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
```

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:` 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 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
Research Marketing I (in-class activity)

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
Research Marketing II (in-class activity)

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
Assignment #12 (20%; due 12/11)
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
MPICH
  Features, Components and Conventions
  Installation, Compilation and Execution
Parallel Computing Examples (MPICH)
  Hello, World!
  Monte Carlo Methods
  Matrix Multiplication
Hybrid (MPICH + OpenMP)
  The Need, Features and Components
  Conventions, Compilation and Execution
  Hello, World!
Research Marketing III (in-class activity)
  Peer Review
Course Summary
  Looking Back
  Looking Ahead
    Portage (Educational HPC Resource)
    Hardware Accelerators
    Self-Paced GPU Programming Course
    Lmod
    Data Formats and Management
    PHP
    WordPress
    Bootstrap
    Google Charts and Highcharts
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 allocated for the term project.

End of semester social @ KBC	5-7 pm 2016-12-09
Online course evaluations	4:59 pm 2016-12-10
Term project	11:59 am 2016-12-11
Email from research advisor	11:59 am 2016-12-12
Save GitHub course repository	11:59 pm 2016-12-16 – 11:59 pm 2016-12-18