



Michigan Tech

UN5390: Scientific Computing I

Fall 2016

Course and Instructor Information

Course # : UN5390 (cross-listed as BE5390, EE5390 and MA5390)
Course name : Scientific Computing I
Location : Fisher Hall 330
Lecture days and time : TR, 8:05 am – 9:20 am

Instructor : Dr. Gowtham
Contact information : EERC B39 · g@mtu.edu · (906) 487-4096
Office hours : By appointment

Course Objectives

1. To gain an exposure to Linux command line, shell scripting, Git revision control system, and free/open source tools and utilities to design and develop computational workflows
2. To acquire/enhance good programming and communication etiquette with an emphasis on readability and clarity of written code
3. To translate science and engineering problems into computer programs, learn compilation, debugging and profiling techniques, and understand various sources of error
4. To learn parallel programming techniques using OpenMP, and data visualization
5. To learn about the use of hardware accelerators (time permitting)

Suggested References

There is no prescribed/required text book for this course. Listed below are useful references and are usually available from the university library. Much of the material deemed necessary by the instructor will be made available to you.

1. [Numerical Recipes – The Art of Scientific Computing](#)
W. Press, S. Teukolsky, W. Vetterling, B. Flannery; 978-0-521-88068-8
2. [The Art of Computer Programming \(vol. 1-4A\)](#)
D. Knuth; 978-0-321-75104-1
3. [The Practice of Programming](#)
B. Kernighan, R. Pike; 978-0-201-61586-9
4. [The Science of Debugging](#)
M. Telles, Y. Hsieh; 978-1-57610-917-5
5. [Linux Command Line and Shell Scripting Bible](#)
R. Blum, C. Bresnahan; 978-1-118-00442-5
6. Language and/or domain-specific literature
Check with your advisor(s), mentor(s) and/or friend(s)

Grading Scheme

Final grade = 50% Assignments + 25% Project + 25% Active Participation

| | |
|-------------------------|----------------------------|
| A (4.00): 93% and above | AB (3.50): 88% – 92.99% |
| B (3.00): 82% – 87.99% | BC (2.50): 76% – 81.99% |
| C (2.00): 70% – 75.99% | CD (1.50): 65% – 69.99% |
| D (1.00): 60% – 64.99% | F (0.00): 59.99% and below |

Active participation (AP) is measured by attendance, how well you come prepared, your ability to lead the problem solving process in front of the class, etc. There is no *curving*, i.e., the grade you get is the grade you earned. Anything less than a B for the final grade could jeopardize your enrollment, funding and/or immigration status. Demonstrating preparation, consistency and quality in the work you do, a willingness to help others in a kind and graceful manner, and *I will do more than what is asked* behavior are critical to earn a reference letter for graduate school/internship/fellowship/job applications.

General Guidelines

1. Show up on time. If the door is closed, stay out and do not bother coming in
2. Show up prepared, and in a presentable and professional manner. You might be randomly picked on any given day to lead a problem-solving process in front of the class
3. No drinking, eating, facebooking, gaming, instagramming, sleeping, snapchatting, texting, tweeting, etc. during class. Cell phones must be in silent mode as well
4. Course material and assignments will be distributed, and assignments and project work must be submitted via GitHub. You may turn in partially completed assignments, without the fear of penalty even if you believe the solution is incorrect, to show timely and continuous work. You may incorporate my suggestions, if any, into your assignment and turn it in for grading. Late submissions will not be accepted.

There are no restrictions on programming languages. You can use any language, more than one if necessary, for this course. The choice of languages should be guided by their applicability to your research endeavors, and their potential for parallelization. You are responsible for learning the language including its features and caveats.

It is expected that you will work on the assignment consistently from the day it's handed out. If you have any questions, concerns and/or need further information, you must get in touch with the instructor at least 48 hours before it's due. Use a method that works best for you – in person (on/off campus), email (with UN5390: or BE5390: or EE5390: or MA5390: in the subject field), phone call, etc.

Assignments and project reports must be typeset in L^AT_EX using the provided template. Microsoft Word, Notepad, handwritten notes, etc. will not be accepted. There is no need to explicitly include the code in the .tex document.

