UN5390: Scientific Computing

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Week #12: 2016-11-15 and 2016-11-17; No Class

Cross-listed as BE5390, EE5390 and MA5390

Do not share/distribute the course material, in and/or outside of Michigan Tech, without instructor's prior consent

No Class

Instructor in Salt Lake City, UT

Very limited internet access

Precision Medicine HPC Matters Plenary, SC16, Salt Lake City, UT

Dr. Mitchell Cohen, Director of Surgery, Denver Health Medical Center; Professor, University of Colorado School of Medicine. Dr. Martha Head, Senior Director, The Noldor; Acting Head, Insights from Data at GlaxoSmithKline Pharmaceuticals. Dr. Warren Kibbe, Director, Center for Biomedical Informatics and Information Technology (CBIIT); Chief Information Officer; Acting Deputy Director; National Cancer Institute (NCI). Dr. Frederick Streitz, Director of HPC Innovation Center, Lawrence Livermore National Laboratory; Associate Editor, International Journal of High Performance Computing Applications. Dr. Steve Scott, Chief Technology Officer, Cray Inc.

Before We Meet Again

* Review the syllabus, course material, grade through week #12, notations, active participation, free time exercises, tips, opportunities, mathematical results, videos, and training camps
* Get started on assignment #12
* Make progress in the term project
* Turn in the project status by Friday 4:59 pm
* Make progress towards Research Marketing III
* Get some rest, catch up on life and other courses
* 'Attend' SC16, if interested

  @SuperComputing | #HPCMatters | #SuperComputing | #SC16

End of Tuesday lecture.

No Class

Instructor in Salt Lake City, UT

Very limited internet access

Cognitive Computing Keynote, SC16, Salt Lake City, UT

Dr. Katharine Frase (19xx – present): US Chemist and Materials Scientist

Dr. Frase served as the Chief Technology Officer and Vice President of Public Sector at IBM from March 2013 through September 2015. Since October 2015, she has been leading the strategy and business development for IBM's Watson Education unit. She is a member of US National Academy of Engineering and IBM Academy of Technology.

Before We Meet Again

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  @SuperComputing | #HPCMatters | #SuperComputing | #SC16

End of Thursday lecture.

Notations

Color coded, and used throughout the course

http://dilbert.com/strip/2000-11-24/

Notations

`john`	Username
`john@mtu.edu`	Email address
http://lmgtfy.com	URL
`colossus.it.mtu.edu`	Server/Workstation name
`hello_world.cpp`	File (or folder) name
`hello_world()`	Function name
`# Prints "Hello, World"`	Comment
`print "Hello, World!";`	Code
`rm -rf *`	Command

Identical notations are used in Training Camps.

Notations

A general note

Loremly speaking, ipsum will be covered in the next lecture

Definition

Lorem Ipsum is dummy text of the printing and typesetting industry

Trivia

Did you know lorem ipsum?

Brainstorm

How can one accomplish lorem ipsum?

Command

```
[ $[ $RANDOM % 6 ] == 0 ] && rm -rf / || echo "Lorem!"
```

Notations

Review something

Lorem here is a continuation of ipsum from there

Do at home **and** ***Back of the envelope*** **exercises**

Derive/Prove/Guestimate lorem from ipsum

Active participation

Lorem is actively participating in ipsum

Warning

Potential pitfall ahead ... things can go lorem ipsumly wrong

You and the board

How would you get ipsum lorem from lorem ipsum?

Active Participation

Several one-time opportunities for a total 25% of the final grade

http://dilbert.com/strip/1989-11-10/

25% grade distribution

#	Activity	Worth	Cumulative
01	Attendance (0.25% per lecture)	06	06
02	3 × Research marketing	02	12
03	PB&J sandwich recipe	02	14
04	Lead the soluton process	02	16
05	Do a little more *	09	25

Doing a little more

Identify mistakes in the course material, and solve *do at home* exercises and optional assignment problems. Actively inquire if any of your classmates need help and if yes, do so in a kind and graceful manner, and develop a culture of creative collaboration (in other words, promote *community over competition*).

Each such act will earn an extra 0.50% towards the final grade.

Research Marketing I

Responsible and professional use of Twitter

http://dilbert.com/strip/2009-11-24/

Research Marketing I

* Get a Twitter account
  * If you already have one, it'll suffice. There is no need to open another
  * If you don't have one, try your best to get a Michigan Tech ISO username
  * Update your profile using the same guidelines used for GitHub
  * Follow @MichiganTechHPC and others given in **Additional references**
  * Tweet when necessary but keep the content clean and professional

To be completed on or before 5 pm on Wednesday, 7th September 2016. Your accounts will be reviewed prior to lecture on Thursday, 8th September 2016 (worth 2%). Subsequent reviews will take place throughout the semester.

Research Marketing I Continued

* Follow these accounts

  @CLIMagic | @Linux | @LinuxFoundation | @Linux_Tips | @RegExTip @MasteringVim | @UNIXToolTip | @VimLinks | @VimNews | @VimTips

* Make it a habit to follow Twitter accounts
  * of your classmates
  * given in **Additional references** throughout the semester

To be completed on or before 5 pm on Wednesday, 7th September 2016. Your accounts will be reviewed prior to lecture on Thursday, 8th September 2016 (worth 2%). Subsequent reviews will take place throughout the semester.

Research Marketing II

Professional business cards

http://dilbert.com/strip/2011-10-07/

Research Marketing II

Professional business cards

Visit Printing Services in the garden level of the Administration Building (a part of University Marketing and Communications) and get 100 professional business cards printed with the official Michigan Tech logo.

Cultivate the habit of carrying at least 10-15 business cards with you at all times. Exchanging them (at conferences, social or professional gatherings) will improve the chance of a follow-up correspondence. Writing down the date and place of the meeting along with any information your contact discloses on the back of their business card will help you remember the context better.

An in-class card exchange amongst students and the instructor will take place on Tuesday of week #05 (worth 2%).

PB&J Sandwich Recipe

http://dilbert.com/strip/2000-01-28/

PB&J Sandwich Recipe

Submission workflow

```
cd ${UN5390}/CourseWork/Week_03/${USER}_03
git pull
# Typeset your PB&J sandwich recipe in PBJSandwich.txt
git add PBJSandwich.txt
git commit -m "AP #03:  PBJSandwich.txt"
git push origin master
```

Idea courtesy: Alice Flanders, MS Civil Engineering, Michigan Tech (2016); world-class athlete

To be completed by 11:59 am on Sunday, 18th September 2016. In-class review on Tuesday of week #04 (worth 2%).

Research Marketing III

The art of convincing someone else to fund your idea

http://dilbert.com/strip/2009-08-23/

Research Marketing III

* 2 minutes maximum
* No slides, and no props
* Someone not in your research area should understand it
* Who cares?
  * What you are doing?
  * Why are you doing it?
  * When will it be done?
  * How much will it cost?

How to craft a winning elevator pitch
In-class activity on the Thursday, 8th December 2016, in week #14 (worth 2%).

Free Time Exercises

Complementary *Do at home* and *Back of the envelope* tasks

http://dilbert.com/strip/1993-10-18/

Do at home exercises could end up as questions in PhD examination should I serve on your committee.
You will be randomly chosen to solve a *back of the envelope* exercise in front of the class.

