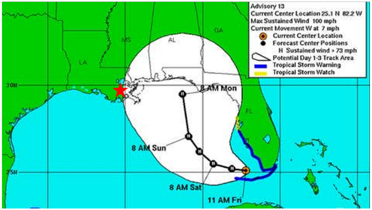
Hurricane Katrina – **11 AM**, August 26th, 2005



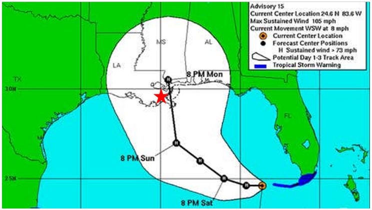
UNIVERSITY OF South Carolina

Motivating examples : Weather Prediction

Hurricane Katrina – **11 AM**, August 26th, 2005

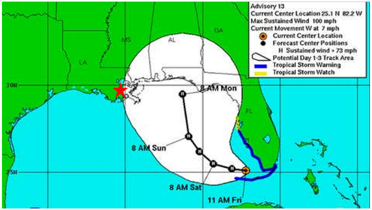


Hurricane Katrina – **11 PM**, August 26th, 2005

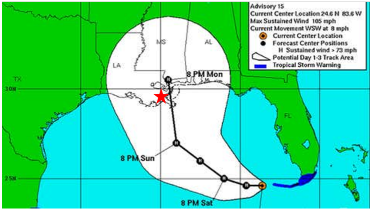


Motivating examples : Weather Prediction

Hurricane Katrina – **11 AM**, August 26th, 2005



Hurricane Katrina – **11 PM**, August 26th, 2005



Uncertainty quantification helps implement simulation models and handle decision making

Motivating examples : 3D Fluid Dynamics

The Navier-Stokes equations for a viscid, incompressible flow in cartesian coordinates :

$$\frac{\partial \mathrm{u}}{\partial t} + (\mathrm{u} \cdot \nabla)\mathrm{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathrm{u} + \mathrm{f} \quad (1)$$

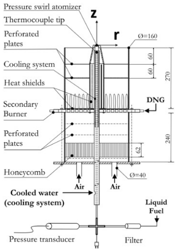
$$\nabla \cdot \mathrm{u} = 0 \quad (2)$$

where :

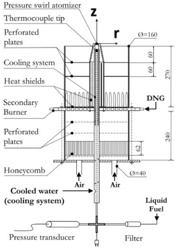
- u is the velocity vector field of the fluid,
- t is time,
- ρ is the fluid density,
- p is the pressure,
- ν is the kinematic viscosity,
- f represents body forces (e.g., gravity),
- $\nabla \cdot \mathrm{u} = 0$ ensures the incompressibility of the fluid.

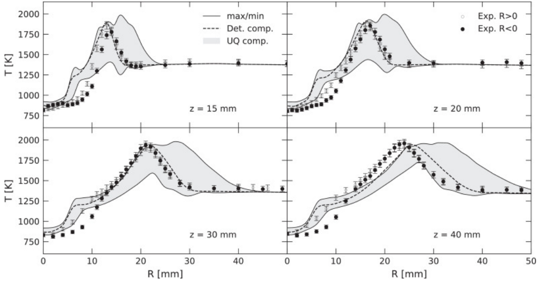
UNIVERSITY OF South Carolina

Motivating examples : Fluid dynamics



Motivating examples : Fluid dynamics





From [4]

Motivating examples : Disease spread

A common, simple ODE model for explaining disease spread is the **suceptible, infected, and recovered (SIR) model** :

Motivating examples : Disease spread

A common, simple ODE model for explaining disease spread is the **suceptible, infected, and recovered (SIR) model** :

$$\frac{dS}{dt} = \mu N - \mu S - \eta k I S \tag{3}$$

$$\frac{dI}{dt} = \eta k I S - (\gamma + \mu) I \tag{4}$$

$$\frac{dR}{dt} = \gamma I - \mu R. \tag{5}$$

Motivating examples : Disease spread

A common, simple ODE model for explaining disease spread is the **suceptible, infected, and recovered (SIR) model** :

$$\frac{dS}{dt} = \mu N - \mu S - \eta k I S \tag{3}$$

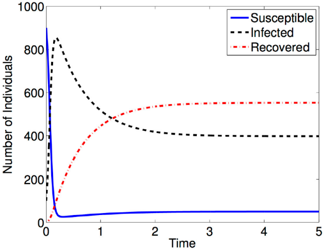
$$\frac{dI}{dt} = \eta k I S - (\gamma + \mu) I \tag{4}$$

$$\frac{dR}{dt} = \gamma I - \mu R. \tag{5}$$

Here, $S(0), I(0)$, and $R(0)$ are the (uncertain) initial conditions, and $\boldsymbol{\theta} = \{\mu, \eta, k, \gamma\}$ are the (uncertain) *model parameters*.

