Scientific and Technical Computing SDS 335/394 Course Syllabus

Course Unique Number: 57020/57130

Fall 2017 FAC 101B

2:00 pm to 3:15 pm Tuesdays and Thursdays

Instructors:

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I Course Aims and Objectives

I.1 Aims

Computing is the third pillar of science, complementing both experiment and theory. The modern scientist is required to use programs effectively. The skill set required for scientific computing vary greatly from the standard programming practices in other disciplines. This course is an introduction to techniques and practices of scientific and technical computing.

I.2 Specific Learning Objectives

We will cover the topics and skills that are necessary to realize computational science on modern architectures. For this, the lecture sessions will cover computer architecture including parallel architectures, machine arithmetic, the sources or large computational problems and the techniques for solving them efficiently. Practical topics covered will concern the development and maintenance of scientific software. We also include lectures of scientific libraries and analysis, post-processing and visualization tools and data analysis.

By the end of this course, students will:

- Understand the architecture of the most common research compute clusters.
- Be familiar with programming techniques and tools.
- Be able to apply scientific libraries for application of numerical methods.
- Be able to program and analyze basic scientific algorithms for applications.

II. Course Assumptions

This course will include a certain amount of coding and analysis of mathematical models. Students will be expected to have mastered the material taught in SSC 222/292 and Mathematics 408D or 408M, these courses are listed as requirements but they have not been enforced during the registration process. The skills they teach are essential. A partial list of these skills include:

- Programming experience, i.e., more than 5K lines of code
- Understanding Linux programming environment, especially use of compilers and text editors.
- Working understanding of C/C++ or Fortran.
- Common data types and structures, control structures, algorithms.
- An understanding of multivariate calculus and matrix operations
- Parametric equations, sequences, functions of several variables,
- Infinite series, power series,
- Vectors, vector calculus,
- Partial derivatives, gradients, and multiple integrals.
- While any single criteria above is not a reason to drop the course, if there are more than two you will spend a non-trivial amount of time catching up on the subjects.

III Format and Procedures

A class will consist of a lecture and often some time for lab tutorials. 5 assignments will be given at the end of topics, and will be due at assigned times. All assignment will be assessed a 1 point penalty for each hour late.

IV Tentative Course Schedule

This syllabus represents our current plans and objectives. As we go through the semester, those plans may need to change to enhance the class learning opportunity. Such changes, communicated clearly, are not unusual and should be expected.

Week	Main Topics	Description
1, Th	Introduction to course	Syllabus, TACC account, canvas and piazza
2, T	Types of computers	Architectures (laptop, cluster, supercomputer). What computers look like and how the pieces interact

Week	Main Topics	Description
2, Th	Unix tools and environment, part 1	How to interact with a linux box and edit files
3, T	Unix tools and environment, part 2	Using TACC systems. ssh and remote access. How to transfer files and manipulate a machine remotely
3, Th	Unix tools and environment, part 3	Advanced Unix, tips and tricks
4, T	Version control	Overview of version control systems, Using Git
4, Th	Version control	
5, T	Representation of numbers	Floating point error and related numerical representation issues with computers
5, Th	Computing environments	Machines, operating systems, tools, differences
6, T	Compilers	What they are, how they work, and why we need them, how to use them
6, Th	Compilers	
7, T	Make	An introduction to build automation tools and how to
7, Th	Scientific libraries	BLAS, LAPACK and FFTW
8, T	Scientific libraries	

Week	Main Topics	Description
8, Th	Debugging	How to find bugs, and software to use for doing this
9, T	Performance analysis	How to find performance bottlenecks and bugs, and software to use for doing this
9, Th	Software testing/documentation	Best practices in software testing and documentation
10, T	Software testing/documentation	
10, Th	Intro to parallel computing	Overview, MPI, OpenMP
11, T	Intro to parallel computing	
11, Th	Scientific Data	What file formats are available, what metadata is, best practices for I/O on HPC systems
12, T	Computer graphics	Graphics pipeline, rendering, openGL and Matrix Transforms and Operations
12, Th	Numerical Linear algebra	Intro to Interactive Methods
13, T	Numerical Linear algebra	
13, Th	No Class Thanksgiving Holiday (Thursday Nov 23)	

Week	Main Topics	Description
14, T	Intro to Sci Vis	Introduction to Data Vis, Sci Vis and Paraview
14, Th	Intro to Sci Vis	
15, T	Data analysis/vis tools	Introduction to Info Vis tools (python/matplotlib, RShiny, d3)
15, Th	Immersive/Interactive visualisation	Tools/Libraries for data explorations with VR/AR

Feedback Statement

During this course we will be asking you to give us feedback on your learning in informal as well as formal ways, including through anonymous surveys about how our teaching strategies are helping or hindering your learning. It is very important for me to know your reaction to what we are doing in class, so we encourage you to respond to these surveys, ensuring that together we can create an environment effective for teaching and learning.

