CSC 435 / S22 High Performance Scientific Computing

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I feel the need, the need for speed. - Maverick and Goose, "Top Gun"

CSC 435 is a course to introduce students the foundational principles of High Performance Scientific Computing. Students in CSC 435 will be exposed to the fundamentals of single machine code optimization as well as coding techniques for shared memory parallel programming, distributed memory parallel programming, and massively parallel architectures. Much of the course will focus on parallel programming strategies for large scale numerical problems encountered in science and engineering. The use of public domain libraries and packages for message passing and numerical computation will be demonstrated. Symbolic algebra packages like *Octave* and *Mathematica* will also be used in the class to develop parallel numerical algorithms.

Students taking CSC 435 are expected to have a working knowledge of a high level programming language such as C, C++, Fortran, or JAVA. To assure complementarity with existing numerical and parallal API's, all coding will be done in C/C++ and a modern implementation of Fortran. Strategies for high performance code development and project management with these languages will be discussed during the course. Students in CSC 435 are expected to read at the college level and also have a working knowledge of differential and integral calculus as well as a knowledge of numerical analysis commensurate with completion of CSC/MAT 335. Topics from multivariable calculus, linear algebra, and differential equations will be introduced as needed.

Class Meeting Times and Locations

Lecture: MWF 11:15 a.m. – 12:05 p.m., Room 218 GSC

Course Materials

REQUIRED: Introduction to High Performance Computing for Scientists and Engineers, Hager and Wellein RECOMMENDED: Pthreads Programming, Buttlar, Ferrill, and Nichols Scientific Calculator Reference Material from Class Webpage (http://theochem.mercer.edu/csc435)

Course Structure

Topics from fourteen chapters of the texts will be covered during the semester in the order listed on the class schedule. The lecture time will be used to expound on and augment the text, discuss problem solving strategies, and demonstrate algorithms. A significant amount of the class period will be devoted to actually utilizing the parallel computing cluster and HPC systems. Students are responsible for all material covered in class as well as the material from the textual sections listed in the class schedule. Several small exercises and three semester-long projects will be submitted for grading. Each of the semester long projects will have multiple deliverables and due dates. One of the semester-long projects will be a group collaborative project. Students will also be required to do a presentation related to their components of the group project. The details of each project and the description of the deliverables for each project will be provided to the students in writing. A midterm and a final exam will be administered per the class schedule.

Grad	ling	
	In-Class Assignments/Homework	$20\% \\ 60\% \\ 10\%$
	Programming Projects/Papers	
	Midterm Exam	
	Final Exam	10%
	Total Possible	100 %
	The following grading scale is assure $\mathbf{A} \ge 90 \%$	ed but may be slightly lowered based on test results.
	$\mathbf{B}+ \stackrel{-}{\geq} 88 \%$	
	$\mathbf{B} \geq 80 \%$	
	$C+ \geq 78 \%$	
	$\mathbf{C} > 70 \%$	

$\mathbf{D} \geq 60 \%$

F <60 %

General Information

Honor Code: All students in CSC 435 are expected to adhere to the Mercer University Honor Code. Any suspected violations will be reported to the Honor Council for further investigation.

Many students have difficulty in determining how to apply the Mercer honor code to Computer Science courses. A few general guidelines should help you in deciding whether you are violating the honor code or not.

- 1. You are allowed to receive help on your programs from other students, provided the purpose of the help is to help you understand your own program better, not to write your program for you.
- 2. You are NOT allowed to use copies of programs written by other students, or copies of programs from published sources unless you are explicitly given permission to do so, even if you plan to modify them extensively.
- 3. You are NOT allowed to give copies of your programs, or parts of your programs, to other students in any form.
- 4. In short YOU MUST WRITE YOUR OWN CODE. DO NOT COPY PROGRAMS OR PARTS OF PROGRAMS FROM ANY SOURCE UNLESS I TELL YOU TO DO SO. If you have any questions about using a published resource, just ask me.
- 5. Any attempt to gain unauthorized access to the computing systems or to in any way damage the parallel computing systems and job schedulers so as to hinder the work of others will not only result in an honor code violation but will infringe upon intellectual property rights and **could result in criminal prosecution**.

