Syllabus for Introduction to Scientific Computing
Math/CS 471
Fall, 2019, University of New Mexico
Version 1, Dated August 12, 2019

Time and Place: Tuesday/Thursday, DSH 144, 9:30am-10:45am

Course webpage: http://math.unm.edu/~schroder/2019_Fall_471/index.html

Instructor: Prof. Jacob B. Schroder, jbschroder@unm.edu

Office Hours: SMLC 332

1. Tuesday: 11:30am-1:00pm
2. Wednesday: 2:30pm-4:00pm
3. By request

Please note that I highly respect parents who are also students. Children are always welcome at my office hours, and I usually have a few toys from my son lying around.

Prerequisites:

1. Math 314 or Math 321 or Math 316 AND
2. Programming skills.

Text (optional): V. Eijkhout (with E. Chow and R. van de Geijn), Introduction to High Performance Scientific Computing
https://zenodo.org/record/49897/files/EijkhoutIntroToHPC.pdf

Important Dates:

- CARC Tutorial on Sept. 17 and 20 [attend only one tutorial]
- Fall Break: October 10th and 11th [No class on Thursday, October 10th]
- Thanksgiving Break: November 28th and 29th [No class on Thursday, November 28th]
- **Final Project Due: Tuesday, December 10 at midnight Mountain Standard Time**

Course Description: This is an introductory course in scientific computing. The course is broad and exposes you to a variety of concepts and algorithms for scientific computing, covering hardware, software, and an emphasis on parallel programming.

This is a required course for all mathematics majors with a concentration in Computational Mathematics.

Schedule of Topics:

Part 1

- Overview of Linux shell computing, remote logins, version control, etc…
- Structure of a standard report for scientific computing using Latex
- Iterative methods and measuring convergence
  - Solving nonlinear systems with Newton's method
- Usage of community-standard numerical Python (Matplotlib, NumPy, SciPy)
  - Usage of PDB debugger
- Numerical quadrature (Newton-Cotes, Gauss Quadrature, Curtis-Clenshaw)
- Finite differencing and sparse linear algebra
  - Usage of compressed sparse row matrices for finite differencing
- Numerical timings of finite difference computations in Python

Part 2

- Introduction to parallel computing
  - Threaded programming versus message passing
  - Parallel computing at CARC
- Computing finite difference approximations in 2D
  - Impact of 2D stencil on parallel communication
- Ordinary differential equations
  - Euler's method, Runge-Kutta methods, stability regions
  - N-body problems
- Iterative methods for linear systems
  - Jacobi, Gauss-Seidel, possibly more
- Time-dependent numerical partial differential equations
  - Simulate heat equation and/or wave equation
  - Use threaded-level parallelism
  - Use message-passing parallelism
- Parallel performance studies: weak and strong scaling
- Advanced topics as time allows (e.g., multigrid, Monte Carlo, etc…)

Goals:

- Introduce you to the field of scientific computing. Broadly speaking, this means teaching you how to apply numerical methods to carry out computational simulations, often of real-world phenomena (like heat transfer or waves).
  - Understand how to apply parallel computing resources to carry out these simulations in a fast and efficient manner
- Teach you how to write and document scientific computing projects in well-organized reports using Latex.

Learning Outcomes

- Understand both the mechanics and mathematical theory behind key numerical techniques for scientific computing (e.g., iterative methods, ODEs, finite-difference approximations, quadrature/integration)
  - Know how to implement these numerical techniques
- Understand how machine architectures impact the performance and design of scientific software, e.g., shared memory versus distributed memory
- Have hands-on experience using scripting to both automate your computations and analyze your computational results.
- Understand some aspects of performance optimization for scientific computing
- Understand the basic concepts of parallel computing and know how to write parallel programs for shared and distributed memory models.
  - Have implemented a parallel program on a large-scale computer.
- Understand how to use Latex to document and effectively describe a scientific computing project using precise, logically correct, and clear statements.

Grading: Your grade for this course is based on 5 homework sets (600 points), a final project (200 points), and in-class work and attendance (50 points). This allows for a total of 850 points.

The final grade for the class will be based on each student's percentage of the total points available. Letter grades will be assigned as follows:

- A, 90% or above
- B, 80% or above
- C, 70% or above
- D, 60% or above
- F, below 60%

The instructor reserves the right to curve grades to offset unforeseen circumstances. Such a curve will never decrease a student's letter grade below that from the above scheme.

