CS4/591:Special Topics: High Performance Computing

Last changed on December 4, 2024

Lectures will be held in the CARC workshop room (1601 Central Ave).

Contents

1 Lecture Slides

- Lecture 1: A Brief History
- Lecture 2: iDRAC
- Lecture 3: Configure Your Linux Machine
- Lecture 4: Vector Operations and User Accounts
- Lecture 5: Devices
- Lecture 6: Filesystems
- Lecture 7: Networking
- Lecture 8: Anatomy of a Machine Room
- Lecture 9: Booting and the Kernel
- Lecture 10: Systemd
- Lecture 11: Compiler Optimisation
- Lecture 12: Shared Memory Parallelism
- Lecture 13: Process and Resource Monitoring
- Lecture 14: Slurm
- Sample Midterm
- Lecture 15: Warewulf
- Lecture 16: Slurm Installation and Configuration
- Lecture 17: High Performance Linpack
- Lecture 18: Distributed Computing
- Lecture 19: Scaling
- Lecture 20: GPU Computation
- Lecture 21: HPCG and Singularity
- Lecture 22: Network Throughput and RAID
- Sample Final

2 ChangeLog

1. Updated Schedule for Second Half (2024-9-23)
2. Added Lecture Slide Links Up Front (2024-9-22)
3. Specified that Ryan's office hours are on Fridays (2024-9-18)
4. Added Homework 3 dates (2024-9-18)
5. Corrected typo in due date for Homework 2 (2024-9-11)
6. Added Project Assistant Info (2024-9-6)
7. New presurvey link added (2024-9-6)
8. Removed the erroneous 18 hours expectation under Time Expectations (8/18/2024).
9. Added Overleaf and JupyterHub links under Resources (2024-8-18).
10. Changed office hours (2024-08-18).

3 Description

This course is a senior/grad level introduction to high performance computing (HPC). The goal of the course is to familiarise students with building a cluster and how modern hardware architectures impact software performance. The skills taught in this course will prepare students to enter the HPC workforce as systems engineers and to better understand how to optimise code for use on HPC systems as end users. Topics include basics of Linux and its administration, building a high-performance computing cluster, optimisation of compiled code for HPC architectures (caching and

accelerators), deployment and use of industry standard HPC tools such as spack, Slurm, warewulf, and hardware aware deployment. We will use benchmarks such as stream and HPL to understand the hardware. This course will not go into detail on MPI since that is covered in the Parallel Processing Course. Most of the work for this course will be team project based since that reflects the reality of devops for most professional systems analysts and programmers.

This syllabus is intended to make course expectations and policies clear so that you, the student, have the best chance possible of meeting those expectations. If anything is unclear please let me know so I can update the syllabus accordingly.

This syllabus is likely to be revised throughout the semester.

4 Contacts and Office Hours

Instructor: **Research Associate Prof. Matthew Fricke**
Email: mfricke@unm.edu
Website: http://www.cs.unm.edu/~mfricke
Office Hour: Friday 10-11am. Farris Engineering Center 3330.

Class Assistant: **Maisy Dunlavy**
Email: mdunlavy@unm.edu
Office Hour: Noon-1:00pm, Wednesdays
CARC Workshop Room

Project Assistant: **Ryan Scherbarth**
Email: rscherbarth@unm.edu
Office Hour: Fridays, 2:00-3:00pm.
Farris Engineering Center 3320

5 Format

This is a three credit hour course consisting of three 50 minute lectures per week to be held on Monday, Wednesday, and Friday at 11:00am.

5.1 Classroom and Workstations

Classes will be held in the CARC workshop room. This workshop room is equiped with Linux workstations that you will be expected to use for in class assignments. You are welcome to being a laptop to class, but due to the variety of possible OS configurations I will not be able to help you carry out the in class assignments on your laptop.