Any violation of the above policies will be treated as academic dishonesty and a violation of the Mercer Honor Code.

Attendance: Attendance will be taken the first three weeks of class and then randomly during the semester. The attendance grade will based on the percentage of absences on the randomly chosen days. For each 10 pecentage points below 100%, the students final letter grade will drop one letter grade. At a minimum, attendance will be taken on ten days of class. Students are still accountable for all material covered in class as well as any announcements made during the lecture period.

Missed Exams: Anyone missing an exam for *any* reason (personal illness, death in the immediate family, or other emergency) must notify Dr. Pounds in advance. The absence will be considered unexcused otherwise. Make-up exams will be individually scheduled.

Partial Credit: Partial credit will not be awarded on any exam unless individuals show their work and clearly delineate how they arrived at their answers.

Re-grading Policy: If a student suspects that an error was made in the grading of a submitted work, they may return the paper for re-grading with the understanding that the entire work will be re-graded and not only the portion in question.

Posting of Grades: Grades will not be posted. If you are curious about your cumulative grade, see Dr. Pounds.

E-mail Listserve: I maintain an e-mail listserve which I use use copiously to send information to the class and which you can use to communicate with each other. To sign up for the listserve and to learn how to send information to it, please go to: http://theochem.mercer.edu/mailman/listinfo/csc435.

GitLab: Students must maintain their programming projects on the departmental *GitLab* server name anvil.cs.mercer.edu. Specific instructions on how the repositories should be structured will be included in in each assignment description. Code for this class will be submitted via anvil.

Class Web Page: I maintain a web page for the class outside of the University CANVAS system with I regularly update with material for the class. I address is http://theochem.mercer.edu/csc435. I will notify the class whenver changes are made to this web page. CANVAS will be used for turning in any in-class assignment or papers.

Course Evaluations: In an ongoing effort to improve the quality of instruction, each student enrolled in this course is required to complete an end-of-semester course evaluation. Details about the evaluation process will provided at the end of the term.

Final Exam: The final exam is scheduled for Tuesday, May 3rd at 2 p.m.

University Compliance Statements

Accommodations and ADA/504: "Students in need of accommodation due to a disability should contact the Access and Accommodation Office to complete the verification process to become approved for services. In order to receive accommodations, each term, students will request accommodation and faculty notification forms through the Access Office online system Accommodate. Students are strongly encouraged to schedule a meeting with each professor in a timely manner to discuss arrangements. Accommodations are not retroactive in nature. Note - Disability accommodations or status are not reflected on academic transcripts. Students with a history of a disability, perceived as having a disability or with a current disability who do not wish to use academic accommodations are also strongly encouraged to complete the verification process with the Access Office. Students must request accommodations in a timely manner to receive accommodations in a timely manner.

The Access Coordinator for Macon Campus is

Katie Johnson, Director and ADA/504 Coordinator. Phone: (478) 301-2778; email: johnson_kc@mercer.edu Website: https://access.mercer.edu

Please note the following additional information from the Access and Accommodation Office (AAO):

In compliance with Section 504 of the Rehabilitation Act of 1973 (504) and the Americans with Disabilities Act Amendments Act of 2009 (ADAAA), "otherwise qualified" students with disabilities are protected from discrimination and may be entitled to "reasonable accommodations" intended to ensure equal access to all courses, programs, and services without a change of curriculum. Examples of accommodations include but are not limited to: testing accommodations, providing alternative format textbooks and tests, note-taking support, and modifications of policies or procedures. Equal Access may require moving a class or event to a physically accessible room, making websites accessible to screen readers, providing sign language interpreters, and captioning videos. All students requesting to be recognized as a student with a disability or requiring accommodations must first self-identify by requesting accommodations with the designated Access Coordinator for their campus or program and complete the verification process."

Mental Health and Wellness: "Mercer University faculty and staff recognize that mental health concerns can impact academic performance and interfere with daily life activities. Please notify your faculty member or academic advisor for academic assistance, as needed. The office of Counseling and Psychological Services (CAPS) can also provide support if you are feeling stressed, overwhelmed, anxious, depressed, lost, or are struggling with personal issues. Please call (478) 301-2862 or visit the CAPS website for more information. These services are free and confidential, and support non-traditional, graduate, and undergraduate students. The CAPS office on the Macon campus is located in Linden House (attached to the MEP Residence Hall)."

