Syllabus for:
COE 322: Scientific Computation

Victor Eijkhout

2020 Fall semester

Contents

1 Basic information

Number and title	Scientific Computation (13370)
Instructor	Victor Eijkhout
	`eijkhout@tacc.utexas.edu`
Co-instructor	Susan Lindsey
&`slindsey@tacc.utexas.edu`	
Time and place	online only, TTh 3:30–5:00
Office hours	online on request
Teaching assistent	Kendrick Shepherd
Teaching assistent	Chase Tessmer
	contact through Canvas or Slack

2 Rationale

Computers were invented over 60 years ago to solve mathematical equations, especially in science and engineering. Over the last 20 years, computers have become ubiquitous in our lives: increasing productivity, enhancing communications and connectivity, ensuring safety, and providing entertainment. The pervasiveness of computers in business and consumer environments – and the resulting revenues – has caused a shift in the computer languages and skills taught in computer science departments today. Introductory programming classes are now commonly taught in Java, and focus on skills needed for industry careers in web development, at the expense of offering scientific computing classes formerly taught for the benefit of technical computing – science and engineering departments at universities as well as the R&D departments in numerous industries. This has occurred even though computers have become increasingly fundamental to the conduct of science and engineering, two fields vital for increasing economic productivity, ensuring national security, and addressing many important societal problems.

There are recent signs of a reversal of this trend: new degree programs in computational science, new emphasis in federal spending on computational technologies and R&D, and even a return of some scientific computing classes in some computer science departments, etc. However, the need for well-trained computational scientists and engineers is still urgent. Fortran, C and C++ remain the most powerful general purpose programming languages for developing scientific software: they offer the best features and flexibility for designing robust, high-performance applications. These languages are constantly evolving and growing, new trends and concepts for software development in both languages frequently arise and are rapidly disseminated. The SDS 322/392 course provides a unique opportunity to learn modern usage of these languages.

3 Course Aims and Objectives

3.1 Course aim

This course teaches the basic of C++ (2017 standard) and Fortran (2003 standard), but it does so as part of a discipline of programming. Notions of program organization, even correctneses, will be taught along basic matters of syntax.

The course stresses active command of the material taught: each lecture section is accompanied by multiple short programming exercises.

By the end of the course, students have the opportunity to demonstrate their command of the material by doing a larger programming project. This project is the equivalent of two weeks of programming, and explores some scientific simulation.

3.2 Course organization

The course is organized as a sequency of topics, each one or two sessions, that cumulatively instill active command of the languages C++ and Fortran. There will be tutorials,

especially early in the course, on the use of Unix, and programmer tools.

Topics taught are, in sequence:

1. data types
2. expressions
3. control structures
4. scoped constructs such as functions
5. classes and objects
6. further object-oriented techniques such as inheritance,
7. arrays
8. I/O and string manipulation.

Time permitting, advanced topics will be taught such as:

- Pointers
- Modular programming
- Dynamic memory
- Templates
- Libraries

By the end of this course, the students will:

- have understanding and active command of the commonly used scientific programming languages C++ and Fortran, sufficient for undertaking scientific programming projects in their further studies;
- have mastered a basic discipline of program development and of debugging the code;
- have familiarity with the Linux Operating System and basic knowledge of its tools.

3.3 Relationship of Course to Program Outcomes

This course contributes to the ABET Criterion 3 student outcomes that took effect with the Fall 2019 semester. For more information, see Criteria for Accrediting Engineering Programs, 2019 – 2020 at https://www.abet.org/accreditation/accreditation-criteria/criteria-for-accrediting-engineering-programs-2019-2020/

Student outcomes:

- 5: an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives

ABET Program Criteria Achieved:

- P: Computer Usage

4 Instructors' Biographical Information

Victor Eijkhout is a research scientist in the High Performance Computing group at the Texas Advanced Computing Center (TACC). His degree is in numerical analysis, and he has longtime experience in programming scientific codes and libraries, especially on parallel computers. His research interests include numerical linear algebra, parallel computing, machine learning, processor performance. He has written several widely used textbooks, as well as many scientific papers.

Susan Lindsey has a degree in computer science from The University of California San Diego. She has a strong track record in the field of High-Performance Computing, with over twenty years at the San Diego Supercomputer Center and now at the Texas Advanced Computing Center. Susan is currently an integral member of User Services at TACC and has contributed to a wide variety of programming projects and technical documentation. She also has previous teaching experience in both C and assembly language programming.

5 Format and Procedures

Class periods will feature both a lecture and lab part, as well as discussions of homework. We encourage a lively participation during the lectures and expect that you participate by asking and answering questions. Active participation makes for a better and more interesting class for you and for us, and allows us to assess your progress and to adjust the class material and/or teaching progress accordingly.

Student progress in this class will be evaluated through homework, quizzes, one exam over C++ and Fortran each, and one major programming project. There will be no final examination. We expect timely notification if you cannot take a quiz/exam as scheduled, or if you are unable to meet a submission deadline.

6 Other course information

6.1 Prerequisites

Elementary knowledge of Unix (logging in, file and directory manipulation) is assumed. Students lacking this knowledge need to do a tutorial by the first week of class.

Familiarity with basic mathematics (trigonometry, linear algebra) is assumed.

6.2 Course materials, further readings

Lectures slides, a textbook, and other materials are distributed electronically through a Git repository.

https://github.com/TACC/coe322fall2020

6.3 Computing Resources

Students will be given access to a TACC machine that has the necessary software loaded. Having a personal computer with the appropriate compilers is convenient but not needed.

It is allowed and possible to do homework on a personal machine, but the test of labs and homework submissions is whether they compile and execute correctly on the TACC machine.

6.4 Online discussion

Students are required to join the `tacc-learn` Slack space:

`tacc-learn.slack.com`

7 Grading Procedures

- There will be once or twice weekly graded homework exercises, counting for 70 percent of the total grade.
- There will be one major programming project counting for 30 points.
- There will be no final examination during the finals period. The programming project is due on the last day of classes.

Participation in class may cause your grade to be rounded up.

8 Formal and informal policies

Covid-19 specific policies

This class observes university guidelines:

`https://provost.utexas.edu/syllabus-guidance-fall-2020#safety-and-class`

In particular:

- Since all instruction will be online, no mask / face covering policies apply.
- Since all course materials are electronic, and assignments will be administered electroniclly, sharing of materials does not apply.
- Classes **will be recorded** and viewable through UT's Zoom/Canvas integration.
- There are no further hybrid or in-person components to the class.

Class attendance and participation policy

We expect students to attend and participate in class in accordance with the UT Honor Code (see below). Students are encouraged to ask questions, especially relating to material used in their projects.

Absences, in particular on exam days, should be communicated with the instructors as early as possible.

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.

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. 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.

Other University Notices and Policies

Students with Special Concerns
Students with special concerns - be they athletes who might miss class meetings, students with religious observances that interfere with class meetings, or students with disabilities who need special accommodation - are all supposed to notify us about these special needs by the 12th class day which is 13th September 2013.

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-mail 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 .

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 (video phone). Faculty is not required to provide accommodations without an official accommodation letter from SSD. Please notify us 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 us 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.).

a notice that students with disabilities may request appropriate academic accommodations from the Division of Diversity and Community Engagement (DDCE), Services for Students with Disabilities (SSD) at http://ddce.utexas.edu/disability.

Behavior 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.

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.

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 us in writing during the first week of class.
- In the event of an evacuation, follow the instructions of class instructors.

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