



# Michigan Tech

## UN5390: Scientific Computing I

Fall 2016

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### 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](mailto: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<sup>A</sup>T<sub>E</sub>X 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

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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  
 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)  
 Looking Back and Looking Ahead  
 Hardware Accelerators  
 Data Management  
 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.