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

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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
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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 LaTeX 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 of Supercomputing
  Introduction
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 of Supercomputing
  Aerospace
  Fairchild Notebooks
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 of Supercomputing
  Batteries
  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

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 of Supercomputing
  Diapers, Detergents and Shampoo
  Margaret 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 of Supercomputing
- Entertainment

Assignment #07 (15%; due 11/06)

Week 08

Numerical Methods – Differential Equations
- Overview
- Euler's Method
- Adams-Bashforth (AB2) Method
- Adams-Moulton (AM2) Method

Guest Lecture
- Secret Life of Big Data
  - Dr. Genevieve Bell, Intel

Impact of Supercomputing
- 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

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.