Homework/Project: There will be 5 sets of homework assignments and one final project. They have the following point values, 50, 100, 150, 150, 150, 200, respectively, making a total of 800 points. Each homework and the project may consist of a combination of theoretical problems and programming tasks.

You are strongly encouraged to work in pairs (a group of two students) for the homework and project, and hand in a single report. It is expected that both of you can explain the material and the computer outputs. Groups of more than two students are not allowed. For the write-ups of the assignments we will use a version control system.

Homework may be submitted late up to a week for 50% credit. ***Homework grading disputes must be submitted in writing within one week after the work is returned.***

Software: The languages used for this course are ***MPI and Python***.

Credit Hour Statement: This is a three credit-hour course. Class meets for two 75-minute sessions of direct instruction per week for fifteen weeks during the Fall 2019 semester. Students are expected to complete a minimum of six hours of out-of-class work (or homework, study, assignment completion, and class preparation) each week.

Absences Policy: It is expected that each student regularly attend class.

- Course follows UNM handbook https://handbook.unm.edu/d170/
- Note, the handbook says "A student with excessive absences may be dropped from a course by the instructor with a grade of W/P or W/F."
- If you need to miss more than two classes during the semester, please contact the instructor.

Academic Integrity: Each student is expected to maintain the highest standards of honesty and integrity in academic and professional matters. The University reserves the right to take disciplinary action, including dismissal, against any student who is found responsible for academic dishonesty or otherwise fails to meet the standards. Any student judged to have engaged in academic dishonesty in course work may receive a reduced or failing grade for the work in question and/or for the course.

Academic dishonesty includes, but is not limited to, dishonesty on quizzes, tests or assignments; claiming credit for work not done or done by others; and hindering the academic work of other students; misrepresenting academic or professional qualifications within or

without the University; and nondisclosure or misrepresentation in filling out applications or other University records.

Accommodation Statement and Americans with Disabilities Act: In accordance with University Policy 2310 and the Americans with Disabilities Act (ADA), academic accommodations may be made for any student who notifies the instructor of the need for an accommodation. It is imperative that you take the initiative to bring such needs to the instructor's attention, as I am not legally permitted to inquire. Students who may require assistance in emergency evacuations should contact the instructor as to the most appropriate procedures to follow. Contact Accessibility Resource Center at 277-3506 or http://arc.unm.edu for additional information.

If you need an accommodation based on how course requirements interact with the impact of a disability, you should contact me to arrange an appointment as soon as possible. At the appointment, we can discuss the course format and requirements, anticipate the need for adjustments and explore potential accommodations. I rely on the Disability Services Office for assistance in developing strategies and verifying accommodation needs. If you have not previously contacted them I encourage you to do so.

Title IX: In an effort to meet obligations under Title IX, UNM faculty, Teaching Assistants (TAs), and Graduate Assistants (GAs) are considered "responsible employees" by the Department of Education (see page 15, http://www2.ed.gov/about/offices/list/ocr/docs/qa-201404-title-ix.pdf). This designation requires that any report of gender discrimination which includes sexual harassment, sexual misconduct and sexual violence made to a faculty member, TA, or GA must be reported to the Title IX Coordinator at the Office of Equal Opportunity (http://oeo.unm.edu). For more information on the campus policy regarding sexual misconduct, see: https://policy.unm.edu/university-policies/2000/2740.html

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Citizenship and/or Immigration Status: All students are welcome in this class regardless of citizenship, residency, or immigration status. Your professor will respect your privacy if you choose to disclose your status. As for all students in the class, family emergency-related absences are normally excused with reasonable notice to the professor, as noted in the attendance guidelines above. UNM as an institution has made a core commitment to the success of all our students, including members of our undocumented community. The Administration's welcome is found on our website: http://undocumented.unm.edu/

Disclaimer: I reserve the right to make reasonable and necessary changes to the policies outlined in this syllabus. Whenever possible, the class will be notified in advance of such changes. An up-to-date copy of the syllabus can always be found on the course website. It is your responsibility to know and understand the policies discussed therein and to be up-to-date. If in doubt, please ask questions.