

**AOE/CS/ME 6444: Verification and Validation in Scientific Computing
Spring 2014, Time and Location TBD**

Course Description: Models found in the computational sciences and engineering (continuum mechanics, thermal analysis, nonlinear dynamics, etc.) are usually described by partial differential or integral equations. Verification, validation, and uncertainty quantification provide a formal framework for assessing the predictive capability of numerical simulations of these scientific computing models. Verification addresses the accuracy of the numerical approximations required to solve complicated models. Validation addresses the ability of the model itself to predict the state of a system. Uncertainty quantification deals with the propagation of uncertainty through the simulations. Engineers, scientists, program managers, and policy makers increasingly rely on scientific computing for decision making. This course addresses the fundamental question of: “How accurate is the simulation prediction?”

Prerequisites: The student must have experience with the numerical solution to differential equations (e.g., finite difference, finite volume, finite element methods) in their chosen area of study.

Textbook: W. L. Oberkampf and C. J. Roy, *Verification and Validation in Scientific Computing*, Cambridge University Press, Cambridge, 2010.

References: P. J. Roache, *Fundamentals of Verification and Validation*, Hermosa Publishers, New Mexico, 2009.
P. Knupp, K. Salari, in: K.H. Rosen (Ed.), *Verification of Computer Codes in Computational Science and Engineering*, Chapman and Hall/CRC, Boca Raton, FL, 2003

Instructor: Dr. Chris Roy, Associate Professor, Aerospace and Ocean Eng. Dept.

Goals: The broad goals of this course are to 1) explain the modern terminology used in assessing the reliability of scientific computing, 2) discuss the many possible sources of error and uncertainty, and 3) to provide a framework for quantifying these errors and uncertainties for use in establishing the total predictive capability of a simulation.

Topics and approximate class time (~14 weeks total):

1. Fundamental concepts and terminology (1 week)
2. Elements of scientific computing (1 week)
3. Software engineering, code verification, and exact solutions (2 weeks)
4. Elements of solution verification (1 week)
5. Discretization error (2 weeks)
6. Model validation fundamentals (1 week)
7. Design and execution of validation experiments (1 week)
8. Quantitative assessment of model accuracy (2 weeks)
9. Predictive capability (3 weeks)

Draft Syllabus

Grading:	Homework	20%
	Project	40%
	Midterm Exam	20%
	<u>Final Exam</u>	<u>20%</u>
	Total	100%

Office Hours: I prefer that you come in during office hours; however, if my office door is open then I am usually free to answer questions.

Dr. Chris Roy, Rm. 330 Randolph Hall, (540) 231-0080, cjroy@vt.edu
Office Hours: TBD

TA: TBD

Project: While a number of small programming assignments will be given as part of the homework, a project will also be assigned during the semester. This is an individual project which will be graded in the following phases: 1) programming and code verification, 2) solution verification, 3) model validation, and 4) uncertainty quantification. The choice of programming language is left up to you; however, the instructor will be able to help with programming language syntax mainly for Fortran. Other recommended programming languages are C/C⁺⁺ and MATLAB. Note that MATLAB will likely run slower than both Fortran and C/C⁺⁺.

Test/Exam Policy: All tests and exams will be open notes and open book.

Class Web Page: via Scholar (<https://scholar.vt.edu>)

Attendance Policy: You are expected to attend all class lectures. However, I plan to make recorded versions of the lectures available via Centra.

Special Needs: Students who need accommodations are asked to arrange a meeting with me during office hours the first week of classes, or as soon as possible if accommodations are needed immediately. If you have a conflict with my office hours, an alternate time can be arranged. To set up this meeting, please contact me by Email.