Adjacent to the workshop room is the Roadrunner room. The Roadrunner room houses the class clusters. The Roadrunner room also houses sensitive equipment for CARC. You will not be permitted access to the Roadrunner room unless I am present. After the first 2 weeks physical access should become unnecessary.

5.2 Curriculum Format

Classes will be taught using a mixture of lectures and hands on activities. The material you will learn is divided into two areas: 1) Linux and HPC Cluster Management and 2) High performance application management and benchmarking. Material on each topic will be presented each week. At first you will conduct your benchmarking on the UNM CARC clusters, but once your own clusters are deployed you will include them in your application deployment and benchmarking tasks.

5.3 Individual Homework

During the course you will be assigned homework to complete individually. See the "What I allow" section for guidelines, but you must write up the assignment in your own words, plots and/or code (i.e don't copy).

5.4 Team Projects

You will be assigned to a team for each project. Team membership will change for each project. Random assignment is essential for determining final grades. Requests to work with particular students will not be entertained. Projects will be assigned on Fridays. Your team will be given two weeks to complete your project with a progress update due on the first Friday.

5.5 Presentations

During the last week of the semester and the final exam week teams present the report from one of their projects. The audience will be HPC experts from industry, academia, and the national labs.

5.6 Exams

From time to time I will give in class exams. Exams will be announced at least 2 weeks ahead.

6 Resources

6.1 Slack Workspace

The slack workspace serves several purposes. 1) I will make announcements about the class on slack. There is no guarantee that I will also make those announcements in class. I may also make announcements in class that are not repeated on slack. You are responsible for both. 2) Slack allows class-wide discussion. Feel free to post questions about the material presented in class, the code you are writing for your assignments, and logistic questions related to the class.

Join the class slack workspace

6.2 Center for Advanced Research Computing (CARC)

CARC is the UNM high performance computing center. All students will be provided with a CARC account so you can compare the performance of the code you build on different hardware.

Create a CARC account

6.3 Overleaf

Assignments will be distributed through Overleaf. If you associate your CS email address with your overleaf account you get the premium version.

6.4 Jupyter Notebooks

You will use Jupyter Notebooks to make plots for your homework and projects. You can install jupyter on your own machine or use JupyterHub on the Wheeler or Hopper CARC clusters.

6.5 Class Cluster

Students will be assigned to teams. Each team will be responsible for assembling and configuring their own small cluster using parts provided by CARC. The cluster will be housed in the Roadrunner room at CARC but teams will be able to access their assigned cluster remotely. These clusters will be used over the course of the semester. Team composition will change each project.

7 Schedule

This is the planned schedule, any changes will be recorded here.

The schedule will follow two parallel tracks. 1) Building and Administering an HPC cluster, and 2) HPC Applications. Each week we will cover topics in each. This is so you don't have to wait until you have deployed your clusters to start learning about how they are used. The goal is to have these two track merge at the end of the semester.

For UNM semester dates and deadlines are here:
https://registrar.unm.edu/semester-deadline-dates/fall-2024.html

7.1 Week 1 (Aug 19 - 25): Introduction

General

- Presurvey: Presurvey
- Course Introduction
- Syllabus Review
- Running on CARC Systems
- A Brief History of HPC

Lecture Slides

- Lecture 1: A Brief History

Assignments

- Homework 1 Assigned. Complete the Presurvey. Due by Monday 9th, Sept at 5:00pm.

7.2 Week 2 (Aug 26 - Sept 1st)

System Administration

- IPMI, iDRAC

Lecture Slides

- Lecture 2: iDRAC
- Lecture 3: Configure Your Linux Machine

Assignments

- Homework 1 Presurvey. Due by Monday 9th, Sept at 5:00pm.

7.3 Week 3 (Sept 2 - Sept 8)

Sept 6th - Last Day to Add Classes. Last day to DROP without "W" grade and receive a 100% tuition refund

System Administration

- Linux: Devices, Disks

Applications

- Vector Operations

System Administration

- User Accounts

Lecture Slides

- Lecture 4: Vector Operations and User Accounts
- Lecture 5: Devices

Assignments

- Homework 2 on Vector Instructions Assigned. Due before Midnight on Sunday, Sept 15th.

