Validation and Uncertainty Quantification in Computational Models
CSCI 7000-008
Spring 2025

Instructor:
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Class details:
Class meetings: T-Th 12:30 - 1:45, KITT Central S161
Office hours: W 1:30 - 2:30 and by appointment

Materials:
Lecture notes (R. Morrison and R. Moser)
Various papers and book chapters, all available on Canvas

Course description

This is a course on assessing the reliability of computational models. Computational models are used to describe physical and engineering systems in nearly every aspect of our lives, from the way an airplane wing interacts with turbulent air to how the human heart pumps blood. We consider the (common) setting in which the system of interest is described by a mathematical model, which in turn is implemented and solved by the computational model. There are three major reasons model results might not be reliable: (1) The mathematical model may not be a good representation of the system of interest; (2) The inputs to the mathematical model (e.g., parameters, initial and boundary conditions) may be uncertain; and (3) The computation may yield results that are not consistent with the solution of the mathematical model. The first two are assessed through validation and uncertainty quantification, respectively. The third is the domain of verification and, while important, it is not considered here. In this course, we will learn to formulate and analyze representations of uncertainty and validation tests for computational models.

Course objectives

In this course, students will learn how to:

- Analyze mathematical models and identify potential sources of uncertainty
- Use and interpret probabilistic representations of uncertainty
- Apply Bayes' theorem in various settings
- Express incomplete information using the principle of maximum entropy
- Characterize the uncertainties in observational data
- Formulate representations of model inadequacy
- Perform model calibration and model selection using Bayesian inference

- Formulate and apply probabilistic validation criteria
- Assess the reliability of extrapolative predictions
- Communicate, via scientific writing, the (sometimes complex or nuanced) concepts we have reviewed in class

Course work and grading

To review and solidify the basic concepts of the course, students will solve a series of exercises as homework. There will also be some small "projects" to apply the concepts of the course to example problems, to be done in small groups. We will conclude the semester with final projects, in which students will apply the course concepts to an example of their choice. Selecting an area that is relevant to the student's research is encouraged.

Grades will be determined based on the following: homework (25%), group projects (25%), and final project (50%).