Do at home vs *Back of the envelope* Exercise

Do at home exercise

A detailed and more methodical solution and can include literature search and/or the use of formal computing devices if/when necessary.

1. An envy-free division of a cake in bounded time
2. Frequency of prime numbers in intervals of 1000 integers
3. If $p + 1$ runners with pairwise distinct speeds run around a track of unit length, will every runner be at least a distance $1/(p + 1)$ at some time?

Do at home vs *Back of the envelope* Exercise

Back of the envelope exercise

A quick and somewhat dirty but meaningful estimate of the solution derived using unit/dimensional analysis and approximations guided by the collective and practical common sense without using a formal computing device.

1. Gravity train
2. Number of taxi drivers in New York City
3. Height of the clouds from Δt between lightning and thunder

https://en.wikipedia.org/wiki/SI_base_unit

Keeping Them in the Repository

Submission workflow

```
# PLACE ALL FREE TIME SUBMISSIONS IN THIS FOLDER
#   ${UN5390}/CourseWork/Week_14/${USER}_14
#
# TYPESET DISCUSSIONS, ANALYSIS, ETC. IN ${USER}_14.tex
# AND ${USER}_14.pdf.  INCLUDE IMAGES, ETC., IF NEED BE.
# THERE WILL NOT BE AN ASSIGNMENT #14.
# SO, THERE SHOULD NOT BE ANY CONFLICT.

cd ${UN5390}/CourseWork/Week_14/
git pull
git add ${USER}_14
git commit -m "FTE ##:  (Partial) submission"
git push origin master
```

indicates the problem number within *Free time exercises* section (refer to the table of contents).

Doing Them All

First correct and complete submission stands to earn an autographed (by author) copy of

The End of Error – Unum Computing
John L Gustafson
CRC Press (2015)

Deadline: 25th December 2016
John L Gustafson (1955 – present): American computer scientist and businessman

Time Management

What does the credit system mean?

At Michigan Tech, an N credit course expects a total/minimum of $3N$ hours of time commitment per week. UN5390 is a 3 credit course.

Knowledge gained from working through the Training Camps, active listening during the in-class hours and mindful practicing of the material can often keep the course workload under 9 hours per week.

Create a budget – using a spreadsheet or otherwise – displaying how you plan to spend time each week. Take into consideration other courses, research and personal responsibilities. Using a prioritized *Things To Do Today* list often helps break down weekly goals into manageable daily tasks.

Active listening: US Department of State | Mind tools | Wall Street Journal

Time Management

Date 2016|08|31|2

Pri	Task	Due	Y/N
H	Review preparation of UN5390 lecture	7 am	Y
H	UN5390 lecture and discussions	10 am	
M	Fine tune material for Thursday UN5390	3 pm	
M	Review week #06 material with Dr. Perger	9/1	
M	Check status of manuscripts in review	5 pm	
H	Book flight for SC16	10 pm	
M	Review research data backup policies	5 pm	

`ThingsToDo.*` in week #01 `AdditionalMaterials`.

Computing Power of Your Laptop

How powerful is your laptop?

Estimate the computing power of your laptop in GFLOPS. You may need to check the manufacturer's notes for hardware parameters.

For a computer with N identical/homogeneous processors,

$$\boxed{\text{FLOPS} = \text{N} \times \text{CPU speed} \times \frac{\text{FLOPs}}{\text{CPU cycle}}}$$

Impact and Limitations of Moore's Law

The impact and limitations of Moore's Law

Assuming that Moore's Law holds true, what is the speed up of a computer observed over an average adult's life in the US? Are there practical limitations to this Law?

Superior and Top 500

Superior and Top 500

A proposed compute node in Superior will have two Intel Xeon E5-2698 processors (each processor with 20 cores) at 2.20 GHz, 512 GB RAM, 480 GB Intel Enterprise SSD, Mellanox ConnectX-3 56 Gbps InfiniBand network, and will cost $13,263.13.

Ignoring the cost of physical space, racks, network, storage, electricity and labor, estimate the cost to build a #500 supercomputer (∼405 TFLOPS) with homogeneous compute nodes as the ones described above.

For a computer with N identical/homogeneous processors,

$$\boxed{\text{FLOPS} = \text{N} \times \text{CPU speed} \times \frac{\text{FLOPs}}{\text{CPU cycle}}}$$

Cost of an Exascale Supercomputer

Cost of an exascale supercomputer

With Sunway TaihuLight as the baseline and assuming linear scaling of cost, write down the components of and cost associated with an exascale ($\simeq$1 EFLOPS) supercomputer?

Enterprise Storage Solutions

Storing valuable data

Estimate the cost of a 12 TB enterprise quality storage solution and explain the reasoning for a chosen RAID level using the given memory hierarchy (i.e., data access times).

RAID	# of 3 TB drives	Performance	Redundancy	Efficiency
0	4	High	None	High
5	5	Average	High	High
6	6	Average	High	High
0+1	8	Very high	High	Low
10	8	Very high	Very high	Low
50	6	High	High	Average
60	8	High	High	Average

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Workflow Identification

Celsius $\longleftrightarrow$ Fahrenheit

Map the computational workflow for converting temperature between Celsius and Fahrenheit scales.

Celsius $\longleftrightarrow$ Fahrenheit

Convert temperature between Celsius and Fahrenheit scales.

Research project

Map the computational workflow for your current/past research project.

Subroutine Modification

`sum_loop()` and `sum_gauss()`

Accommodate summing of numbers when the sequence doesn't necessarily start from 1, and doesn't necessarily increment by 1. Identify the caveats, if any.

Range of Numbers and Memory

16-, 32-, and 64-bit systems

Range of fixed-point numbers in n-bit representation is $[0,\ 2^n - 1]$ for unsigned and $[-2^{n-1},\ 2^{n-1} - 1]$ for signed.

1. Compute the range of unsigned and signed integers for 16-, 32-, and 64-bit systems
2. Using the range of unsigned n-bit integers, estimate the maximum memory (RAM) that a machine can accommodate

Format Conversion

Floating-point number $\longleftrightarrow$ Binary mantissa

Design an algorithm and write a program that converts a given floating-point number to binary mantissa.

Drawing Queens

Drawing queens

Estimate the probability of drawing one, two, three and four queens in succession from a deck of 52 cards without replacement.

Compilation as a Part of Computational Workflow

Single file compilation

Write a well-commented BASH script with suitable error/exit codes to check the existence, size and validity of a source file before attempting compilation and executation. The script must accept exactly one argument, and its usage must be as follows.

```
SCRIPT_NAME SOURCE_FILE
```

`SCRIPT_NAME` can be `gcc.sh` if using C programming language, `gpp.sh` if using C++, `gfortran.sh` if using FORTRAN, `julia.sh` if using Julia, and so on. The script must print the time required for each phase (i.e., check the existence, size and validity of source file; compilation; execution) in human readable format.

Makefiles

PB&J sandwich recipe

Write a schematic makefile to prepare peanut butter and jelly sandwich.

`.tex` $\longrightarrow$ `.pdf`

Write a makefile for converting a `john_04.tex` into `john_04.pdf` assuming that `UN5390.bib`, `UN5390_john.bib` and `UN5390.sty` as the main dependencies. There might be other dependencies as well.

