# Syllabus for:
# Scientific & Technical Computing

**Instructors: Victor Eijkhout and Lars Koesterke**

**2020 Fall semester**

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|---|---|
| Number and title | Scientific and technical computing, 56265, 56415 |
| Time and place | online-only, TTh 2:00-3:30pm |
| Listed instructor | Victor Eijkhout |
| | eijkhout@tacc.utexas.edu |
| Co-instructor: | Lars Koesterke |
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## 1 Course Information

The field of scientific and technical computing covers a wide range of topics. Traditionally, it was motivated by the solution of problems arising in simulation sciences (physics, chemistry, various engineering disciplines), which were expressed as ordinary and partial differential equations. More recently, fields such as life sciences, data science, machine learning, have been motivating their own flavors of high performance computing. Despite these different provinances, however, computations show a great deal of commonality.

Thus, this course aims to provide an introductory perspective on the basic tools and techniques of scientific computing. The goal is to give students across a wide range of disciplines skills and background knowledge to perform computations at high efficiency.

The content of this class is roughly divided into two parts: tools, and scientific computing fundamental knowledge.

Fundamental topics for computing include:

- The architecture of a single processor, in particular its memory system. This section will have a practical discussion of the factors that influence the performance of code;
- Computer arithmetic, which is of prime importance to floating point computations. Students will learn both the design of floating point arithmetic, and its implications for computations;
- Parallelism: the structure of parallel computers and theory of parallel computing; discussion of parallelism in applications;

- Linear algebra from a computational point of view;
- Finally, performance and scalability aspects of certain important operations in scientific applications.

Tools discussed include:

- Unix fundamentals including shell scripting;
- Compilers, compiler optimizations, linker conventions and language interoperability;
- Build systems such as Make and CMake;
- The LaTeX ecosystem for documentation;
- Source code control through git and mercurial.
- Time permitting, there can be a discussion of major scientific software libraries.

All sections will incorporate exercises.

Proposed time table:

| Week | Lecture | Segment | Topic |
|---|---|---|---|
| 1 | 1 | | Class intro |
| 2 | 2 | 1 | Architecture |
| | 3 | 3 | Unix basics |
| 3 | 4 | 1 | Architecture |
| | 5 | 3 | Unix scripting |
| 4 | 6 | 1 | Architecture |
| | 7 | 3 | Compilers, intro |
| 5 | 8 | 1 | Architecture |
| | 9 | 3 | Compilers and linkers |
| 6 | 10 | 1 | Architecture |
| | 11 | 3 | Debugging |
| 7 | 12 | 1 | Architecture |
| | 13 | 3 | Make |
| 8 | 14 | 1 | Architecture |
| | 15 | 3 | git |
| 9 | 16 | 1 | Architecture |
| | 17 | 1 | Architecture |
| 10 | 18 | 1 | Architecture |
| | 19 | 3 | LaTeX |
| 11 | 20 | 2 | Computer arithmetic |
| | 21 | 2 | Computer arithmetic |
| 12 | 22 | 2 | Linear algebra: Gaussian elimination |
| | 23 | 2 | Linear algebra: Sparse matrices |
| 13 | 24 | 2 | Linear algebra: iterative methods |
| | 25 | 2 | HPC: parallelism and collectives |
| 14 | 26 | 2 | HPC: scaling of dense operations |
| | 27 | 3 | the PETSc library |
| 15 | 28 | 3 | the PETSc library |

### 1.1 Course Prerequisites

Students must have prior programming experience in Fortran or C/C++, since there will be extensive discussion of the intricacies of compiled languages. Mathematical prerequisites are linear algebra (specifically matrix algebra) for undergraduate students, and basic knowledge of ordinary and partial differential equations for graduate students.

### 1.2 Course Materials

The lecture content is derived from many different sources, including reference manuals, journal articles and conference presentations. The official lectures notes will be the book 'Introduction to High Performance Scientific Computing', by the lead instructor.

All course material will be distributed electronically through this repository:

`https://github.com/TACC/sds335fall2020`

For further reading:

- Scientific Computing: An Introductory Survey, Second Edition by Michael T. Heath, published by McGraw-Hill, New York, 2002, http://www.cse.uiuc.edu/heath/scicomp/notes/ *This book covers methods in applied mathematics and numerical analysis*
- Computer Architecture: A Quantitative Approach, by D. A. Patterson and J. L. Hennessy, Morgan Kaufman Publishers, 1996, ISBN 1-55860-372-2, 760 pp. plus appendices. *This is the standard book about computer design, chip design, memory subsystems*
- Parallel Programming, by Barry Wilkinson and Michael Allen, Prentice-Hall, ISBN 0-13-671710-1 *This book covers parallel architectures and general parallel programming*

### 1.3 Instructors

**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.

**Lars Koesterke** Lars Koesterke joined TACC in the fall of 2007. He is a member of the High Performance Computing (HPC) group, with emphasis on Performance, Evaluation and Optimization of parallel programs. Before coming to TACC, he held positions at the Astronomy Department at The University of Texas at Austin, NASA's Goddard Space Flight Center and the Universities of Potsdam and Kiel (both Germany). His work focuses on serial and parallel optimization, parallel computing with OpenMP and MPI, and Fortran.

**Guest lecturers** There may be occasional guest lectures by other TACC staff.

### 1.4 Homework and Programming Assignment

Assignments will be performed on one or more of TACC's high performance computing resources. Accounts will be handed out during the second week of class.

Students will use their own PCs/Macs/workstations to access the machines through SSH.

### 1.5 Grades

The final grade will consist equally of grades for the three sections, each of which evaluated through a combination (different per section) of small quizzes, class participation, and programming assignments.

As per university policy, incomplete grades will be granted only for work unavoidably missed at the semester's end and only if 70% of the course work has been completed. An incomplete grade must be resolved within eight (8) weeks from the first day of the subsequent long semester. If the required work to complete the course and to remove the incomplete grade is not submitted by the specified deadline, the incomplete grade is changed automatically to a grade of F.

## 2 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 hybrid or in-person components to the class. This specifically includes office hours with the instructors or the TA: these are all conducted online.

**Class attendance and participation policy**

We encourage students to attend the class as it happens, 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.

Students watching the recorded lecture should finish quizzes within 24 hours of the class period.

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.).

Contact Services for Students with Disabilities at 471-6259 (voice) or 1-866-329-3986 (video phone) or reference SSD's website for more disability-related information: `http://www.utexas.edu/diversity/ddce/ssd/for_cstudents.php`

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.