ISC 5316: Applied Computational Science II

This course provides students with high-performance computational tools necessary to investigate problems arising in science and engineering, with an emphasis on combining them to accomplish more complex tasks. A combination of course work and lab work provides the proper blend of theory and practice with problems culled from the applied sciences. Topics include mesh generation, stochastic methods, basic parallel algorithms and programming, numerical optimization, and nonlinear solvers.

Credit

3 semester hours

Prerequisites

ISC 5315: Applied Computational Science I, or the permission of the instructor.

Course Objectives

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

- build simple parallel computer programs,
- implement Fast Fourier transform to solve problems computationally,
- use optimization and programming algorithms to solve relevant problems,
- carry out solutions of partial differential equations in 2D (2 spatial dimensions or 1 spatial dimension and time) computationally,
- build statistical models to analysis and solve relevant problems.

Course Topics

The topics covered under this course broadly include: Fourier transforms, parallel computing, numerical solution of partial differential equations, optimization and nonlinear equations and statistical methods.

Contact Information

Instructor: Tomasz Plewa
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Office hours: WF, 2pm-3pm, or by appointment.

Teaching Assistant: Benjamin McLaughlin
Office: 451A DSL
E-mail: mbm09m@my.fsu.edu
Office hours: by appointment.

Homework Submission

Each homework assignment or project must be submitted as a single pdf document via email to TA (bm09m@fsu.edu) with a copy to the Instructor (tplewa@fsu.edu).

Grading

The course grade will be based on class tests (3 in total, 45%), computer laboratory homework assignments (50%), and ad hoc essays (5%). Because the laboratory and homework effort is substantial, no mid-term or final exams will be given. Late homework submissions will be subject of 10% points reduction per day, with 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

Required: E. Ward Cheney, David R. Kincaid, *Numerical Mathematics and Computing* (Cengage Learning), 2012, 7th edition, ISBN-10: 1133103715, ISBN-13: 978-1133103714

Choice: Michael T. Heath, *Scientific Computing: An Introductory Survey* (The McGraw-Hill Companies, Inc.), 2002, 2nd edition, ISBN-10: 0072399104, ISBN-13: 978-0072399103

Choice: R. J. Barlow, Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences (Wiley), 1993, ISBN-10: 0471922951, ISBN-13: 978-0471922957

Website

https://campus.fsu.edu/webapps/blackboard/execute/courseMain?course_id=_6401317_1

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://dof.fsu.edu/honorpolicy.htm.)

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.

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)
sdrc@admin.fsu.edu
http://www.disabilitycenter.fsu.edu/

Free Tutoring from FSU

For tutoring and writing help in any course at Florida State University, visit the Academic Center for Excellence (ACE) Tutoring Services' comprehensive list of tutoring options - see http://ace.fsu.edu/tutoring or contact tutor@fsu.edu for more information. 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.

List of Topics

1. Parallel computing (8/26, 8/28, 9/2, 9/4)
Brief introduction to parallel computing; OpenMP and MPI programming techniques

2. Statistical methods (9/9, 9/11, 9/16, 9/18, 9/23, 9/25)
Random variables, distributions, central limit theorem; normal theory inference; hypothesis testing and confidence interval; introduction to statistical models; linear models; nonlinear models

3. Optimization and non-linear equations (9/30 + T1, 10/2, 10/7, 10/9, 10/14, 10/16)
Introduction; unconstrained smooth optimization; line search methods; Conjugate Gradients (CG) methods (linear and nonlinear CG methods); practical Newton methods; quasi-Newton methods (trust region method); linear programming; constrained programming

4. Fourier transform (10/21, 10/23, 10/28)
General definition of integral transforms; Fourier transform (FT); properties and applications of FT and Fourier series; discrete FT; computational implementation and Fast Fourier Transform (FFT); applications

5. Numerical solution of partial differential equations (10/30 + T2, 11/4, 11/6, 11/11, 11/13, 11/18)
Classification of Partial Differential Equations (PDEs); boundary value problems; initial-boundary value problems; physical situations (fluid flow, electro-magnetic field equations, diffusion, reaction-diffusion equations); well-posedness and solvability of PDEs; computational solution of PDEs; finite difference, finite element and finite volume methods; grids and grid generation; convergence and stability of solution; errors and error estimation; computational implementation and examples; survey of software for solving PDEs

6. Molecular dynamics and algorithms (11/20, 11/25, 12/2, 12/4 + T3)
Motivation (physics, chemistry, materials science, biology); atomic and molecular interactions and force fields; statistical foundation; Molecular Dynamics (MD) algorithms; equations of motion; boundary conditions; integration algorithms; typical simulation and analysis