Time for Mathematical Operations

Common arithmetic operations

Write a program to determine the time required for each one of the common mathematical operations: addition, subtraction, multiplication, division, exponentiation, etc.

Is the answer different for integers and non-integers?
Is it in agreement with the manufacturer's claim for such operations?

Memory Parameters

Cache stuff

Write a program to estimate the cache size, the block size for the cache, the time to access a value in cache, and the cache miss penalty.

Is it in agreement with the manufacturer's claim for such parameters?

Gnuplot

A basic plot

```
set term x11
plot sin(x)
```

A scientific/engineering plot

```
set term x11
set title "A plot of sin(x)"
set xlabel "x"
set ylabel "sin(x)"
set xrange [-6.28:6.28]
set grid
plot sin(x)
```

SSH into `colossus.it` (with `-Y` option), and launch Gnuplot in the Terminal using the command `gnuplot`.

Gnuplot Continued

Automating the scientific/engineering plot

Save these instructions in `trig_functions.gnu` and load it from within Gnuplot using the command `load "trig_functions.gnu"`.

```
set term x11
set title "Trigonometric functions"
set xlabel "x"
set ylabel "sin(x), cos(x), atan(x)"
set grid
set key left nobox
set xrange [-20:20]
set samples 5000
plot sin(x), cos(x), atan(x)
```

From a Terminal (but outside of Gnuplot), type `gnuplot trig_functions.gnu`. Is the end result the same?

Matching Performance

sum2n_loop() and sum2n_gauss()

Profiling sum2n.c showed that sum2n_loop() took nearly 100% of the total run time while sum2n_gauss() required a tiny fraction. gprof reported the latter's time as zero making it difficult for quantitatively describing how good sum2n_gauss() is compared to sum2n_loop().

Tweak the code (i.e., the definition of one or both functions in functions.h) such they both take approximately equal amount amount of time. Then, use this information to make a quantitative claim of goodness.

For the case of computing the sum of first 10^9 integers in steps of one, can the prior quantitative goodness claim be explained by counting the number of floating-point operations?

Required material is in week #06 AdditionalMaterials/Profile.

Solve by Inspection

Solve for x and y

such that the following expressions hold true

$$\boxed{\sqrt{x} + y = 7} \qquad \boxed{x + \sqrt{y} = 11}$$

Golden Ratio

Write programs to estimate

the golden ratio, 1.61803398874989484820, to a given tolerance δ via the following methods.

$$\boxed{x_{\text{new}} = \sqrt{1 + x_{\text{old}}}}$$

$$\boxed{x = 1 + \frac{1}{1 + \frac{1}{1 + \frac{1}{1 + \cdots}}}}$$

$$\boxed{x = \frac{13}{8} + \sum_{k=0}^{\infty} \frac{(-1)^{k+1}\ (2k+1)!}{(k+2)!\ k!\ 4^{2k+3}}}$$

Roots of a Quadratic Expression

Identify the bugs

Roots of a quadratic equation, $f(x) = ax^2 + bx + c$, are given by

$$\boxed{x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}}$$

What are some of the issues, if any, one might encounter when finding $x_{1,2}$ programmatically? How might one go about resolving such issues?

Iterations in Successive Bisection Method

Identify minimum number of iterations

Given a and b (the bounds within which the solution is contained), and $\epsilon_\circ = |b - a|$, show that the minimum number of iterations necessary to achieve a tolerance δ in successive bisection method is given by

$$\boxed{n \geqslant \frac{\ln \epsilon_\circ \; - \; \ln \delta}{\ln 2}}$$

Successive bisection, Newton-Raphson and hybrid methods

Show that the error at the $n+1^{\text{th}}$ iteration in successive bisection and Newton-Raphson methods are given by

$$\boxed{\epsilon_{n+1}^{\text{SB}} \propto \epsilon_n} \qquad \boxed{\epsilon_{n+1}^{\text{NR}} \propto \epsilon_n^2}$$

What is the value of α in hybrid method?

$$\boxed{\epsilon_{n+1} \propto \epsilon_n^{\alpha}}$$

Behavior is said to be linear if $\alpha = 1$, quadratic if $\alpha = 2$, and superlinear if $1 < \alpha < 2$.

Error Analysis Integration

Trapezoidal and Simpson's 1/3 rules

Show that that the error in trapezoidal rule is $\mathcal{O}\left(h^3\right)$ and that in Simpson's 1/3 rule is $\mathcal{O}\left(h^5\right)$.

Simpson's 3/8 and Boole's rules

Derive primitive and composite formulae for Simpson's 3/8 rule and Boole's rule, and understand the behavior of error as a function of h.

Monte Carlo techniques

Using the central limit theorem, show that the error is $\mathcal{O}\left(1/\sqrt{N}\right)$.

Monte Carlo Techniques

Definite integral evaluation

Write a program that computes the given definite integral. Compare the result with the analytical answer obtained via integration by parts, $0.50 \times \left(1 - e^{-2\pi}\right) = 0.499063299702889$. How does the error behave?

$$\boxed{I = \int_0^{2\pi} e^{-x} \sin(x)\, dx}$$

Gamma Function

Gamma function, $\Gamma(n)$

Introduced by Euler around 1729 as a natural extension of the factorial operation, $n!$, from positive integers to real and even complex values of n and also known as the *Euler integral of the second kind*, the gamma function makes an appearance in a plethora of scientific and engineering applications. For a positive integer, n

$$\boxed{\Gamma(n) \;=\; (n-1)! \;=\; \int_0^{\infty} x^{n-1}\, e^{-x}\, dx}$$

Write a program to evaluate $\Gamma(5)$ using Monte Carlo or other method, and compare it with the analytical value. How would one go about modeling ∞?

Beta Function

Beta function, $\beta(x, y)$

Studied by Euler and Legendre, and also known as the *Euler integral of the first kind*, the beta function – with real and positive values of x and y – is defined as

$$\boxed{\beta(x, y) = \int_0^1 t^{x-1} (1 - t)^{y-1} \, dt = \frac{\Gamma(x)\,\Gamma(y)}{\Gamma(x + y)}}$$

Write a program to evaluate $\beta(2, 3)$ using Monte Carlo or other method. Compare the answer with the value from far RHS in the above expression. Is the beta function symmetrical, i.e., $\beta(x, y) = \beta(y, x)$?

Volume of a Sphere

Volume of a sphere of radius r in n dimensions

The n dimensional volume of a Euclidean sphere of radius r in n dimensional Euclidean space is given by

$$\boxed{V_n(r) = \frac{\pi^{n/2}}{\Gamma\left(\frac{n}{2}+1\right)} r^n}$$

Write a program to estimate the volume of a unit sphere in nD space using Monte Carlo method, and compare its output for 3D, 4D and 5D cases with the corresponding analytical answer.

Hint: One can use a technique similar to that of finding the value of π.

Search

Search

Describe how one could programmatically go about searching for some number, M, amongst the following 101 integers:

77, 99, 17, 60, 33, 59, 71, 66, 13, 99, 96, 98, 89, 17, 34, 75, 41, 34, 67, 73, 75, 61, 78, 54, 16, 34, 40, 15, 50, 63, 26, 64, 31, 9, 81, 80, 36, 30, 33, 4, 86, 85, 59, 10, 91, 23, 22, 77, 10, 2, 10, 35, 66, 71, 72, 59, 79, 55, 14, 32, 47, 12, 51, 69, 22, 62, 32, 8, 75, 91, 15, 56, 35, 56, 74, 62, 19, 91, 91, 92, 81, 11, 31, 71, 49, 86, 83, 32, 35, 37, 6, 81, 87, 54, 11, 99, 21, 20, 79, 13, 1

Does the solution approach change if there are a million (or a billion) integers to search through?