It is acceptable (and often highly encouraged) to seek help from your classmates and/or others but any such help must be clearly and appropriately cited in the assignment. If you helped someone, you must include that information as well. Absence of proper citation and/or inability to explain your work will mean that someone else authored it. This, in turn, means that you will get no credit for the problem and the incident will be treated as a case of academic dishonesty.

Submissions must be thoroughly spell-checked for typographical and/or grammatical mistakes. If the submissions contain mistakes or be otherwise deemed difficult to understand, you will be required to work with the *Michigan Tech Multiliteracies Center*

5. Academic policies: <http://www.mtu.edu/deanofstudents/academic-policies/>

Tentative Timeline

Week 01 – 02

Tips to Succeed
 Git, GitHub, and UN5390
 Compliance and Security
 A Brief History of Computing
 Computational Workflow
 Programming Etiquette
 Seeking and Citing Help (Guest Lecture)
 Assignment #01 (5%)
 Research Marketing I (AP 2%)
 Watch [Silicon Valley](#) (PBS; not Showtime)

Week 03 – No Class

Instructor at [CASC](#) in Alexandria, VA
 Attend [Webinars\(s\)](#); catch up on life
 PB&J Sandwich Recipe (AP 2%)

Week 04 – 05

Review of Assignment #01
 Statistics, Numbers and Errors
 Journal of Failed Experiments
 Program Compilation
 Debugging and Profiling Programs
 Integrated Development Environment
 Assignment #04 (10%)

Week 06 – 08

Review of Assignment #04
 Numerical Results
 Numerical Methods – Finding Roots
 Numerical Methods – Differential Equations
 Numerical Methods – Integration
 Numerical Methods – Matrices
 Assignment #06 (15%)
 Research Marketing II (AP 2%)

Week 09 – No Class

Instructor at [NSF](#) in Arlington, VA
 Attend [Webinars\(s\)](#); catch up on life
 Assignment #09 (20%)

Week 10 – 11

Review of Assignment #06
 Parallel Computing and Programming
 OpenMP
 Term Project (Starting Week #10; 25%)

Week 12 – No Class

Instructor at [SC16](#) in Salt Lake City, UT
 Attend [Webinar\(s\)](#); catch up on life

Thanksgiving Break

Week 13 – 14

Review of Assignment #09
 OpenMP (Continued)
 Managing and Visualizing Data
 Hardware Accelerators (Time permitting)
 Research Marketing III (AP 2%)
 Semester Summary

Remaining active participation (AP) credit is reserved for attendance (6%), leading a timed problem-solving process in front of the class when chosen randomly (2%), and doing a little more (9%).

A weekly meeting with your research advisor and a weekly status report of research project (worth 1% each) are required during weeks 10 – 14. Your research advisor decides 20% of the grade by 5 pm of the finals week.

Actual Timeline

Week 01

Tips to Succeed
 Revision Control System (Git and GitHub)
 A Brief History of Computing
 Compliance and Security
 Impact on/of Computing
 Introduction
 Richard Phillips Feynman
 Ada Augusta King
 Alan Mathison Turing
 Hard Drives
 Assignment #01 (5%; due 09/11)
 Research Marketing I (AP 2%; due 09/07)
 Research Marketing II (AP 2%; due 09/26)

Week 02

Computational Workflow
 Programming Etiquette
 PB&J Sandwich Recipe (AP 2%; due 09/18)
 Guest Lecture
 The Art of Seeking and Citing Help
 – Sarah Lucchesi, JRVP Library
 Impact on/of Computing
 Aerospace
 Fairchild Notebooks
 Grace Brewster Murray Hopper
 Review of Research Marketing I

Week 03 – No Class

Instructor at [CASC](#) in Alexandria, VA
 Get rest, catch up on life and other courses

Week 04

Review of Assignment #01
 Review of PB&J Sandwich Recipe
 Numbers
 Bits, Bytes and Words
 Fixed-Point and Floating-Point

Statistics

Impact on/of Computing
 Batteries
 Accuracy vs Precision
 The Art of Writing Software
 Silicon Valley (PBS Documentary)
 Assignment #04 (10%; due 10/09)

