CPS 5401 (CRN 11839)
Introduction to Computational Science
Fall 2021
The University of Texas at El Paso
Xianyi Zeng, Instructor

CPS 5401 provides an introduction to basic computational science skills including the Linux operating system, scientific programming using high level languages, parallel computer architectures, parallel programming paradigms, and numerical libraries.

<table>
<thead>
<tr>
<th>Course number:</th>
<th>CPS 5401 (CRN 11938)</th>
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<tbody>
<tr>
<td>Course title:</td>
<td>Introduction to Computational Science</td>
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<tr>
<td>Credit hours:</td>
<td>4</td>
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<td>Term:</td>
<td>Fall 2021</td>
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</table>
| Time & location:      | Lecture: 17:00–18:20pm TR, online or UGLC 340  
Lab: 16:00–16:50pm T, online or Bell Hall 130 |
| Exam dates:           | Midterm exam: in class 10/07/2021 (tentative)  
Term project due: 11:59pm Sunday, 12/12/2021 |
| Drop deadline:        | Friday, October 29, 2021 |
| Prerequisites:        | Instructor approval  
Recommended: Co-enrollment in MATH 5329 |
| Course fee:           | None |
| Instructor:           | Xianyi Zeng  
Office hour: 14:30–16:00pm TR  
Office location: virtually or Bell Hall 202  
Email: xzeng@utep.edu |
| Teaching assistant:   | Christopher Ibarra  
Office hour: 14:30–16:30pm W  
Office location: virtual meeting only  
Email: caibarra5@miners.utep.edu |
| Course website:       | [http://math.utep.edu/faculty/xzeng/2021fall_cps5401](http://math.utep.edu/faculty/xzeng/2021fall_cps5401) |
| Textbook:             | None. Slides and handouts will be posted on the course website. |
Website: [http://pages.tacc.utexas.edu/~eijkhout/istc/istc.html](http://pages.tacc.utexas.edu/~eijkhout/istc/istc.html) |

**General course format**

Our lectures, lab sessions, and office hours will be delivered in hybrid form. The class will meet in the designated classroom and computer lab whenever possible, but the students are not required to attend in person with possible exception for the midterm exam. Live lecture and lab sessions will be recorded and made available in Blackboard after class, unless otherwise announced. Announcements will be made either via email or Blackboard; the students are required to check the emails and the course shell in Blackboard frequently to keep up-to-date. Course materials except the recorded lectures will be posted on the *course website.*
COVID-19 Precaution Statement
Please stay home if you have been diagnosed with COVID-19 or are experiencing COVID-19 symptoms. If you are feeling unwell, please let me know as soon as possible, so that we can work on appropriate accommodations. If you have tested positive for COVID-19, you are encouraged to report your results to covidaction@utep.edu, so that the Dean of Students Office can provide you with support and help with communication with your professors. The Student Health Center is equipped to provide COVID-19 testing.

The Center for Disease Control and Prevention recommends that people in areas of substantial or high COVID-19 transmission wear face masks when indoors in groups of people. The best way that Miners can take care of Miners is to get the vaccine. If you still need the vaccine, it is widely available in the El Paso area, and will be available at no charge on campus during the first week of classes. For more information about the current rates, testing, and vaccinations, please visit epstrong.org.

Technology requirements
Course content is delivered via the Internet through the Blackboard learning management system (announcement, grade distribution, and recorded lectures), the course website (other course materials), and Zoom (live sessions). The students need to have access to a computer/laptop with functional microphone; a webcam is suggested but not required. The students also need to ensure the UTEP e-mail account is working and that they have access to the Web and a stable web browser. Google Chrome and Mozilla Firefox are the best browsers for Blackboard; other browsers may cause complications. When having technical difficulties, update your browser, clear your cache, or try switching to another browser.

Important: The students are encouraged to contact the UTEP Help Desk (https://www.utep.edu/irp/technologysupport) when they encounter course-irrelevant technical difficulties beyond their scope of troubleshooting.

Network etiquette
As communication online can be challenging sometimes, it’s possible to miscommunicate what we mean or to misunderstand what our classmates mean given the lack of body language and immediate feedback. Therefore, please keep these network etiquette guidelines in mind. Failure to observe them may result in disciplinary action.

• Always consider audience. This is an entry-level class for computational sciences; therefore, all communication should reflect polite consideration of others’ ideas.
• Respect and courtesy must be provided to classmates and to the instructor at all times. No harassment or inappropriate postings will be tolerated.
• When reacting to someone else’s message, address the ideas, not the person. Post only what anyone would comfortably state in a face-to-face situation.
• Blackboard is not a public Internet venue; all postings to it should be considered private and confidential. Whatever is posted on in these online spaces is intended for classmates and instructor only. Please do not copy documents and paste them to a publicly accessible website, blog, or other space.
Course format and attendance
The lecture portion of the class will consist of short lectures interspersed with program demonstrations. Lab assignments will reinforce the lecture material. The lecture and lab exercises will make use of computing facilities at the university to be announced later.

All recorded lecture/lab sessions will be uploaded to Blackboard. Attendance of the lectures is not required except for the midterm exam, which will be announced separately.