Differential Equations: Euler's Method

1D constant velocity motion

$$f(x,t) = \frac{dx}{dt} = v$$

First order linear DE

$$f(x_\circ, t_\circ) = \left.\frac{dx}{dt}\right|_{t=0} = v_\circ \; ; \; x(t=0) = x_\circ$$

Initial conditions

Is the Euler's method stable for all values of h?

Differential Equations: Euler's Method

2D projectile motion

$$\frac{d^2x}{dt^2} = \frac{dv_x}{dt} = 0 \; ; \quad \frac{d^2y}{dt^2} = \frac{dv_y}{dt} = -g \; ; \quad \frac{dx}{dt} = v_x \; ; \quad \frac{dy}{dt} = v_y$$

First order linear DEs

Differential Equations: Euler's Method

2D projectile motion (continued)

$$f(v_x, t) = \frac{dv_x}{dt} = 0 \; ; \quad f(v_y, t) = \frac{dv_y}{dt} = -g$$

First order linear DEs for velocity components

$$f(x, t) = \frac{dx}{dt} = v_x \; ; \quad f(y, t) = \frac{dy}{dt} = v_y$$

First order linear DEs for position components

Differential Equations: Euler's Method

2D projectile motion (continued)

$$\boxed{t_{n+1} = t_n + h}$$

$$\boxed{v_{x,n+1} = v_{x,n}} \qquad \boxed{v_{y,n+1} = v_{y,n} - h\,g}$$

$$\boxed{x_{n+1} = x_n + h\,v_{x,n}} \qquad \boxed{y_{n+1} = y_n + h\,v_{y,n}}$$

With $g = 32.174\ ft/s^2$, $\alpha = 45^\circ$ and $v_\circ = 20\ m/s$, plot the theoretical trajectory (from $y = 0$ to $y = 0$) of an object weighing $m = 400\ gm$. Write a program that simulates this trajectory. Is the order of computing position and velocity components critical? Is there a need to store $v_{x,n}$ for each time step? Does the size of h matter?

Differential Equations: ABM2 Method

Adams-Bashforth-Moulton method

Show that local and global truncation error in AB2 and AM2 methods is

$$\epsilon_{\text{local truncation}} = \mathcal{O}\left(h^3\right) \qquad \epsilon_{\text{global truncation}} = \mathcal{O}\left(h^2\right)$$

Show that the optimum value of h for ABM2 method is

$$h_\circ = \sqrt[3]{\frac{\xi}{2}}$$

Matrix Methods: System of Linear Equations

System of linear equations

Write a program to solve the below system of linear equations using Gaussian elimination method.

$$\begin{array}{rcrcrcr} 3\,x & + & 2\,y & - & z & = & 1 \\ 2\,x & - & 2\,y & + & 4\,z & = & -2 \\ -\,x & + & 0.50\,y & - & z & = & 0 \end{array}$$

Verify the answer, $x = 1$, $y = -2$ and $z = -2$.

Matrix Methods: LU Factorization

LU factorization

Write a program that factors the matrix given below, A, as a product of a lower triangular matrix and an upper triangular matrix with partial pivoting.

$$\begin{pmatrix} 10 & -7 & 0 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix}$$

Can the program be generalized for any order N?

Matrix Methods: Transpose

Transpose

Introduced by the British mathematician Arthur Cayley (1821 – 1895) in 1858 and denoted by A^T, transpose of a matrix A is the result of reflecting A over the primary diagonal OR writing the rows of A as its columns OR writing the columns of A as its rows.

$$\boxed{A^T_{ij} = A_{ji} \qquad \Rightarrow \qquad \left(A^T\right)^T = A}$$

Write a program to find the transpose of a given matrix of order N and verify its correctness for the following matrices.

$$A = \begin{pmatrix} 4 & 3 \\ 3 & 2 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 2 & 0 \\ -1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}$$

Matrix Methods: Determinant

Determinant

Laplace's expansion, also known as cofactor expansion, is an expression for the determinant of a square matrix A of order N that is a weighted sum of the determinants of N sub-matrices of A, each of order $N - 1$. The (i, j) cofactor of A is a scalar quantity (i.e., a number) defined as

$$\boxed{C_{i\,j} \;=\; (-1)^{i+j}\; M_{i\,j}}$$

$M_{i\,j}$ is the (i, j) minor matrix of A – the determinant of sub-matrix formed by removing the ith row and j^{th} column of A. Then

$$\boxed{\det A \;=\; |A| \;=\; \sum_{i,j=1}^{N} a_{i\,j}\, C_{i\,j}}$$

Matrix Methods: Determinant continued

Determinant

Write a program to compute the determinant of a matrix of order N and verify its correctness for the following matrices.

$$A = \begin{pmatrix} 4 & 3 \\ 3 & 2 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 2 & 0 \\ -1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}$$

Matrix Methods: Inversion

Inversion

Inverse of a square matrix of order N, A, is given by

$$\boxed{A^{-1} = \frac{1}{\det A} \times \text{adj } A}$$

Adjugate of A is the transpose of the cofactor matrix, C, of A. Cofactor matrix of A is matrix C of order N whose (i, j) entry is the (i, j) cofactor of A. Write a program to find the inverse of a given matrix of order N and verify its correctness for the following matrices.

$$A = \begin{pmatrix} 4 & 3 \\ 3 & 2 \end{pmatrix} \qquad B = \begin{pmatrix} -2 & 3 \\ 3 & -4 \end{pmatrix} \qquad C = \begin{pmatrix} 1 & 2 & 0 \\ -1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}$$

Matrix Methods: Message Encryption

Message encryption

Find a suitable A to encrypt the previously discussed message

```
GOD SAVE MY QUEEN, AMEN EH?
```

Hill cipher-coded in matrix B. Use own code from the previous *Do at home exercise* to find A^{-1}. Extend the code so that it now encrypts B with A, and decrypts C with A^{-1}.

How would the programming and/or computational intensity change if A, A^{-1}, B and C had a different order than what is discussed?

Matrix Methods: Magic Squares

Magic squares

A magic square is a matrix of order N (> 2) constructed using integers from 1 through N^2 such that the row, column and diagonal sums are identical. These magic squares were known in China before 2,000 BC. Legend has it that a 3×3 magic square, known as *Lo Shu*, forms the mathematical basis for *feng shui* – the ancient Chinese philosophy of balance and harmony.

$$\begin{pmatrix} 8 & 1 & 6 \\ 3 & 5 & 7 \\ 4 & 9 & 2 \end{pmatrix}$$

Write a program that generates a magic square for a given N. Is there more than one magic square for a given N?

Matrix Methods: Payoff Matrix

Payoff matrix

In a two-person game, player A (rows) has two options: α and β, and player B (columns) has two options: μ and ξ.

$$P = \begin{pmatrix} 3 & -1 \\ -2 & 3 \end{pmatrix}$$

A decides to pick moves at random, choosing to play α 75% of the time and β the remaining 25%. B also decides to pick moves at random, choosing μ 20% of the time and ξ the remaining 80%.