7.4 Week 4 (Sept 9 - 15)

System Administration

- Linux: Filesystems
- Linux: Networks and Network Configuration
- Linux: Infiniband

Applications

- Compiler Optimisations

Lecture Slides

- Lecture 6: Filesystems
- Lecture 7: Networking

7.5 Week 5 (Sept 16 - 22)

System Administration

- Linux: The Kernel

Applications

- Timing and Profiling (gcov and gprof)
- Top Down Optimisation

Lecture Slides

- Lecture 8: Anatomy of a Machine Room
- Lecture 9: Booting and the Kernel

Assignments:

- Homework 3 assigned Friday, Sept 20th. Due by 11:59pm Friday, Sept 27th. Turn the HW in using Canvas Dropbox. Canvas will reject submissions after 11:59pm Sept 27th.

7.6 Week 6 (Sept 23 - 29)

System Administration

- Linux: Systemd and System V

Applications

- Compiler Optimisation and Profiling

Lecture Slides

- Lecture 10: Systemd
- Lecture 11: Compiler Optimisation

Assignments

7.7 Week 7 (Sept 30 - Oct 6)

System Administration

- Linux: Monitoring Processes and Resources

Applications

- High Performance Languages: C, FORTRAN, and Julia
- Open Multi-Processing (Shared MP)

Lecture Slides

- Lecture 12: Shared Memory Parallelism

Assignments

Fall Break (Oct 10 - 11)

7.8 Week 8 (Oct 7 - 13)

System Administration

- Slurm (end user)

Lecture Slides

- Lecture 13: Process and Resource Monitoring
- Lecture 14: Slurm
- Sample Midterm

7.9 Week 9 (Oct 14 - 20)

System Administration

- Warewulf

Lecture Slides

- Lecture 15: Warewulf

Assignments

7.10 Week 10 (Oct 21 - 27)

System Administration

- Slurm Installation and Administration
- Linux: Shell Scripting, AWK, and Sed

Applications

- Spack and the High Performance Linpack

Lecture Slides

- Lecture 16: Slurm Installation and Configuration
- Lecture 17: HPL

Assignments

7.11 Week 11 (Oct 28 - Nov 3)

System Administration

- Distributed Computing (MPI and Job Arrays)

Lecture Slides

- Lecture 18: Distributed Computing

Assignments

Project 1 Assigned
Due by 11:59pm on Nov 17th.

- Project 1: High Performance Linpack
- Performance of Various Computers Using Standard Linear Equations Software
- The LINPACK Benchmark: past, present and future
- THE PROBLEM WITH THE LINPACK BENCHMARK 1.0 MATRIX GENERATOR
- Toward a New Metric for Ranking High Performance Computing Systems

7.12 Week 12 (Nov 4 - 10)

Nov 8 - Last day to drop without Dean's permission

Applications

- Scaleable Parallel Processing (Amdahl and Gustafson)
- Strategies for Parallelism and Halo Exchange

Lecture Slides

- Lecture 19: Scaling

Assignments:

- Project 1 due by 11:59pm on Nov 17th.

Nov 11th - Last Day to Drop without Dean's Permission

7.13 Week 13 (Nov 11 - 17)

Applications

- CUDA Programming and GPUs
- Benchmarks: HPCG

Lecture Slides

- Lecture 20: GPU Computation
- Lecture 21: HPCG and Singularity

Assignments:

- Project 1 due by 11:59pm on Nov 17th.

Supercomputing Conference (Nov 18th - 24)

7.14 Week 14 (Nov 25 - Dec 1)

System Administration

- RAID

Lecture Slides

- Lecture 22: Network Throughput and RAID

Assignments

- Project 2: High Performance Conjugate Gradient due by 11:59pm on Dec 8th.