V Course Requirements

V.1 Class attendance and participation policy

To make our time together as valuable as possible, we all have to work hard at it. The following basic principles may give us some guidelines: Every student has the right to learn as well as the responsibility not to deprive others of their right to learn. Every student is accountable for his or her actions. In order for you to get the most out of this class, please consider the following:

- Attend all scheduled classes and arrive on time. Late arrivals and early departures are very disruptive and violate the first basic principle listed above.
- Please do not schedule other engagements during this class time. You probably wouldn't appreciate it if we did! We will try to make class as interesting and informative as possible, but we can't learn the material for you.

- If you have trouble hearing the lecture or media presentation because of distractions around you, quietly ask those responsible for the distraction to stop. If the distraction continues, please let us know. It is often impossible for us to hear such things from our position in the classroom.
- Please let us know immediately if you have any problem that is preventing you from performing satisfactorily in this class.

Religious Holy Days

By UT Austin policy, you must notify us of your pending absence at least fourteen days prior to the date of observance of a religious holy day. If you must miss a class, an examination, a work assignment, or a project in order to observe a religious holy day, we will give you an opportunity to complete the missed work within a reasonable time after the absence.

V.2 Course Readings/Materials

Largely we will rely on class notes and manuscripts from the web. Below we list several books that may be used as reference materials but are by no means required.

V.2.1 Class Slides

Class slides will be posted to canvas: https://utexas.instructure.com/courses/1208648/files

V.2.2 Related Texts

Introduction to Scientific and Technical Computing by Frank T. Willmore, Eric Jankowski and Coray Colina

Introduction to High Performance Scientific Computing by Victor Eijkhout with Edmond Chow and Robert van de Geijn.

V.2.3 Use of Canvas in class

In this class we use Canvas—a Web-based course management system with password-protected access at https://utexas.instructure.com/courses/1208648 (Links to an external site.)Links to an external site. —to distribute course materials, to communicate and collaborate online, to post grades, to submit assignments, and to give you online quizzes and surveys if any. You can find support in using Canvas at the ITS Help Desk at 475-9400, Monday through Friday, 8 a.m. to 6 p.m., so plan accordingly.

V.2.4 Use of Piazza in class

In this class we use Piazza, a web-based discussion forum. Students can post discussion topics or questions and suggest answers on Piazza: piazza.com/utexas/fall2017/sds335394. Instructors will make an effort to check the forum at least once a day. Ask your question here before mailing the instructor or TA.

V.3.1 Homework Assignments

Format: Topic and Tutorial homework assignments will be announced in class.

Posting: Assignments and due dates will be posted on Canvas.

Late policy: Every hour late will incur penalty of 1 point.

V.3.2 Final Project

The final project will be worth 30% of your grade. The specific details of the final project and its requirements will be posted to canvas in October. As part of the final project, you can expect to submit version controlled code and a report.

V.3.3 Subject-to-change notice

Assignments and schedule is subject to change at the instructor's' discretion.

Other Electronic Resources

Students can post discussion or questions and suggest answers on Piazza: piazza.com/utexas/fall2017/sds335394

Instructors will make an effort to check the forum at least once a day. Ask your questions here before mailing the instructor or TA.

Programming exercises are to be submitted for grading through a source code repository. Sign up with your utexas.edu email at https://bitbucket.org/ for a free account and invite both instructors and the TA to your project. The use of source code repositories will be explained in class.

VI Grading Procedures

Grades will be based on:

20% Quizzes

50% Homework

30% Final project

We reserve the right to curve the grades to the benefit of the student. Final grade will be given according to the scale of

A: [1000, 900],

B: [800,900],

C: [700,800],

D: [600,700],

F: below 600

VII Academic Integrity University of Texas Honor Code

The core values of The University of Texas at Austin are learning, discovery, freedom, leadership, individual opportunity, and responsibility. Each member of the university is expected to uphold these values through integrity, honesty, trust, fairness, and respect toward peers and community.

Each student in this course is expected to abide by the University of Texas Honor Code. [See the UT Honor Code above.] Any work submitted by a student in this course for academic credit will be the student's own work.

You are encouraged to study together and to discuss information and concepts covered in lecture and the sections with other students. You can give "consulting" help to or receive "consulting" help from such students. However, this permissible cooperation should never involve one student having possession of a copy of all or part of work done by someone else.