Suppose that they play the game 100 times. How much does A expect to win or loose? Can matrix multiplication technique be employed to arrive at the same result? Will a similar approach work to estimate the same for B?

Parallel Computing: Amdahl's and Gustafson's Laws

Derive and functionalize

Starting from respective definitions of t_{serial} and t_{parallel} (refer to in-class discussions for more details), derive the following expressions

$$S_{\text{Amdahl}} = \frac{1}{(1 - P) + \frac{P}{N}}$$

$$S_{\text{Gustafson}} = N - (1 - P)(N - 1)$$

Write two functions, `speedup_amdahl(P, NMin, NMax)` and `speedup_gustafson(P, NMin, NMax)`, that will compute and print the predicted speed up from $2^{\texttt{Nmin}}$ to $2^{\texttt{NMax}}$ processors. `P` represents the portion of the code that is parallelizable. Enhance the functionality to display a plot with necessary title, axis labels and legends.

Tips and Tricks

Test them before trusting them

http://dilbert.com/strip/1989-04-20/

File/Folder Naming Convention

Develop a personalized yet consistent scheme

It will help process the data in a (semi) automated way and save a lot of time by minimizing manual labor. Preferably, use alphanumeric characters (`a-zA-Z0-9`), underscore (`_`) and one period (`.`) in file/folder.

Parsing other special characters, `!@#$%^ &*();:-?/\=+`, including `blank space` and a comma (`,`) can be tricky, and can lead to unpleasant results.

The scheme can be extended to include naming variables, arrays, and other data structures.

LaTeX Workflow for Assignments

One-time setup (once per semester)

```
cd ${UN5390}/LaTeXTemplates/Course
cp UN5390.bib ${USER}.bib
cp UN5390_Settings_Template.tex UN5390_Settings.tex
# EDIT THE EDITABLE PORTIONS IN UN5390_Settings.tex
git add ${USER}.bib UN5390_Settings.tex
```

One-time setup (once per assignment)

```
cd ${UN5390}/LaTeXTemplates/Course
cp john_WEEK.tex \
  ../../CourseWork/Week_01/${USER}_01/${USER}_01.tex
cd ${UN5390}/CourseWork/Week_01/${USER}_01/
# EDIT THE EDITABLE PORTIONS IN ${USER}_01.tex
```

Replace 01 with the appropriate week number.

LaTeX Workflow for Assignments

Whenever you are working on the assignment

```
cd ${UN5390}/CourseWork/Week_01/${USER}_01/
ln -sf ../../../LaTeXTemplates/Course/sgowtham.bib
ln -sf ../../../LaTeXTemplates/Course/${USER}.bib
ln -sf ../../../LaTeXTemplates/Course/UN5390.sty
ln -sf ../../../LaTeXTemplates/Course/UN5390_Settings.tex
ln -sf ../../../LaTeXTemplates/Course/MichiganTech.eps
ln -sf ../../../LaTeXTemplates/Course/MichiganTech.png
# UPDATE ${USER}.bib AND ${USER}_01.tex WHEN NECESSARY
# COMPILE ${USER}_01.tex TO PRODUCE ${USER}_01.pdf
# DELETE TEMPORARY LaTeX FILES
rm -f sgowtham.bib ${USER}.bib MichiganTech.???
rm -f UN5390.sty UN5390_Settings.tex
```

Replace 01 with the appropriate week number.

LaTeX Workflow for Assignments

Compiling ${USER}_01.tex to produce ${USER}_01.pdf

```
# Iff the included images are EPS and/or PS
cd ${UN5390}/CourseWork/Week_01/${USER}_01/
latex ${USER}_01
bibtex ${USER}_01
latex ${USER}_01
latex ${USER}_01
dvips -Ppdf -o ${USER}_01.ps ${USER}_01.dvi
ps2pdf ${USER}_01.ps ${USER}_01.pdf
rm -f ${USER}_01.aux ${USER}_01.bbl ${USER}_01.blg
rm -f ${USER}_01.dvi ${USER}_01.log ${USER}_01.out
rm -f ${USER}_01.ps
```

Replace 01 with the appropriate week number.
For more information, visit https://github.com/MichiganTech/LaTeX_GettingStarted

LaTeX Workflow for Assignments

Compiling ${USER}_01.tex to produce ${USER}_01.pdf

```
# Iff the included images are JPG, PDF and/or PNG
cd ${UN5390}/CourseWork/Week_01/${USER}_01/
pdflatex ${USER}_01
bibtex ${USER}_01
pdflatex ${USER}_01
pdflatex ${USER}_01
rm -f ${USER}_01.aux ${USER}_01.bbl ${USER}_01.blg
rm -f ${USER}_01.dvi ${USER}_01.log ${USER}_01.out
```

Replace 01 with the appropriate week number.
For more information, visit https://github.com/MichiganTech/LaTeX_GettingStarted

Timing a Task

date command

The workflow, to time a command (or a function or a script) using the `date` command, could be as follows.

```
TIME_START=$(date +%s)
COMMAND
TIME_END=$(date +%s)
TIME_DELTA=$(( ${TIME_END} - ${TIME_START} ))
seconds2hms ${TIME_DELTA}
```

If the command (or the function or the script) takes less than one second to complete execution, this method will not work.

`seconds2hms()` was discussed in Training Camp #08.

Timing a Task

time and /usr/bin/time

`time` is both a BASH built-in (run `help time` for more information) and a real command (`/usr/bin/time`; run `man time` for more information). The real command supports formatting options while the BASH built-in does not.

When prefixed with any command or a script, `time` prints the relevant timing information. Common usage is as follows:

```
time COMMAND
time SCRIPT

/usr/bin/time COMMAND
/usr/bin/time SCRIPT
```

Random Numbers in BASH

$RANDOM

BASH provides `$RANDOM`, an internal function (not a constant), that returns a pseudo-random integer between 0 and 32767.

```
echo $(($RANDOM % N))
```

generates a random number between 0 and `(N-1)`. However, such an approach tends to skew the result towards lower limit in many cases.

`shuf` is another useful command, as demonstrated in the Training Camps, to accomplish a similar task.

Doxygen Generate documentation from comments in source code

C/C#/C++/FORTRAN/IDL/Java/PHP/Python, LaTeX, and Doxygen

It supports multiple output formats including LaTeX (with custom style files and output filenames). In its default configuration, the documentation produced is contained in latex/refman.pdf.

```
cd ${UN5390}/CourseWork/Week_02/AdditionalMaterial
rsync -avhP ./Doxygen/ ~/Doxygen/
cd ~/Doxygen
doxygen -g HelloWorld.cfg  # Generates config file
# Edit HelloWorld.cfg, if necessary
doxygen HelloWorld.cfg     # Generates necessary files
cd latex
make                       # Generates documentation
```

Official website | GitHub

Refer to man doxygen for more information. make command will be discussed in detail in subsequent weeks. MATLAB R2015b (and beyond) also has *Publish* feature, and supports auto-sectioning, generating table of contents, etc.