Week 05

Program Compilation
 Manual: Single and Multiple Source Files
 Makefile: Single and Multiple Source Files
 Visualization
 Workflow Design and Examples
 Gnuplot
 Impact on/of Computing
 Climate Modeling
 Review of Research Marketing II

Week 06

Errors
 Round-Off and Truncation
 Propagation
 Catastrophic Cancellation
 Approximation (Absolute and Relative)
 Logic and Design
 Compiler and Run Time
 Overflow, Underflow and Undefined
 Journal of Failed Experiments
 Debugging and Profiling Programs
 Integrated Development Environment
 Impact on/of Computing
 Diapers, Detergents and Shampoo
 Margaret Heafield Hamilton

Week 07

Review of Assignment #04
Analytical vs Numerical Methods
Numerical Methods – Finding Roots
 Visual Inspection and Graphical Methods
 Direct Numerical Method
 Iterative Methods: Successive Bisection
 Iterative Methods: Newton-Raphson
 Iterative Methods: Hybrid
 Cognitive Computing
Random Numbers
 Sequence and Seed
 Mapping/Scaling
 Systematic vs Random Sampling
Numerical Methods – Integration
 Overview
 Reimann Sum
 Polynomial Approximations
 Monte Carlo Techniques
Impact on/of Computing
 Entertainment
Assignment #07 (15%; due 11/13)

Week 08

Numerical Methods – Differential Equations
 Overview
 Euler's Method
 Adams-Bashforth (AB2) Method
 Adams-Moulton (AM2) Method
eGuest Lecture (SC13, Denver, CO)
 Secret Life of Big Data
 – Dr. Genevieve Bell (Keynote), Intel
Impact on/of Computing
 Big Data
 Epilepsy and Parkinson's Treatments

Week 09 – No Class

Instructor at NSF in Arlington, VA
Discuss research project (starts week #10)
Get rest, catch up on life and other courses

Week 10

Numerical Methods – Differential Equations
 Runge-Kutta (RK) Method
Numerical Methods – Matrix Methods
 LU Factorization
 Message Encryption
 Graph Theory
 Game Theory
Research Marketing III (AP 2%; due 12/08)
Impact on/of Computing
 Human-Induced Climate Change
 Missing Plane, MH370
Project Status Report (1%; due 11/04)

Week 11

Parallel Computing
 The Need
 Design and Development
 Memory Architecture
 Costs and Limitations
Message Passing Interface
 Definition and Implementation
 Common Workflow
 Types of Communication
OpenMP
 Features, Components and Conventions
 Compilation and Execution
MATLAB
 Features and Conventions
 Code Parallelization and Execution
Parallel Computing Examples
 Hello, World! (MATLAB and OpenMP)
 Eigen Values (MATLAB)
Impact on/of Computing
 Paypal
 Storm Prediction
Project Status Report (1%; due 11/11)

Week 12 – No Class

Instructor at [SC16](#) in Salt Lake City, UT
Get rest, catch up on life and other courses
eGuest Lectures (SC16, Salt Lake City, UT)
 Precision Medicine
 – HPC Plenary (Panel Discussion)
 Cognitive Computing
 – Dr. Katharine Frase (Keynote), IBM
Impact on/of Computing
 Precision Medicine
 Preview of SC11
 Preview of SC12
 Preview of SC13
 Preview of SC14
 Preview of SC15
 Preview of SC17
Project Status Report (1%; **due 11/18**)

Week 13

Review of Assignment #07
Parallel Computing Examples (OpenMP)
 Array Manipulation
 Monte Carlo Methods
 Numerical Integration
 Matrix Multiplication
 Finding Primes
Project Status Report (1%; **due 12/02**)

Week 14

Research Marketing III (in-class activity)
Semester Summary
Project Status Report (1%; **due 12/09**)

The remaining active participation (AP) credit is reserved for attendance (6%), leading a timed problem-solving process in front of the class when chosen randomly (2%), and doing a little more (9%).

A weekly meeting with your research advisor and a weekly status report of research project (worth 1% each) are required during weeks 10 – 14. Your research advisor decides 20% of the grade by 5 pm of the finals week.