CSci 509 Introduction to Computational Sciences

Course Syllabus

Spring 2018

Instructor

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Class Meetings

Lectures and course materials will be distributed through our University's eCollege online course system.

01WWeb Based Class

Course Description

Big scientific data sets are growing exponentially both in size and complexity. Extracting meaningful information from this data requires not only programming skills, but also understanding the analysis work-flows and mathematical models and visualization tools that help to condense large amounts of information into a comprehensible story. Computational science is the scientific investigation of problems through modeling, simulation and analysis of physical processes on a computer. Computational science is now considered by most scientists to be on par with the development of scientific theory and the use of experimentation in order to understand more about our world. Computational science is not the same as computer science. Rather, it is an interdisciplinary blend of scientific models, applied mathematics, computational techniques, and practices. This Introduction to Computational Science course focuses upon simple and intuitive computational models and methods.

Requirements and Objectives

This course forms one of the core subjects in the master's degree program in the Computational Sciences. Computational sciences differs from the traditional computer science discipline in several ways, but most importantly as being focused on applying computational methods to solving large scientific problems. Thus this type of scientific data analysis of large complex data sets is both increasingly crucial to scientific research, as well as being in great demand for practitioners who can apply computational analysis and modeling to such data sets. This course directly addresses this area, and forms a cornerstone subject for any student wishing to understand and practice computational science research.

Goals include:

- Understand the scientific process and the philosophy of science.
- Understand the purpose and value of computational science.
- Be exposed to the common tools and practices of working computational scientists.
- Learn to use basic computational simulation and modeling tools, specifically the Python toolkit stack.
- Be exposed to basic data analysis and modeling concepts and practices.
- Learn about common computational algorithms for performing scientific modeling, including computational integration and differentiation, random Monte Carlo methods, solutions of ordinary differential equations, etc.

Companion Textbooks / Readings

Most materials, work and readings will be provided as iPython notebooks for students to read and experiment with. Many materials were developed using the following sources. Additional readings from these sources are encouraged for a deeper understanding of the topics:

- Langtangen, H.P. (2012). A Primer on Scientific Programming with Python 3rd ed. Springer.
- Newman, M. (2012). Computational Physics. CreateSpace.

Prerequisites

Successful enrollment in Computational Sciences Master's Program. This course assumes a basic proficiency with computer programming and computational concepts. A basic understanding of how a sequential computer works is assumed. Fundamental familiarity with basic CS topics such as algorithms and analysis, data types, data storage, I/O, loops, branches, subprograms and object-oriented programming are also assumed. Fundamental mathematical ability is assumed, such as familiarity with discrete and continuous mathematical models. Enough ability to use vectors, matrices, integration and differentiation. The REAL prerequisite is a desire to learn and explore new ideas.

Evaluation (Tentative)

Your grade for the course will be based on the following (approximate) percentages:

Letter grades will be assigned according to the following scale:

Final Average $(\%)$	Letter Grade
90 - 100	A
80 - 89	В
70 - 79	\mathbf{C}
60 - 69	D
Below 60	F

All assignments and study materials will be distributed and collected through our Universities online eCollege learning system. In addition, we will have two scheduled exams and required exams during the semester. The dates of these exams will be announced before hand, but they will be held during the morning scheduled times we have for this course. These face-to-face exams will not be optional, you will be required to be on campus and attend these meeting in order to take our two course exams in person.

Student's with Disabilities

The Americans with Disabilities Act (ADA) is a federal anti-discrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you have a disability requiring an accommodation, please contact: Office of Student Disability Resources and Services, Texas A&M University-Commerce, Gee Library, Room 132, Phone (903) 886-5150, Student Disability Services@tamuc.edu

Academic Ethics

"All students enrolled at the University shall follow the tenets of common decency and acceptable behavior conducive to a positive learning environment." (See Student's Guide Handbook, Policies and Procedures, Conduct). Ethics also includes the issue of plagiarism, and copying code for programming/lab assignments is just as serious as any other type of plagiarism. If you are caught sharing or using other people's work in this class, you will receive a 0 grade and a warning on the first instance. A subsequent instance will result in receiving an F grade for the course, and possible disciplinary proceedings.

Attendance Policy

Students are expected to follow all instructions and visit eCollege regularly many times weekly to complete the materials for this online course. If a student is unable to submit assignments by the due date for the assignment, they are expected to make alternative arrangements to assure that the assignment is turned in ON TIME, before the assignment is actually due. Any student wishing to withdraw from the course must do so officially as outlined in the class schedule. THE INSTRUCTOR CANNOT DROP OR WITHDRAW ANY STUDENT.

Students are required to be present on campus for the two scheduled face-to-face course exams. You will not be allowed to make up these exams if missed for an unexcused absence.

Course Requirement Deadlines

Credit will be given for ONLY those exam(s), program(s), and/or project(s) turned in no later than the deadline(s) as announced by the instructor of this class unless prior arrangement has been made with the instructor.

Technology Requirements

This course is a web enhanced course, which means all assignments and handouts will be distributed and collected through our University's eCollege online course system.