7.15 Week 15 (Dec 2 - Dec 8)

Dec 5 - Last day to drop with Dean's permission

- December 4th, Sandia National Labs and Los Alamos National Labs HPC representatives will meet with the class.
- Sample Final

Assignments

Project 2 due by 11:59pm on Dec 8th. Homework 6 due by 11:59pm on Dec 8th.

- Synchronous Project 2

May 8 - Last day to DROP with Dean's Permission

7.16 Final Exam Week (Dec 9 - 14)

Final Exam. Wednesday May 8th. CARC Workshop Room

- Group A: 10am-11am.
- Group B: 11am-noon.

Sunday, May 17th, 2:30pm - Upload of Final Grades Expected by UNM.

8 Assignments and Grading

I use a 10 point fractional grading scale:

A+	A	A-	B+	B	B-	C+	I
98-100	93-97	90-92	87-89	83-86	80-82	77-79	Incomplete
C	C-	D+	D	D-	F		W
73-76	70-72	67-69	63-66	60-62	< 60		Withdrew

A+, A, and A- indicate excellent performance.
B+, B, and B- indicate good performance.
C+, C, and C- indicate satisfactory performance.
D+, D, and D- indicate less than satisfactory performance.
F indicates unsatisfactory performance.
W indicates withdrawal from the course.

The course grade is comprised of the following:
Homework: 30% (6 homeworks 5% each)
Projects: 40% (2 team projects 20% each)
Exams: 30% (2 exams 15% each)

8.1 Late Projects

Late homework and projects will not be accepted unless accompanied by an absence note provided by the Dean of Students Office for the period beginning on or before the *day the assignment was due* until the *day before* the assignment is actually submitted. I do this because allowing late submissions without good cause results in more stress for students than having strict deadlines.

9 Attendance

- Please see the UNM policy on class attendance: Class Attendance Policy
- Class attendance will not be recorded.

10 Cheating

10.1 Responsible Learning and Academic Honesty

- See the UNM policy on academic dishonesty: Academic Dishonesty

Cheating and plagiarism (academic dishonesty) are often driven by lack of time, desperation, or lack of knowledge about how to identify a source. Communicate with me and ask for help, even at the last minute, rather than risking your academic career by committing academic dishonesty. Academic dishonesty involves presenting material as your own that has been generated on a website, in a publication, by an artificial intelligence algorithm (AI), by another person, or by otherwise breaking the rules of an assignment or exam. It is a Student Code of Conduct violation that can lead to a disciplinary procedure. When you use a resource (such as an AI, article, a friend's work, or a website) in work submitted for this class, document how you used it and distinguish between your original work and the material taken from the resource.

10.2 Artificial Intelligence and Academic Integrity

A 2023-24 task force led by Dean Leo Lo concluded that current policies on student conduct (RPM 4.8, FH D100, D175, and D176) "reasonably articulate the university's student conduct expectations."

Artificial Intelligence is a useful tool. It is used widely but cautiously by software engineers and system administrators in industry, and is becoming an indispensable tool. I expect you to use tools such as chatGPT to aid your home and project work. Be cautious though, generative AI's guess the answers to questions and frequently get the facts wrong.

10.3 Why it's a bad idea

Cheating is harmful to you, the University, and your fellow students:

- The University warrants that receipt of grades and a degree accurately reflects the knowledge and skills of the recipient. Cheating undermines the value of the degrees and grades awarded by the University.
- Cheating makes assignments and exams look easier than they really are. This encourages instructors to make assignments and exams harder than they would otherwise.
- The desire to cheat indicates that there is an issue with developing the desired skills that needs to be resolved. Please approach lab instructors or the professor to discuss problems with the material and how to honestly do better in the class.
- Cheating indicates that the material is not being sufficiently mastered, this will likely result in difficulties when you take classes in the future that require this course.
- Trading your integrity for a better grade is something that will stay with you for the rest of your life, whether or not you are discovered.
- If you are caught cheating you will receive a failing grade for the course. However, the University may take further action including dismissal from the University.