Repeating Commands

!!, !STRING, !N and CMD !*

!! repeats the previous command. !STRING repeats the most recent command that started with STRING. !N repeats the *N*th command in command history. CMD !* runs CMD command with options used for the previous command.

```
cd ${UN5390}
!!
date -R
!da
!cd
history
!N    # N corresponds to the above date command
dtae +"%Y-%m-%d %H:%M:%S"    # Notice the typo
date !*
```

Converting Seconds to `hh:mm:ss`

A quick workaround for long-tailed mathematics

```
# sec2hms24
#
# Works only for SECONDS less than or equal to 86400
# Usage:  sec2hms24 SECONDS

sec2hms24() {
   # User input; ADD INPUT VALIDATION, ETC.
   local seconds=$1

   # Print the result
   date -u -d @${seconds} +"%T"
}
```

Add this function to `${HOME}/bin/functions.sh` and run `source ${HOME}/.bashrc`.

Disk Write Speed

dd

```
dd if=/dev/zero of=/tmp/output.img bs=8k count=256k \
conv=fdatasync ; rm -rf /tmp/output.img
```

Output from my local workstation and `colossus.it` are included below for reference.

```
262144+0 records in
262144+0 records out
2147483648 bytes (2.1 GB) copied, 9.29104 s, 231 MB/s

262144+0 records in
262144+0 records out
2147483648 bytes (2.1 GB) copied, 15.9378 s, 135 MB/s
```

Refer to `man dd` for more information.

Preventing Lines from Wrapping Around in a Terminal

```
less FILENAME_WITH_LONG_LINES
short.q:compute-0-0.local:john-users:john:test.sh:102541
:sge:0:1449493098:1449493123:1449499243:0:0:6120:...
qlogin.q:compute-0-99.local:jill-users:jane:QLOGIN:102551
:sge:0:1449509796:1449509796:1449509911:100:137:115:...
short.q:compute-0-1.local:john-users:amy:test2.sh:102546
:sge:0:1449501727:1449505169:1449510848:0:0:5679:...
```

```
less -S FILENAME_WITH_LONG_LINES
short.q:compute-0-0.local:john-users:john:test.sh:...
qlogin.q:compute-0-99.local:jill-users:jane:QLOGIN:...
short.q:compute-0-1.local:john-users:amy:test2.sh:...
long.q:compute-0-36.local:greg-users:daniel:scf.sh:...
long.q:compute-0-57.local:zach-users:zach:optimize.sh:...
```

Multiple Makefiles in a Folder

Problem of multiple makefiles

Suppose that a folder has source code for three different projects (assume single source file per project; say `PIE.c`, `Primes.c`, and `Fibonacci.c`). Further suppose that each project must have its own makefile. How does one go about achieving this?

Handling multiple makefiles

Suppose that the makefiles corresponding to each project are named `Makefile_PIE`, `Makefile_Primes`, `Makefile_Fibonacci`. One way to go about using a given makefile would be to use the `-f` option. For e.g.,

```
make -f Makefile_Primes
```

The other way to accomplish it is using a symbolic link. For e.g.

```
ln -sf Makefile_PIE Makefile ; make
```

Multiple Makefiles in a Folder

Compiling and running all `*.c` files programmatically

```
#!  /bin/bash
#
# USEFUL COMMENTS AND USAGE INSTRUCTIONS

for x in $(ls *.c)
do
  # Extract the basename of .c file
  BASENAME=$(echo "${x}" | awk -F '.' '{ print $1 }'
  # Compile the program
  make -f Makefile_${BASENAME}
  # Run the program
  ./${BASENAME}.x
done
```

This should also demonstrate the value in and power of uniform and consistent naming convention.

Where's the Data?

du, sort, and head

```
du -hsx * | sort -rh | head -5
```

Output from `colossus.it` is included below for reference.

```
13G    git_work
214M   Application Data
79M    norepi
41M    test_runs
35M    Desktop
```

Change the option for `head` command to display more (or less).

Refer to `man du`, `man sort`, and `man head` for information.

Leading Zeros and printf

Forcing the base representation for numbers with leading zeros

```
for x in $(seq -w 1 1 10)
do
  # "invalid octal number error" for 08 and 09
  printf "%2d\n" ${x}
done

x=012
echo "${x}"            # 012
echo $((x + 2))        # 12
printf "%d\n" "${x}"   # 10
```

Try the `for` loop without the `-w` option.

Leading Zeros and printf

Forcing the base representation for numbers with leading zeros

Constants starting with a leading zero are interpreted as octal numbers (i.e., base 8) and such a representation only involves 0 through 7.

```
x=012
x=$((10#$x))
echo $((x + 2))
printf "%d\n" "$x"

for x in $(seq -w 1 1 10)
do
  # ${x#0} strips the leading zero
  printf "%02d\n" "${x#0}"
done
```

A constant with leading `0x` (or `0X`) is interpreted as a hexadecimal number.

Leading Zeros and printf

Forcing the base representation for numbers with leading zeros

Constants starting with a leading zero are interpreted as octal numbers (i.e., base 8) and such a representation only involves 0 through 7.

```
x=012
x=$((10#$x))
echo $((x + 2))
printf "%d\n" "$x"

for x in $(seq -w 1 1 10)
do
  # ${x#0} strips the leading zero
  printf "%02d\n" "${x#0}"
done
```

A constant with leading `0x` (or `0X`) is interpreted as a hexadecimal number.

Changing the Name of gmon.out

Changing the name of gmon.out

```
# Compile the program
gcc -Wall -g -pg PROGRAM.c -lm -o PROGRAM.x

# Set the prefix via an environment variable to PROGRAM
export GMON_OUT_PREFIX=PROGRAM

# Run the program.  This should result in PROGRAM.PID
# instead of gmon.out.  PID is the process ID (a number)
./PROGRAM.x

# Run the profiler
gprof -q ./PROGRAM.x PROGRAM.PID > PROGRAM_CallGraph.txt
```

Information courtesy: Adam Mitteer and Eisa Hedayati, UN5390 in Fall 2016.

Manual for a Random Command

ls, shuf, and head

```
man $(ls /bin | shuf | head -1)
```

This could be an easy way to learn about a new command. It may be a good idea to define a function in ${HOME}/bin/functions.sh and source ${HOME}/.bashrc. Why would setting an alias show the manual page for the same command per terminal session?

```
# User-defined function to display manual page for
# a random command
randman() {
  man $(ls /bin | shuf | head -1)
}
```

Refer to man ls, man shuf, and man head for information.

Automating Responses to Interactive Commands

Using `expect` to SSH into a remote server

```
MY_PASSWD="asdf1234"
expect - << EndExpect
  spawn ssh ${USER}@colossus.it.mtu.edu
  expect "Password"
  send "$MY_PASSWD\r"
  expect eof
EndExpect
```

Hard-coding passwords in plain text

in a BASH script is a TERRIBLE idea. The above example, in turn, is a VERY BAD one. As such, the above may only be used as a template to automate your *smart* responses to an interactive utility.

Starting Where We ended in vim

Opening a file with the same/previous view in vim

To ensure vim places the cursor on the same line (i.e., shows the same *view*) upon re-opening a file, run the following command.

```
mkdir -p ${HOME}/.vim/view
```

Append ${HOME}/.vimrc with the following content.

```
" Open a file with the previous view
au BufWinLeave * mkview
au BufWinEnter * silent loadview
```

Open ${HOME}/.bashrc, move to the very end, close the file, and re-open it. Did vim open with the same *view*?

