Syllabus for Methods and Practice of Scientific Computing (Fall 2019)
NERS 590-004

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Course Description:
This course is designed for graduate students who are developing the methods, and using the tools, of scientific computing in their research. With the increased power and availability of computers to do massively scaled simulations, computational science and engineering as a whole has become an integral part of research that complements experiment and theory. This course will teach students the necessary skills to be effective computational scientists and how to produce work that adheres to the scientific method. A broad range of topics will be covered including: software engineering best practices, computer architectures, computational performance, common algorithms in engineering, solvers, software libraries for scientific computing, uncertainty quantification, verification and validation, and how to use all the various tools to accomplish these things.

Format:

Bi-weekly Lectures on	M/W	4:00 PM - 5:30 PM, G906 Cooley
Weekly Lab on	F	9:00 AM - 11:00 AM, GGBL 2517

Grading:

Lecture Quizzes	10%
Homework	15%
Lab	40%
Project	35%

Policies

- Deliverables for assignments must be completed in the appropriate format. Format for assignment deliverables will be given on a case by case basis. Expected formats are:
  - Typed documents
  - Source code
  - LaTeX
  - Google forms
  - Program output
  - Repository commits
  - Canvas quizzes
- Late Assignments
  - Late homework assignments are penalized with a 5-day half-life
  - Late lab assignments are penalized with a 7-day half-life
  - Late project deliverables are penalized with a **3-day half-life**
- Announcements
  - Canvas: https://umich.instructure.com/
- Honor code: **http://ossa.engin.umich.edu/honor-council/**

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Schedule:

Date	Lecture	Lab	Topic
09/04/2019	1		Course Overview & Introduction to Linux
09/06/2019		1	*Introduction to Linux*
09/09/2019	2		Programming Languages: C, C++, Fortran
09/11/2019	3		Intermediate Linux: Bash Scripting & Intro to Python
09/13/2019		*2*	*Scripting*
09/16/2019	4		Elements of Development: Configuring, Compiling, Linking
09/18/2019	5		Tools of the Trade: Version Control, Text Editors, Dev. Env
09/20/2019		*3*†*	*ARC-TS/CAEN: Introduction to Flux/Great Lakes*
09/23/2019	6		Algorithms for Linear Algebra
09/25/2019	7		Sci. Computing Libs: BLAS, LAPACK, PETSc, Trilinos
09/27/2019		*4*	*Working with Third Party Libraries*
09/30/2019	8		Software Engineering Practices & Development Workflows
10/02/2019	9		Object-Oriented Programming, Design Patterns, UML
10/04/2019		*5*	*Workflows in Practice*
10/07/2019	10		Serial and Parallel Architectures
10/09/2019[a]	11		Performance and Profiling
10/11/2019		*6*	*Micro-Benchmarks and Measuring Performance*
10/14/2019	FALL BREAK		
10/16/2019	12		Serial Optimization Techniques
10/18/2019		*7*	*Basic Optimizations*
10/22/2019	13		Parallel Programming Models
10/24/2019	14		OpenMP
10/26/2019		*8*	*Parallel Computing: OpenMP*
10/28/2019	15		The Message Passing Interface I
10/30/2019	16		The Message Passing Interface II
11/01/2019		*9*	*Parallel Computing: MPI*
11/04/2019	17		Heterogeneous Architectures
11/06/2019	18		Parallel Debugging & Optimization Tools
11/08/2019		*10*	*Hardware Abstraction with Kokkos*
11/11/2019[a]	19†		Data Format Libraries: HDF5, NetCDF, SILO
11/13/2019[a]	20		Mesh Libraries: Libmesh, Exodus, others
11/15/2019		*11*	*Working with Data Libraries*
11/19/2019	21†		Visualization Tools
11/20/2019	22†		Testing, Verification, and Validation
11/22/2019	NO LAB - Work on Term Projects		
11/25/2019[a]	23†*		Misc. Topics: QA, deployment, copyrights, and licensing
11/27/2019	THANKSGIVING BREAK		
11/29/2019			
12/02/2019	Project Presentations		
12/04/2019			
12/06/2019	NO LAB - Work on Term Projects		
12/09/2019	Project Presentations		
12/11/2019			

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* Guest Lecturer † Subject to change

Associated Readings and General References:

Lecture	Topic
1	None
2	Modern Fortran C/C++ programmer's reference
3	Bash Quick Start Guide Learning Python
4	None
5	Pro Git
6	Finite Difference Methods Finite Element Methods The Method of Weighted Residuals and Variational Principles Multigrid Methods Matrix Analysis Vol. 1 and Vol. 2 Iterative Methods for Sparse Linear Systems Model Reduction and Approximation Accuracy and Reliability of Scientific Computing Accuracy and Stability of Numerical Algorithms
7	LAPACK User's Guide ScaLAPACK User's Guide Numerical Recipes in Fortran (Online PDF) Numerical Recipes in C (Online PDF)
8	Code Complete Agile Development in the Real World
9	Scientific Software Design: The Object-Oriented Way The Unified Modeling Language Design Patterns
10	Numerical Linear Algebra for High-Performance Computers
11	Parallel Processing for Scientific Computing
12	Performance Optimization of Numerically Intensive Codes
13	Patterns for Parallel Programming
14	Using OpenMP
15	Using MPI
16	Using Advanced MPI
17	None
18	None
19	None
20	None
21	None
22	None
23	None

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Anticipated Homework Assignments

HW	Description	Supporting Lectures
1	LaTeX and Programming in C/C++ and Fortran	1,2
2	Using scientific software libraries for sparse linear algebra	1,4,6,7
3	Draft Project Proposal and TBD	
4	Maybe	

Anticipated Lab Assignments

Lab	Description	Supporting Lectures
1	Hands on walkthrough of Linux.	1
2	Bash and Python Scripting	1,3
3	Hands on walkthrough of Flux/Great Lakes	1,4
4	Working with BLAS	1,4,7
5	Perform a workflow and setup basic git and CMake	1,5,8,9
6	Computer performance. Collect data in lab, finish analysis outside	1,4,10,11
7	Performance Profiling and Optimizations. Start in lab, finish outside	1,4,11
8	OpenMP simulated annealing parallel programming. Mostly in lab	1,4,6,10,14
9	MPI simulated annealing parallel programming. Mostly in lab	1,4,6,10,15,16
10	Heterogeneous Computing in lab work only	1,4,17
11	Using HDF5 in lab only.	1,4,20

Project Assignments

Deliverable	Description	
Proposal	3-5 page document	
Presentation	10-15 minute presentation	
Report	10-20 page typed document	