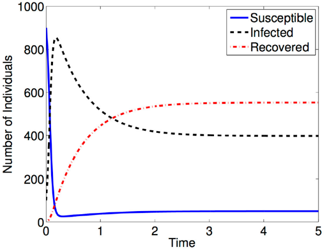
UNIVERSITY OF South Carolina

Motivating examples : Disease spread

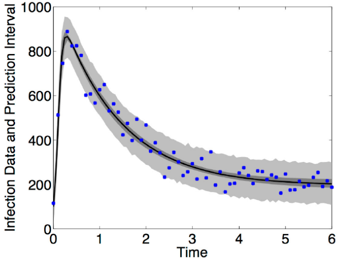


Typical Output

Motivating examples : Disease spread



Typical Output



Uncertain infected predictions

Motivating example : Blood flow models

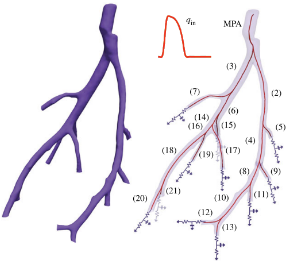
A common, reduced order blood flow model is given by the single spatial (or "one-dimensional) fluid flow equations :

$$\frac{\partial A}{\partial t} + \frac{\partial q}{\partial x} = 0, \tag{6}$$

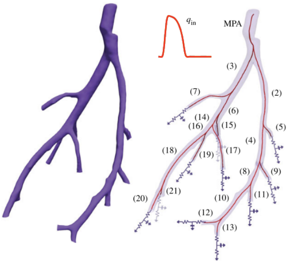
$$\frac{\partial q}{\partial t} + \Gamma \frac{\partial}{\partial x}\left(\frac{q^2}{A}\right) + \frac{A}{\rho}\frac{\partial p}{\partial x} = \mathcal{F}\left(\frac{q}{A}\right), \tag{7}$$

UNIVERSITY OF South Carolina

Motivating example : Blood flow models

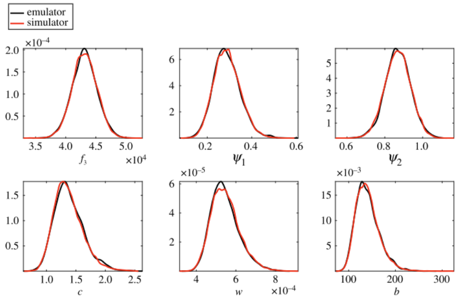


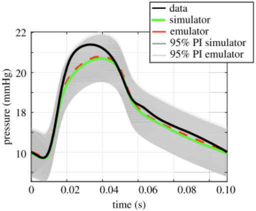
Motivating example : Blood flow models



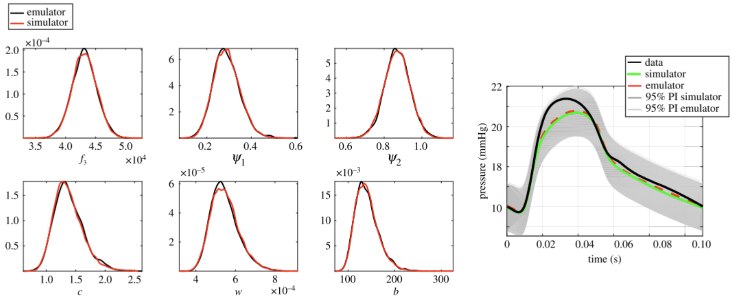
If we solve reduced order PDEs in an uncertain domain, with uncertain parameters, how can we establish credibility in our model outputs ?

Motivating example : Blood flow models





Motivating example : Blood flow models



Calibrate, validate, and perform uncertainty quantification. [5]

UNIVERSITY OF South Carolina

Some definitions

- **Mechanistic models** : Mathematical equation(s) that embed underlying hypotheses about the processes of a system
- **Statistical models** : Relationships between observables that are rooted in underlying frequentist and/or Bayesian statistics
- **Data-driven models** : computational methods that seek to group, relate, or transform observable data for a specific task or objective

Some definitions

- **Model Parameters :** Unknowns in the model that can determined from data (literature or actual data instances)
  - Notes : parameters can be fixed in models, but are distinguished from constants
- **Observation/Data :** Any measurable output of a given system
- **Constants :** Any variable that can be scientifically assumed to be constant in value (e.g., gravitational acceleration on earth)
- **Model Response :** The output or response of a model system (e.g., a vector field or ODE state variable)
- **Quantity of Interest :** The model response that will be analyzed or used in decision making

UNIVERSITY OF
South Carolina

Know the difference

There are three, commonly confused terms in computational science and engineering :

- **Calibration :** The process of updating a model such that the parameters (or inputs) of the model explain or match given observations
- **Verification :** Quantifying the accuracy of computer simulation codes in representing mathematical equations
- **Validation :** Determining the accuracy of a model in its ability to replicate an underlying system
  - Note : validation requires the use of generaltized behavior or data **not used for calibration**

UNIVERSITY OF South Carolina

References

https://en.wikipedia.org/wiki/Uncertainty_quantification

https://www.nist.gov/itl/sed/topic-areas/measurement-uncertainty

Ralph Smith
Uncertainty Quantification : Theory, Implementation, and Applications (Second Edition)
Society for Industrial and Applied Mathematics

Enderle, Benedict, et al.
"Non-intrusive uncertainty quantification in the simulation of turbulent spray combustion using polynomial chaos expansion : A case study."
Combustion and Flame 213 (2020) : 26-38.

Paun, L. Mihaela, et al.
"Assessing model mismatch and model selection in a Bayesian uncertainty quantification analysis of a fluid-dynamics model of pulmonary blood circulation."
Journal of the Royal Society Interface 17.173 (2020) : 20200886.

UNIVERSITY OF South Carolina