Electronic Submission of Materials: "Students bear sole responsibility for ensuring that papers or assignments submitted electronically to a professor are received in a timely manner and in the electronic format(s) specified by the professor. Students are therefore obliged to have their e-mail client issue a receipt verifying that the document has been received. Students are also strongly advised to retain a copy of the dated submission on a separate disk. Faculty members are encouraged, but not required, to acknowledge receipt of the assignment."

Cell Phones and Pagers: "Out of courtesy for all those participating in the learning experience, all cell phones and pagers must be turned off, or placed on vibrate, before entering any classroom, lab, or formal academic or performance event."

FERPA and Assessment: The College of Liberal Arts is keenly interested in assuring the quality and integrity of its general education program. Every semester, randomly selected samples of student work from general education courses will be independently and objectively assessed. No personally identifiable information about any student will be used for the purposes of this assessment, and assessment results will have no bearing whatsoever on student grades.

Tentative Class $Schedule^1$

Week Starting	Chapter	Lecture Topics
January 9 th	Chapter 1 [HPC]	Introduction
		Numerics and the Dusty Deck
		Code Maintenance
		Code Timing
January 16 th	Chapter 2 [HPC]	Single Processor Tuning
-		Performance Tuning Tools
		Cache and Memory Optimization
		Compiler Switches and a review of <i>makefiles</i>
January 23 rd	Chapter 3 [HPC]	Data Access
		Loop Optimization
		Interlanguage Communication
		Vector Computers, SIMD, and Pipelines
January 30 th	Chapters 4 and 5 [HPC]	Parallel Computers
		Basics of Writing Parallel Code
February 6 th	Chapters 1 and 2 [PTH]	Introduction to <i>Pthreads</i>
		Designing Threaded Programs
		Embarassingly Parallel Computations
		Monte Carlo Integration
February 13 th	Chapter 3 [PTH]	Mutexes, Deadlock, Barriers,
		and Syncronization
		Data Dependence
February 20 th	Chapter 6 [HPC]	Introduction to OpenMP
February 27 th	Chapter 7 [HPC]	Data Dependencies
		MIDTERM EXAM, $3/4/22$
March 6 st		SPRING BREAK
March 13 th	Chapter 9 [HPC]	Introduction to MPI
		Preparations for Parallel Cluster Work
		Network Mapping and Characteristics
March 20 th	Chapter 10 [HPC]	Data Dependence, Location, and Placement
		Work and Data Decomposition
		Locating Parallel Regions
March 27 nd		Distributed Barriers and Synchronization
		Performance Tuning
		Benchmarking Cluster Calculations
April 3 rd	Special Topic - CUDA	Introduction to Massively Parallel Computations
		Environment Setup, CUDA Hardware
		Memory Structure, Code Management,
		Data Locality, Placement, and
		Memory Management
April $10^{\rm th}$		Optimizing CUDA Code
		CUDA Kernels and Hardware
		Benchmarking CUDA
April 17 th	Chapter 11 [HPC]	Hybrid High Performance Computing
April 24 th		Benchmarking Hybrid Code
May 1 st		FINAL EXAM, 5/3/22, 2 p.m.
		(Tuesday)

 $^{^{1}\}mathrm{I}$ reserve the right to modify this schedule as situations warrant.

University Health and Safety Protocols for the Spring 2022 Semester

Office of the Provost 478-301-2110

Campus Health's 24/7 COVID-19 Hotline 478-301-7425

The Pledge

All students are expected to commit to the following pledge:

I pledge to protect myself and others by following the safety guidelines put forth by the University.

I pledge to protect myself and others by reporting immediately to the Campus Health COVID-19 Hotline (478-301-7425) if I become symptomatic of COVID-19. I pledge to test for COVID-19 as directed by the University and isolate until cleared by Mercer Medicine if I test positive for the coronavirus.

I pledge to protect myself and others by respecting the rights of others and acting responsibly to reduce the spread of COVID-19.

Students are expected to monitor and adhere to all policies and guidelines pertaining to COVID-19 found on the <u>University's COVID-19 website</u>.