10.4 What I do allow

You may use any resources to complete the projects including learning from other students and taking information from the internet and getting help from artificial intelligences, such as large

language models. I encourage learning from your classmates. Make sure to document your sources. You will not lose points for citing your sources.

10.5 What I don't allow

Exams will be used to test whether you have developed an individual understanding HPC fundamentals covered in the course. No collaboration or exam aids such as notes or devices may be used during the exam. Failure to follow this policy will result in an F on the exam or quiz, possibly the course, and may result in disciplinary action by the University. You may not copy quiz answers from other students. Resources such as other students, artificial intelligence, the internet, etc may not be used in your projects and homework without being cited. You will not lose points for using these resources as long as you cite them. You do not have to cite information you got in class or from the slides. Even if you cite a resource you may not copy from it *verbatum*. Write up the assignment in your own words, plots and/or code (i.e don't copy). The only exception is if you are presenting a command or number with just one sensible representation.

11 Innovative Teaching Study

This class is paid for by a Department of Education Grant and funds from the School of Engineering Innovative Teaching Program. As part of those programs we will be collecting information about the class and your interactions. This requires IRB review and your consent. I will be distributing consent forms at the start of the semester. There is no obligation to participate and the data gathered will have no bearing on your grade in the class.

12 Time Expectations

(This statement is mandated by University Accreditation) Credit-hour statement: This is a three credit-hour course. Class meets for three 50-minute sessions of direct instruction for fifteen weeks during the Fall 2024 semester. Please plan for a minimum of six hours of out-of-class work (or homework, study, assignment completion, and class preparation) each week.

13 UNM Resources and Student Rights

13.1 Student Support

UNM has many resources and centres to help you thrive, including opportunities to get involved in campus life, research experiences, mental health resources, academic support such as tutoring, resource centres for people like you, free food at Lobo Food Pantry, jobs on campus and financial capability support. Your advisor, staff at the resource centres and Dean of Students, and I can help you find the right opportunities for you.

Resources to support study skills and time management are available through Student Learning Assistance at the Center for Teaching and Learning in Zimmerman Library or online.

13.2 Student Health and Counselling (SHAC)

"SHAC provides quality health and counseling services to all UNM students to foster student success."

https://shac.unm.edu/

505.277.3136 (24-hr number)

13.3 Center for Academic Program Support

https://caps.unm.edu/index.php

"CAPS is the University of New Mexico's learning center. We are a free service that provides academic support for undergraduate students at UNM through peer-tutoring. Our tutors are UNM students who are trained to create comfortable and welcoming spaces for students to learn and thrive in. We are passionate about helping students achieve individual academic success at UNM through peer tutoring and interactions."

13.4 Wellness

If you do need to stay home due to illness or are experiencing a wellness challenge, please take advantage of the resources below. You can communicate with me through email and I can work with you to provide alternatives for course participation and completion. Let me, an advisor, or another UNM staff member know that you need support so that we can connect you to the right resources. UNM is a mask friendly, but not a mask required, community. If you are experiencing COVID-19 symptoms, please do not come to class.

13.5 Accessibility Resource Center

https://arc.unm.edu/

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 my 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 for additional information.

If you need an accommodation based on how course requirement 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.

13.6 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.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/.

13.7 Equal Educational Opportunities

Our classroom and our university should always be spaces of mutual respect, kindness, and support, without fear of discrimination, harassment, or violence. Should you ever need assistance or have concerns about incidents that violate this principle, please let me know and/or access the resources available to you on campus, especially the LoboRESPECT Advocacy Center and the support services listed on its website (http://loborespect.unm.edu/).