In the second half of the course, the students will need to access on-campus computing resource or the CPS computing facility for parallel computations.

Course objectives
The course will cover three major aspects of computational science in three parts:

• Part I consists of a practical introduction to Linux, scientific programming using high level languages, and tools for managing source code and data files.
• Part II covers computer architecture and its implication in writing correct and efficient programs both in serial and in parallel.
• Part III involves parallel programming using both OpenMP and MPI.

Grading
The final grade for the course will be based on the following:

• 30% homework.
• 20% lab assignments.
• 20% midterm exam.
• 30% term project.

Late homework or lab assignments will be not accepted under any circumstances. However, the lowest among all homework scores and the lowest among all lab assignment scores will be dropped towards calculating the final grade.

Missed exam cannot be made up, either; exceptions can be given only in extraordinary and unavoidable circumstances with reasonable proofs, and with advance notice in written.

The term project will be announced in the middle of the semester and submission is due by the end of December 12th, 2021. Aspects of the project will be discussed throughout the semester and the students are encouraged to start building the product as early as possible. Students will form groups of two (or three, in case there are odd number of students) to work on the project. Each group must submit one copy of the project; whereas each student must submit a report that specifies individual work.

The letter grade will be guaranteed at the following levels: A (90 - 100%), B (80 - 89%), C (70 - 79%), D (60 - 69%). Depending on circumstances, the thresholds for each of the four letter grades could be lowered, but will be equal among all students. The letter grade F will be given if the final score does not reach the D threshold.

Accommodations for students with disabilities
If the student has a disability and need classroom/exam/homework accommodations, please contact The Center for Accommodations and Support Services (CASS) at 747-5148, or by email to cass@utep.edu, or visit their office located in UTEP Union East, Room 106. For additional information, please visit the CASS website at http://www.sa.utep.edu/cass.
Academic honesty policy
The students are required to understand the UTEP academic honesty policy. Sharing ideas are encouraged among the students; but collaboration of any form in the written homework, lab assignment, and exam is strictly prohibited. If the instructor has reason to believe that the students have cheated on the exam, and if the homework or program code is suspected of being duplicated or copied, the case will be referred to the Dean of Students for adjudication.

Military statement
A military student with the potential of being called to military service and/or training during the course of the semester, the students are encouraged to contact as soon as possible.

Course drop deadline
October 29 is the university fall drop/withdrawal deadline. The college of science will not accept drop/withdrawal requests of any form after October 29.

Course topics
1. Linux:
   - Shell commands, environment variables, and shell programming;
   - File system and job control;
   - Build system and source code control.
2. Scientific programming languages:
   - Compiling and linking; C and C++;
   - Python and SciPy;
   - Scientific libraries for linear algebra tasks.
3. Computer architecture:
   - Cache-based microprocessors;
   - Memory hierarchy;
   - Shared memory parallel computers;
   - Distributed memory parallel computers.
4. Parallel programming paradigms:
   - Data and task parallelism;
   - Shared memory parallel programming using OpenMP;
   - Distributed memory parallel programming using MPI.

Learning outcomes
1. Manage program and data files on a Linux system.
2. Implement basic matrix operations and linear algebra algorithms in the C/C++ scientific programming language.
3. Implement scientific programming workflows using Python.
4. Select the appropriate computer architecture and programming model for a given problem.
5. Implement basic matrix operations and numerical linear algebra algorithms in parallel on shared and distributed memory computers using C/C++ together with OpenMP (shared memory) and MPI (distributed memory).
6. Call linear algebra library routines correctly from a program written in C/C++.
Course schedule
Below is a tentative schedule for this course.

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<th>Week 01 (08/24, 08/26)</th>
<th>Introduction to Linux. The Unix shell.</th>
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<tr>
<td>Week 02 (08/31, 09/02)</td>
<td>The Unix shell. The C programming language.</td>
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<td>Week 03 (09/07, 09/09)</td>
<td>The C programming language.</td>
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<td>Week 04 (09/14, 09/16)</td>
<td>The C programming language. Review of numerical linear algebra.</td>
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<td>Week 05 (09/21, 09/23)</td>
<td>Scientific libraries. The C++ programming language.</td>
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<td>Week 06 (09/28, 09/30)</td>
<td>The C++ programming language. GNU Make. CMake.</td>
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<td>Week 07 (10/05, 10/07)</td>
<td>The version control system. Midterm exam.</td>
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<td>Week 08 (10/12, 10/14)</td>
<td>Single-processor architecture.</td>
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<td>Week 09 (10/19, 10/21)</td>
<td>Multicore architecture.</td>
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<td>Week 10 (10/26, 10/28)</td>
<td>Parallel computing with OpenMP.</td>
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<td>Week 11 (11/02, 11/04)</td>
<td>Parallel computing with OpenMP. Parallel computing with MPI.</td>
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<td>Week 12 (11/09, 11/11)</td>
<td>Parallel computing with MPI.</td>
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<td>Week 13 (11/16, 11/18)</td>
<td>Python.</td>
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<td>Week 14 (11/23)</td>
<td>Application of Python in SVM or ANN.</td>
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<td>Week 16</td>
<td>Work on the term project. No final exam.</td>
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