Violations of these policies may include but are not limited to the following:

- A review of the University's student code of conduct charges
- Removal of a student from a particular University activity
- A registration hold on a student's account
- Deactivation of a student's Bear Card
- Dismissal from class
- A review of the standards of professional conduct penalties (by academic program)

Violations of any policy should be reported immediately to

- o the Student Affairs professional in your academic area,
- o the Office of Student Affairs (Macon 478-301-2685 or Atlanta 678-547-6823),
- the Director of Regional Academic Center Operations, Mr. Scott Mahone, at 678-547-6551 (for Center students),
- o or Mercer Police (Macon 478-301-2970 or Atlanta 678-547-6358).

What You Need to Know

In order to promote safe campuses, students are required to follow these COVID-19 protocols:

- As COVID-19 conditions evolve, the University will post updates on our <u>COVID-19 website</u>. Also, please continue to check your Mercer email frequently for important messages.
- Each faculty member has the authority to decide if masks are required during class meetings and advising.
- If you are vaccinated for COVID-19, submit a copy or photo of your vaccine card to <u>myvaccine@mercer.edu</u>. Type your full legal name and MUID in the subject line of the email.
- If you are <u>symptomatic of COVID-19</u>, whether vaccinated or unvaccinated, you cannot attend inperson classes, labs, orientations, clinical/field experiences, other on-campus activities, or work on campus. You should immediately call Campus Health's 24/7 COVID-19 Hotline at (478) 301-7425 for a testing appointment or get tested immediately at an off-campus location.

If you are <u>asymptomatic</u> and would like to get tested, go to <u>go.mercer.edu/covidappt</u> to schedule an appointment at the Macon or Atlanta Campus Health Center.

There have been recent changes to insurance coverage for COVID-19 testing. As a result, Mercer Medicine will bill your insurance company for COVID-19 testing if you are symptomatic or have been exposed recently to someone who has tested positive for COVID-19. If you are tested for other reasons, you will be required to pay \$90 at the time of testing.

- Testing locations:
 - o Macon Campus Health Center, Drake Field House, Macon Campus
 - Atlanta Campus Health Center, Sheffield Building, Atlanta Campus
 - Savannah Memorial University Medical Center, Savannah Campus (Drs. Shelly or Baxter)
 - Columbus Mercer University School of Medicine, Columbus Campus (Dr. House)
 - Henry and Douglas Counties Contact the Provost's Office at <u>provost@mercer.edu</u> for a list of testing facilities near the Mercer centers.
- An off-campus test must be a <u>nasal swab PCR test.</u> Mercer Medicine does not accept antigen tests (known as rapid tests) or antibody tests.

All students must provide off-campus, **positive COVID-19 results** to Campus Health at <u>mytestreport@mercer.edu</u>. In the subject line of the email, type "Macon Test" (for Macon, Savannah, and Columbus students) or type "Atlanta Test" (for Atlanta, Henry, and Douglas students). Be sure to include your full legal name and MUID in the body of the email.

- If you have a health or other disability-related reason that would warrant a reasonable accommodation with respect to <u>COVID-19 testing</u>, please contact the Office of the Provost at <u>provost@mercer.edu</u> or 478-301-2110.
- As you remember, the University discontinued mandatory surveillance testing during the fall semester. If
 mandatory surveillance testing is reinstated, you will be informed of the requirement via your Mercer email
 and the University's COVID-19 website. The University will cover the cost of surveillance testing.
- If you test at the Campus Health Center and are positive, a Campus Health staff member will call you from a Mercer phone number with the positive results. With negative results, you will receive an email in your Mercer email account.
- Students <u>do not submit COVID-19 results</u> directly to faculty, the Dean's Office, or Student Affairs for <u>COVID-related</u>, excused absences. All COVID-related absences must be processed through Campus Health and the Office of the Provost. Faculty are then notified of a student's COVID-related, excused absence(s).
- Faculty are required to provide academic accommodations to students who are in isolation after either testing positive at the Campus Health Center or submitting off-campus, positive test results to Campus Health at mytestreport@mercer.edu. Also, if a symptomatic student has been tested and is awaiting results, the student must isolate and be provided academic accommodations during this brief isolation period.
- You must be cleared from isolation by Campus Health/Mercer Medicine before you can return to campus.