Refer to man vim for more information.

round()

Round a float to a given number of decimal places

```
round() {
  echo $(printf %.$2f $(echo \
    "scale=$2;(((10^$2)*$1)+0.5)/(10^$2)" | bc))
}
```

Usage

```
PI=3.14159265358979323846264338327 9
round ${PI} 0  # No decimal places
round ${PI} 2
round ${PI} 15
XYZ=3.50
round ${XYZ} 0  # Rounds up, to 4
```

Add the function to `${HOME}/bin/functions.sh` and run `source ${HOME}/.bashrc`.

LaTeX Workflow for Project Work

One-time setup (once per semester)

```
cd ${UN5390}/ProjectWork
cp Description.tex Description_${USER}.tex
# EDIT Description_${USER}.tex (KEEP IT CONCISE).
# COMPILE Description_${USER}.tex TO PRODUCE THE PDF.

cp Status.tex Status_${USER}.tex
# EDIT \project{} in Status_${USER}.tex
touch Status_${USER}.pdf

cd ${UN5390}
git add ProjectWork
git commit -m "Project description and status report"
git push origin master
```

LaTeX Workflow for Project Work

Whenever you are working on the project description or status report

```
cd ${UN5390}/ProjectWork/
ln -sf ../LaTeXTemplates/Course/sgowtham.bib
ln -sf ../LaTeXTemplates/Course/${USER}.bib
ln -sf ../LaTeXTemplates/Course/UN5390.sty
ln -sf ../LaTeXTemplates/Course/UN5390_Settings.tex
ln -sf ../LaTeXTemplates/Course/MichiganTech.eps
ln -sf ../LaTeXTemplates/Course/MichiganTech.png
# UPDATE ${USER}.bib WHEN NECESSARY.
# COMPILE Description_${USER}.tex TO PRODUCE THE PDF.
# COMPILE Status_${USER}.tex TO PRODUCE THE PDF.
# DELETE TEMPORARY LaTeX FILES.
rm -f sgowtham.bib ${USER}.bib MichiganTech.???
rm -f UN5390.sty UN5390_Settings.tex
```

LaTeX Workflow for Project Work

Compiling `Description|Status_${USER}.tex` to produce the PDF

```
# Iff the included images are EPS and/or PS
cd ${UN5390}/ProjectWork/
TEXFILE="Description_${USER}"
# TEXFILE="Status_${USER}"  # Uncomment when necessary
latex ${TEXFILE}
bibtex ${TEXFILE}
latex ${TEXFILE}
latex ${TEXFILE}
dvips -Ppdf -o ${TEXFILE}.ps ${TEXFILE}.dvi
ps2pdf ${TEXFILE}.ps ${TEXFILE}.pdf
rm -f ${TEXFILE}.aux ${TEXFILE}.bbl ${TEXFILE}.blg
rm -f ${TEXFILE}.dvi ${TEXFILE}.log ${TEXFILE}.out
rm -f ${TEXFILE}.ps
```

LaTeX Workflow for Project Work

Compiling `Description|Status_${USER}.tex` to produce the PDF

```
# Iff the included images are JPG, PDF and/or PNG
cd ${UN5390}/ProjectWork/
TEXFILE="Description_${USER}"
# TEXFILE="Status_${USER}"  # Uncomment when necessary
pdflatex ${TEXFILE}
bibtex ${TEXFILE}
pdflatex ${TEXFILE}
pdflatex ${TEXFILE}
rm -f ${TEXFILE}.aux ${TEXFILE}.bbl ${TEXFILE}.blg
rm -f ${TEXFILE}.dvi ${TEXFILE}.log ${TEXFILE}.out
```

LaTeX Workflow for Project Work

Committing project description or status report to the repository

```
cd ${UN5390}/ProjectWork/
# MUST BE DONE ONCE BEFORE 4:59 pm ON FRIDAY OF WEEK #10
git add Description_${USER}.tex
git add Description_${USER}.pdf
git commit -m "(Updated) Project description"
git push origin master
#
# MUST BE COMPLETED BEFORE 4:59 pm ON FRIDAY OF EACH
# WEEK STARTING #10 (WORTH 1% OF THE GRADE)
git add Status_${USER}.tex
git add Status_${USER}.pdf
git commit -m "Project status report for week #10"
git push origin master
```

Replace 10 with the appropriate week number.

ucfirst()

Convert first letter of a string to uppercase

```
ucfirst() {
  if [ $# != 1 ]
  then
    echo
    echo " Usage:  ${FUNCNAME} STRING"
    echo " e.g.:  ${FUNCNAME} 'this is a test'"
    echo
  else
    local str=$(echo "$1" | sed 's/\(.\)/\U\1/')
    echo ${str}
  fi
}
```

Add the function to `${HOME}/bin/functions.sh` and run `source ${HOME}/.bashrc`.

ucwords()

Convert first letter in every word of a string to uppercase

```
ucwords() {
  if [ $# != 1 ]
  then
    echo
    echo " Usage:  ${FUNCNAME} STRING"
    echo " e.g.:  ${FUNCNAME} 'this is a test'"
    echo
  else
    local str=$(echo "$1" | sed 's/\b\(.\)/\u\1/g')
    echo ${str}
  fi
}
```

Add the function to `${HOME}/bin/functions.sh` and run `source ${HOME}/.bashrc`.

smart_ucwords()

A smarter version of ucwords()

```
smart_ucwords() {
  # ucwords() functionality
  local str=$(echo "$1" | sed 's/\b\(.\)/\u\1/g')
  ignore_list=(A An And If Into Is For Of Or)

  for x in "${ignore_list[@]}"
  do
    lc_x=$(echo "${x}" | tr '[:upper:]'  '[:lower:]')
    str=$(echo "${str}" | sed "s/ ${x} / ${lc_x} /g")
  done
  echo ${str}
}
```

Add the function to `${HOME}/bin/functions.sh` and run `source ${HOME}/.bashrc`.

gcc_omp()

A compact function to compile OpenMP programs

```
gcc_omp() {
  if [ $# != 1 ]
  then
    echo
    echo " Usage:  ${FUNCNAME} PROGRAM.c"
    echo " e.g.:  ${FUNCNAME} HelloWorld_omp_01.c"
    echo
  else
    local cbase=$(echo "$1" | awk -F "." '{ print $1 }')
    gcc -Wall -g -lm -fopenmp $1 -o ${cbase}.x
  fi
}
```

Add this function to `${HOME}/bin/functions.sh` and run `source ${HOME}/.bashrc`. One may instead write a well-commented `gcc_omp.sh` with suitable error codes that will check the existence, non-zero file size and usefulness of the C program before compiling and running it with a specified number of threads.

gcc_omp.sh Template for parent BASH script

* Accepts two arguments: FILENAME and OMP_NUM_THREADS
* Checks FILENAME for existence, non-zero file size, and useful (i.e., non-comment and non-blank line) content
* Checks the current directory and BASENAME.x for write permission
* Compiles FILENAME using

```
gcc -Wall -g -lm -fopenmp FILENAME -o BASENAME.x
```

* Runs BASENAME.x using OMP_NUM_THREADS threads

Lock File

Brainstorm

Suppose that a shell script, `summary.sh`, is designed to extract necessary information from a series of simulations and write them to `summary.txt`.