- To fully participate in online courses you will need to use a current browser, such as Mozilla Firefox or Google Chrome.
- You will need regular access to a computer with a broadband internet connection. The minimum computer requirements are:
 - 512 MB of RAM, 1 GB or more preferred.
 - Broadband connection required by courses that are heavily video intensive.
 - Video display capable of high-color 16-bit display 1024 x 768 or higher resolution.
- You must have a:
 - Sound card, which is usually integrated into your desktop or laptop computer.
 - Speakers or headphones.

Access and Navigation

This course will be facilitated using Pearson LearningStudio, the learning management system used by Texas A&M University-Commerce. To get started with the course, go to myLeo and from the top menu ribbon select eCollege. Then on the upper left side of the screen click on the My Courses tab. http://www.tamuc.edu/myleo.aspx

You will need your campus-wide ID (CWID) and password to log into the course. If you do not know your CWID or have forgotten your password, contact the Center for IT Excellence (CITE) at 903.468.6000 or helpdesk@tamuc.edu.

Note: It is strongly recommended you perform a "Browser Test" prior to the start of your course. To launch a browser test login to Pearson LearningStudio, click on the My Courses tab, and then select the Browser Test link under Support Services.

Texas A&M University-Commerce provides students technical support for the use of Pearson LearningStudio. Technical assistance is available 24/7 (24 hours, 7 days a week). If you experience LearningStudio (eCollege) technical problems, contact the LearningStudio helpdesk at 1-866-656-5511 (toll free) or visit Pearson 24/7 Customer Support Site http://247support.custhelp.com/

Accessing Help from within Your Course: Click on the 'Tech Support' icon on the upper left side of the screen inside the course. Then you will be able to get assistance via online chat or by phone.

Note: Personal computer and internet connection problems do not excuse the requirement to complete all course work in a timely and satisfactory manner. Each student needs to have a backup method to deal with these inevitable problems. These methods might include the availability of a backup PC at home or work, the temporary use of a computer at a friend's home, the local library, office service companies, Starbucks, a TAMUC campus open computer lab, etc.

myLeo Support: Your myLeo email address is required to send and receive all student correspondence. Please email helpdesk@tamuc.edu or call us at 903-468-6000 with any questions about setting up your myLeo email account. You may also access information at myLeo. https://leo.tamuc.edu

Nondiscrimination Notice

Texas A&M University-Commerce will comply in the classroom, and in online courses, with all federal and state laws prohibiting discrimination and related retaliation on the basis of race, color, religion, sex, national origin, disability, age, genetic information or veteran status. Further, an environment free from discrimination on the basis of sexual orientation, gender identity, or gender expression will be maintained.

Campus Concealed Carry Statement

Texas Senate Bill - 11 (Government Code 411.2031, et al.) authorizes the carrying of a concealed handgun in Texas A&M University-Commerce buildings only by persons who have been issued and are in possession of a Texas License to Carry a Handgun. Qualified law enforcement officers or those who are otherwise authorized to carry a concealed handgun in the State of Texas are also permitted to do so. Pursuant to Penal Code (PC) 46.035 and A&M-Commerce Rule 34.06.02.R1, license holders may not carry a concealed handgun in restricted locations.

For a list of locations, please refer to the Carrying Concealed Handguns On Campus document and/or consult your event organizer.

 $Web\ url:\ http://www.tamuc.edu/aboutUs/policiesProceduresStandardsStatements/rulesProcedures/34SafetyOfEmployeesAndStudents/34.06.02.R1.pdf$

Pursuant to PC 46.035, the open carrying of handguns is prohibited on all A&M- Commerce campuses. Report violations to the University Police Department at 903-886-5868 or 9-1

Course Schedule (Preliminary)

W	Date	Topic / Activity	Assg	Test
1	2/1	Introduction to Computational Science and Course, Introduction to Python		
2	2/5	NumPy - Python Numerical Computing Library		
3	2/12	Matplotlib, Mathematical Functions and vectorization, Discrete Approximations	#1	
4	2/19	Speed and Accuracy in Numerical Simulations	#2	
5	2/26	Sequences and Difference Equations		
6	3/5	Taylor Expansion	#3	
7	3/12	Integration and Differentation		
8	3/19	Integration and Differentation	#4	Midterm
9	3/26	Numerical Solutions of Ordinary Differential Equations		
10	4/2	Numerical Solutions of Ordinary Differential Equations	#5	
11	4/9	System of Equations, Discrete Grid/Cell Models		
12	4/16	System of Equations, Discrete Grid/Cell Models	#6	
13	4/23	Random Numbers, Statistics and Monte Carlo Simulations		
14	4/30	Random Numbers, Statistics and Monte Carlo Simulations	#7	
15	5/7	Large Scale Network Models and Network Science Methods	#8	
	5/7	Finals Week		Final

Student Learning Outcomes

- 1. Be able to apply numerical solutions to scientific modeling problems.
- 2. Apply computational techniques to tackling scientific research questions.
- 3. Familiarize with standard tools of computational science: HPC, R/Python/Numpy/Scipy toolkit stack, markup and documentation systems, plotting and visualization, etc.
- 4. Understand stochastic models and be able to apply to building simple Monte Carlo simulations.
- 5. Be familiar with fundamental building blocks of numerical modeling and discrete calculus for computational approximation.

6. Understand importance of series and difference equations for discrete approximations of numerical methods.

Learning outcomes will be measured through mapping assignment and test questions to specific outcome items, as well as through exit surveys of student experiences with the outcome familiarity.