I am committed to building with you a positive classroom environment in which everyone can learn. I reserve the right to intervene and enforce standards of respectful behaviour when classroom conduct is inconsistent with University expectations. Interventions and enforcement may include but are not limited to required meetings to discuss classroom expectations, written notification of expectations, and/or removal from a class meeting. Removal from a class meeting will result in an unexcused absence. [Insert number] or more unexcused absences may result in permanent removal and a drop from the course (see attendance policy). The University of New Mexico ensures freedom of academic inquiry, free expression and open debate, and a respectful campus through adherence to the following policies: D75: Classroom Conduct, Student Code of Conduct, University Policy 2240 – Respectful Campus, University Policy 2210 – Campus Violence.

Several Federal civil rights laws prohibit discrimination in programs or activities that receive Federal funds from the Department of Education. These laws prohibit discrimination on the basis of race, colour, and national origin (Title VI of the Civil Rights Act of 1964), sex (Title IX of the Education Amendments of 1972), age (Age Discrimination Act of 1975) and disability (The Americans with Disabilities Act of 2008). The Office for Civil Rights enforces these rights: `https://www2.ed.gov/about/offices/list/ocr/know.html`.

Please note that because the teaching assistants and I are considered "responsible employees" by the Department of Education, we are required to report any disclosure of gender discrimination (including sexual harassment, sexual misconduct, and sexual violence) to the university's Title IX coordinator. For more information on the campus policy regarding sexual misconduct, please see: UNM Policy.

13.8 Title IX

The University of New Mexico and its faculty are committed to supporting our students and providing an environment that is free of bias, discrimination, and harassment. The University's programs and activities, including the classroom, should always provide a space of mutual respect, kindness, and support without fear of harassment, violence, or discrimination. Discrimination on the basis of sex includes discrimination on the basis of assigned sex at birth, sex characteristics, pregnancy and pregnancy related conditions, sexual orientation and gender identity. If you have encountered any form of discrimination on the basis of sex, including sexual harassment, sexual assault, stalking, domestic or dating violence, we encourage you to report this to the University. You can access the confidential resources available on campus at the LoboRESPECT Advocacy Center (https://loborespect.unm.edu), the Women's Resource Center (https://women.unm.edu), and the LGBTQ Resource Center (https://lgbtqrc.unm.edu). If you speak with an instructor (including a TA or a GA) regarding an incident connected to discrimination on the basis of sex, they must notify UNM's Title IX Coordinator that you shared an experience relating to Title IX, even if you ask the instructor not to disclose it. The Title IX Coordinator is available to assist you in understanding your options and in connecting you with all possible resources on and off campus. For more information on the campus policy regarding sexual misconduct and reporting, please see

https://policy.unm.edu/university-policies/2000/2740.html and CEEO's website.

If you are pregnant or experiencing a pregnancy-related condition, you may contact UNM's Office of Compliance, Ethics, and Equal Opportunity at ceeo@unm.edu. The CEEO staff will provide you with access to available resources and supportive measures and assist you in understanding your rights.

UNM's Title IX Coordinator, Angela Catena, can be reached at acatena@unm.edu.

13.9 Accommodations

UNM is committed to providing equitable access to learning opportunities for students with documented disabilities. As your instructor, it is my objective to facilitate an inclusive classroom setting, in which students have full access and opportunity to participate. To engage in a confidential conversation about the process for requesting reasonable accommodations for this class and/or program, please contact Accessibility Resource Center (https://arc.unm.edu/) at arcsrvs@unm.edu or by phone at 505-277-3506.

14 Land Acknowledgement

Founded in 1889, the University of New Mexico sits on the traditional homelands of the Pueblo of Sandia. The original peoples of New Mexico Pueblo, Navajo, and Apache since time immemorial, have deep connections to the land and have made significant contributions to the broader community statewide. We honour the land itself and those who remain stewards of this land throughout the generations and also acknowledge our committed relationship to Indigenous peoples. We gratefully recognise our history.)