SYLLABUS

ISC 5316: Applied Computational Science II
Fall 2013

Instructors: Prof Ionel M Navon

Scientific Computing Department
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Office hours Monday 10:00 am -12:00 noon
Friday 2:00 pm -4:00 pm
Textbook Numerical Mathematics and
Computing 7-th Edition
E. Ward Cheney, David R. Kincaid
Class Time Tuesday, Thursday 11:00 AM --12:15 DSL 0468

Place HCB 0217

Lab time Tuesday 03:30 PM 06:00 PM

Place DSL 0152

Catalogue description

ISC 5316: Applied Computational Science II (4).

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 works 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

Prerequisites

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

List of Topics

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

Course Objectives

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

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

Grading & Exam Policy

The student's grade for this course will be determined by his/her performance in homework and lab assignments.

Homework, including other special assignments:	50%
Laboratory work, including reports	50%

There will be six lab assignments. Each assignment will culminate in a written report by the student, complete with summary, introduction, solution, results, tables, figures, and conclusions. Each lab report is due one week past the end of the particular lab sequence. Dates will be confirmed by instructor each time an assignment is given.

Because the laboratory and homework effort is substantial, no mid-term or final exams will be given. The instructors might give short quizzes during the semester.

Attendance Policy

Students are required to attend all classes unless there is a reason to be absent; please see university rules regarding absence.

Students are responsible for bringing themselves up to date both on subject matter and all other related class activities, e.g., homework assignments, laboratory projects, etc. Students who have to miss a class or more are encouraged to talk to the instructors before and/or after their absence.

Reading List

1. Instructor handouts
2. Literature specified by instructors for each section

All course materials will be posted on the course website.

Announcements

The instructors will periodically make announcements about homework assignments and due dates, solution, course materials, etc.

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.)

ADA

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/

Syllabus (detailed list of topics)

1. Optimization and non-linear equations (8/30, 26, 9/1, 6, 8, 13)

   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

2. Statistical methods (9/15, 20, 22, 27, 29, 10/4)

   Random variables, distributions, central limit theorem; normal theory inference; hypothesis testing and confidence interval; introduction to statistical models; linear models; nonlinear models

3. Parallel computing (10/ 6, 11, 13, 18)

   Brief introduction to parallel computing; Open MP and MPI programming techniques

4. Fourier transform (10/20, 25, 27)

   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 (11/1, 11/3, 8, 10, 15, 17)

   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 (11/22 24, 29, 12/1)

   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