

ISC 5314 **Verification and Validation in Computational Science**

Computer simulation is of critical importance in several engineering and basic science applications. Frequently it is the only way to study complex physics phenomena, design new or improve the existing engineering systems. Verification and validation is a centerpiece of modern computer code development environment and of critical importance for creating successful simulation tools.

This course addresses the needs of students with interest in scientific computation, development, maintenance and application of computer codes to both basic physics and real world problems. The course covers both theory and practice of verification and validation in computational sciences. Students will learn basic terminology, procedures and practical methods used in software implementation verification and solution verification, use of exact and manufactured solutions, and elements of software quality assurance. Essential data analysis techniques will be introduced and a review of software development and maintenance tools will be given.

Examples from physical sciences and engineering will be used to illustrate aspects of code validation including validation hierarchy, validation benchmarks, and uncertainty quantification and simulation code predictive capabilities. Computational laboratory will be an essential part of the course.

Credit

3 semester hours

Prerequisites

MAC 2312, or the permission of the instructor; basic programming skills in Fortran, C, and/or C++.

Course Objectives

At the end of the course, the student will be able to

- conduct reliable scientific computations,
- use effective methods in code development and maintenance,
- design large scale physics simulation,
- conduct scientific problem analysis and identify its critical elements,
- estimate errors of the computer model and offer strategies for improving it,
- visualize and present simulation results in form suitable for publication in scientific literature.

Course Topics

- elements of modern science: observation and experiments, theory, computations;
- the role of scientific computations in engineering and basic physics applications;
- accuracy verification of computer codes;
- error estimation and error control in computer modeling;
- code validation in engineering and basic physics applications;
- sensitivity analysis;
- code certification;
- software quality engineering.

Contact Information

Instructor: Tomasz Plewa
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Office phone: 850.644.1959
E-mail: tplewa@fsu.edu
Office hours: by appointment.

Teaching Assistant: none
E-mail:
Office hours:

Homework Submission

Each homework assignment or project must be submitted as a single pdf document describing the solution process and presenting results with relevant code sources, input files, graphs, and images via email to the Instructor (tplewa@fsu.edu).

Grading

The course grade will be based on 3 tests (30% contribution toward the grade), homework assignments (20%), and computer lab-type projects (50%). No mid-term or final exams will be given.

Late homework submissions will be subject of 10% points reduction per day, with the maximum of 50% points reduction.

The scale for the grades will be: A (90-100%), A- (87-89%), B+ (83-86%), B (77-82%), B- (73-76%), C+ (69-72%), C (63-68%), C- (59-62%), D+ (55-58%), D (50-54%), and F (<50%).

Textbooks

- online lecture and computational laboratory materials
- required: [W. L. Oberkamp & C. J. Roy, *Verification and Validation in Scientific Computing* \(CUP\) ISBN-10: 0521113601](#)
- optional: [Knupp, P., & Salari, K., *Verification of Computer Codes in Computational Science and Engineering* \(Chapman & Hall/CRC: Boca Raton\) ISBN-10: 1584882646](#)

Website

<https://canvas.fsu.edu/courses/225248>

http://people.sc.fsu.edu/~tplewa/Teaching/ISC_5314/index.html

University Attendance Policy

Excused absences include documented illness, deaths in the family and other documented crises, call to active military duty or jury duty, religious holy days, and official University activities. These absences will be accommodated in a way that does not arbitrarily penalize students who have a valid excuse. Consideration will also be given to students whose dependent children experience serious illness.

Academic Honor Policy

The Florida State University Academic Honor Policy outlines the University's expectations for the integrity of students' academic work, the procedures for resolving alleged violations of those expectations, and the rights and responsibilities of students and faculty members throughout the process. Students are responsible for reading the Academic Honor Policy and for living up to their pledge to ". . . be honest and truthful and . . . [to] strive for personal and institutional integrity at Florida State University." (Florida State University Academic Honor Policy, found at <http://fda.fsu.edu/Academics/Academic-Honor-Policy>.)

Americans with Disabilities Act

Students with disabilities needing academic accommodation should: (1) register with and provide documentation to the Student Disability Resource Center; and (2) bring a letter to the instructor indicating the need for accommodation and what type. This should be done during the first week of class.

Please note that instructors are not allowed to provide classroom accommodation to a student until appropriate verification from the Student Disability Resource Center has been provided.

This syllabus and other class materials are available in alternative format upon request.

For more information about services available to FSU students with disabilities, contact the:

Student Disability Resource Center
874 Traditions Way
108 Student Services Building
Florida State University
Tallahassee, FL 32306-4167
(850) 644-9566 (voice)
(850) 644-8504 (TDD)
<mailto:sdrc@admin.fsu.edu>
<http://www.disabilitycenter.fsu.edu/>

Free Tutoring from FSU

On-campus tutoring and writing assistance is available for many courses at Florida State University. For more information, visit the Academic Center for Excellence (ACE) Tutoring Services' comprehensive list of on-campus tutoring options - see <http://ace.fsu.edu/tutoring> or contact tutor@fsu.edu. High-quality tutoring is available by appointment and on a walk-in basis. These services are offered by tutors trained to encourage the highest level of individual academic success while upholding personal academic integrity.

Syllabus Change Policy

Except for changes that substantially affect implementation of the evaluation (grading) statement, this syllabus is a guide for the course and is subject to change with advance notice.

2022-23 Syllabus Statement on Pandemic Protocols

The CDC recommends that all individuals, even vaccinated individuals, wear proper and well-fitting masks in public indoor spaces, like classrooms, especially where social distancing is not possible and virus rates are high. The CDC assesses the infection rate in Leon County as **HIGH** (see details at <https://www.cdc.gov/coronavirus/2019-ncov/your-health/covid-by-county.html>) and continues to recommend masking in indoor public spaces, especially when social distancing is not possible.

Florida is experiencing a surge of the Omicron BA.5 variant, the most easily transmissible Covid variant to date, which is able to evade previous immunity from infection and vaccination. It is a much more transmissible variant than the original virus, the Delta variant, or even the earlier Omicron variants. It can infect even vaccinated individuals and can be spread by them to others. It poses a special threat to members of the community with underlying health conditions and family members vulnerable to the

virus. The best way to protect against serious illness is to be fully vaccinated, but not everyone among us can be.

For these reasons, FSU expects each of us to continue cooperating with common-sense [public health protocols](#), including (1) getting vaccinated and boosted, (2) testing for the virus if you have symptoms, (3) staying home and away from others if you are sick (in such exceptional cases a virtual meeting room will be made available), and (4) masking in public indoor spaces to protect yourself and others whenever there is reason for concern. In our classroom together, I will wear a proper, well-fitting mask, and I invite you to join me in order to reduce the spread of BA.5 and protect the vulnerable among us.

Please remember that you should **NOT** attend class in person if you have tested positive for Covid-19 or are in quarantine.

Course Timeline

week	topics covered
1	Verification and validation terminology, three legs of science
2	Decision making, biases, engineering disasters
3	Differential equations, discretization, convergence, Lax Theorem
4	Code verification activities: static and dynamic testing
5	Forward and backward problems, manufactured solutions
6	Solution verification for time-dependent problems
7	Solution verification for multiphysics and multiscale problems
8	Elements of uncertainty quantification; aleatory and epistemic uncertainties
9	Sensitivity analysis, Bayes' Theorem, screening methods
10	Validation pyramid, validation experiments
11	Experimental diagnostic, validation metric
12	Design and execution of validation experiments for smooth problems
13	Design and execution of validation experiments for discontinuous problems
14	Code-to-code comparison procedure