Should copying occur, both the student who copied work from another student and the student who gave material to be copied will both automatically receive a zero for the assignment. Penalty for violation of this Code can also be extended to include failure of the course and University disciplinary action.

Sharing Code

Coding is a major aspect of this course. While discussion of ideas on the material is acceptable, one should never use a code without attributing. You are expected to code the solutions yourself. If someone helps you with some part of the code, attribute, but always put their code aside and write a solution from top to bottom.

It is also unacceptable to use another code rather than implementing the assignment yourself. While not attributing code is plagiarism, using another code as your own with attribution and turning it in for your assignment is misleading. Both cases will be reported to the Student Judicial Services.

VIII Other University Notices and Policies

VIII.1 University of Texas Honor Code

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Each student in this course is expected to abide by the University of Texas Honor Code. [See the UT Honor Code above.] Any work submitted by a student in this course for academic credit will be the student's own work. Collaborations will be allowed for the course project.

You are encouraged to study together and to discuss information and concepts covered in lecture and the sections with other students. You can give "consulting" help to or receive "consulting" help from such students. However, this permissible cooperation should never involve one student having possession of a copy of all or part of work done by someone else, in the form of an e-mail, an e-mail attachment file, a diskette, or a hard copy.

Should copying occur, both the student who copied work from another student and the student who gave material to be copied will both automatically receive a zero for the assignment. Penalty for violation of this Code can also be extended to include failure of the course and University disciplinary action.

During examinations, you must do your own work. Talking or discussion is not permitted during the examinations, nor may you compare papers, copy from others, or collaborate in any way. Any collaborative behavior during the examinations will result in failure of the exam, and may lead to failure of the course and University disciplinary action.

VIII.2 Use of E-mail for Official Correspondence to Students

All students should become familiar with the University's official e-mail student notification policy. It is the student's responsibility to keep the University informed as to changes in his or her e-mail address. Students are expected to check e-mails on a frequent and regular basis in order to stay current with University-related communications, recognizing that certain communications may be time-critical. It is recommended that e-mail be checked daily, but at a minimum, twice per week. The complete text of this policy and instructions for updating your e-mail address are available at http://www.utexas.edu/its/help/utmail/1564.

VIII.3 Documented Disability Statement

Any student with a documented disability who requires academic accommodations should contact Services for Students with Disabilities (SSD) at (512) 471-6259 (voice) or 1-866-329-3986 (videophone). Faculty are not required to provide accommodations without an official accommodation letter from SSD. (Note to Faculty: Details of a student's disability are confidential. Faculty should not ask questions related to a student's condition or diagnosis when receiving an official accommodation letter.)

- Please notify me as quickly as possible if the material being presented in class is not accessible (e.g., instructional videos need captioning, course packets are not readable for proper alternative text conversion, etc.).

- Please notify me as early in the semester as possible if disability-related accommodations for field trips are required. Advanced notice will permit the arrangement of accommodations on the given day (e.g., transportation, site accessibility, etc.).
- Contact Services for Students with Disabilities at 471-6259 (voice) or 1-866-329-3986 (video phone) or reference SSDs website for more disability-related information: http://www.utexas.edu/diversity/ddce/ssd/for_cstudents.php

VIII.5 Concerns Advice Line (BCAL)

If you are worried about someone who is acting differently, you may use the Behavior Concerns Advice Line to discuss by phone your concerns about another individual's behavior. This service is provided through a partnership among the Office of the Dean of Students, the Counseling and Mental Health Center (CMHC), the Employee Assistance Program (EAP), and The University of Texas Police Department (UTPD). Call 512-232-5050 or visit http://www.utexas.edu/safety/bcal.

VIII.6 Drop Policy

The State of Texas has enacted a law that limits the number of course drops for academic reasons to six (6). As stated in Senate Bill 1231:

“Beginning with the fall 2007 academic term, an institution of higher education may not permit an undergraduate student a total of more than six dropped courses, including any course a transfer student has dropped at another institution of higher education, unless the student shows good cause for dropping more than that number.”

VIII.7 Emergency Evacuation Policy

Occupants of buildings on the UT Austin campus are required to evacuate and assemble outside when a fire alarm is activated or an announcement is made. Please be aware of the following policies regarding evacuation:

- Familiarize yourself with all exit doors of the classroom and the building. Remember that the nearest exit door may not be the one you used when you entered the building.
- If you require assistance to evacuate, inform me in writing during the first week of class.
- In the event of an evacuation, follow my instructions or those of class instructors.

Do not re-enter a building unless you're given instructions by the Austin Fire Department, the UT or Austin Police Department, or the Fire Prevention Services office.

We welcome feedback; please address questions, suggestions, and requests for more information to info@tacc.utexas.edu (Links to an external site.)Links to an external site..