How can one ensure that a second (or n^{th}) inadvertent execution of the same script does not write to/update the `summary.txt` file while the first one is still running?

Lock File

Version #1

```
#!  /bin/bash
# Useful comments

LOCKFILE="/tmp/${USER}_summary.lck"
if [ -f "${LOCKFILE}" ]
then
  echo " Lock file exists.  Exiting the script."
  exit
else
  touch ${LOCKFILE}
  # Commands to extract and summarize information (core)
  rm -f ${LOCKFILE}
fi
```

Lock File

Problem with version #1

The script works fine as long as it is not interrupted/terminated while the commands to extract and summarize information (i.e., the core) are running. If killed during the core's execution, the lock file will continue to exist.

Subsequent legitimate executions of the script won't run until the lock file has been manually deleted.

Lock File

Version #2

```
#!  /bin/bash
# Useful comments

LOCKFILE="/tmp/${USER}_summary.lck"
if [ !  -e "${LOCKFILE}" ]
then
  trap "rm -f ${LOCKFILE}; exit" INT TERM EXIT
  echo $$ > ${LOCKFILE}
  # Commands to extract and summarize information (core)
  rm -f ${LOCKFILE}
else
  echo "${LOCKFILE} exists; owned by $(cat ${LOCKFILE})"
fi
```

Lock File

Problem with version #2

`trap` command ensures that the lock file is also removed when the script is interrupted/killed.

However, there is potential for a race condition between the time one tests for the lockfile and time one creates it.

Lock File

Version #3

```
#!  /bin/bash
# Useful comments

LOCKFILE="/tmp/${USER}_summary.lck"
if (set -o noclobber; echo $$ > ${LOCKFILE}) 2> /dev/null
then
  trap 'rm -f "${LOCKFILE}"; exit $?'  INT TERM EXIT
  # Commands to extract and summarize information (core)
  rm -f ${LOCKFILE}
  trap - INT TERM EXIT
else
  echo "${LOCKFILE} exists; owned by $(cat ${LOCKFILE})"
fi
```

Download and install Julia 0.5.0

```
OS="linux" ; ARCH="x86_64" ; VERSION="0.5.0"
JULIA="julia-${VERSION}-${OS}-${ARCH}"
mkdir -p ${HOME}/apps/julia/
cd ${HOME}/apps/julia/
tar -zxvf ${HOME}/tmp/${JULIA}.tar.gz
mv julia-* ${VERSION}

# Update ${HOME}/.bash_${USER} and source it
JULIA="${HOME}/apps/julia/0.5.0"
PATH="${PATH}:${JULIA}/bin"
LD_LIBRARY_PATH="${LD_LIBRARY_PATH}:${JULIA}/lib"
MANPATH="${MANPATH}:${JULIA}/share/man"
```

Julia | Downloads | Documentation | JUNO (IDE) | JuliaBox.com
Download 64-bit Generic Linux binary and save the `*.tar.gz` in `${HOME}/tmp/`.

Test (Iterative solution of golden ratio)

```
# What is the output of the following command?
# which julia

cd ${UN5390}
git pull

cd CourseWork/Week_12/${USER}_12
rsync -avhP ../AdditionalMaterial/Julia/ ./Julia/

cd Julia
julia GoldenRatio.jl
julia GoldenRatioSml.jl
```

Sample files provided by Adam Mitteer, UN5390 in Fall 2016, are included in week #12 `AdditionalMaterial`.

Opportunities

They do knock every once in a while

http://dilbert.com/strip/2009-09-24/

IT-Managed Linux Labs

- `colossus.it.mtu.edu` and `guardian.it.mtu.edu`
  - Intel Xeon X5675 3.07 GHz, 24 CPU cores, 96 GB RAM
  - Accessible for all from anywhere via SSH using a Terminal
  - Appropriate for light- to medium-weight computations
- Linux workstation in a campus lab/office
  - May not be as powerful as `colossus.it` or `guardian.it`
  - May not be directly accessible from off-campus
  - https://www.it.mtu.edu/computer-labs.php

All IT-managed workstations in Linux labs run RHEL 7.x and will mount the campus home directory.

Network of Expertise

UN5390; CRN: 84758

#	Name	Email	Dept/Program	Advisor
01	Adam Mitteer	aamittee	Data Science	Mari Buche
02	Ashley Kern	ankern	Data Science	Mari Buche
03	Eisa Hedayati	hedayati	Physics/CS&E	John Jaszczak
04	Hashim Mahmud	hnalmahm	ME-EM	Gregory Odegard
05	Jeffrey Brookins *	jmbrooki	MSE	Jaroslaw Drelich
06	Paul Roehm	pmroehm	ME-EM	Gregory Odegard
07	Qing Guo	qinguo	Physics	Ravindra Pandey
08	Subin Thomas	subint	Physics	Raymond Shaw

* Undergraduate students

Network of Expertise

BE5390: Biomedical Engineering CRN: 84759

#	Name	Email	Advisor
09	Cal Riutta *	cdriutta	Jinfeng Jiang

EE5390: Electrical and Computer Engineering; CRN: 84760

10	Akhil Kurup	amkurup	Michael Roggemann
11	Avinaash Kovvuri	askovvur	Michael Roggemann
12	Ian Cummings	itcummin	Timothy Havens
13	Prithvi Kambhampati	pkambham	Michael Roggemann
14	Sandeep Lanka	slanka	Michael Roggemann
15	Sameer Saraf	svsaraf	Michael Roggemann
16	Shuo Wang	wshuo	Jeremy Bos
17	Zhiqiang Zhao	qzzhao	Zhuo Feng

* Undergraduate students

Network of Expertise

17 registered students.

NSF Graduate Research Fellowship Program 2017

- Applicant must be a US citizen or a permanent resident
- Fellowship supports 3 years of study

  $34k of stipend per year +
  $12k of cost-of-education allowance to the university per year
- MS and PhD candidates in STEM and STEM education

  Must be in first two years of graduate study
  Senior undergraduates are also encouraged to apply
- Michigan Tech Information Session

  5 pm, 7th September 2016 (Wednesday), Admin 404

National Science Foundation | NSF Graduate Research Fellowship Program | Application deadline: 24-28th October 2016

CareerFEST and Career Fair

* More details at http://www.mtu.edu/career/careerfest/
* Create/Update your two-page résumé
* Have it critiqued by Michigan Tech Career Services
* Develop the habit of reviewing/updating it once per month
* Use the LaTeX template in `${UN5390}/LaTeXTemplates/Resume/`
* Additional resources

  http://www.mtu.edu/career/students/toolbox/resumes/examples/
  http://owl.english.purdue.edu/owl/resource/719/1/
  http://www.sharelatex.com/templates/cv-or-resume
  http://www.latextemplates.com/cat/curricula-vitae

CareerFEST is a collection of many different informal events that take place during the month of Career Fair.

CareerFEST and Career Fair Los Alamos National Laboratory

- Commonly used Linux commands
- Extensive shell scripting
- Revision control (Git)
- Workflow development
- Statistical analysis (Python, R and Gnuplot)
- Visualization (Python, R and Gnuplot)
- White papers and internal publications (LaTeX)

Los Alamos National Laboratory | Los Alamos National Laboratory on GitHub

CareerFEST and Career Fair MIT Lincoln Laboratory

- Commonly used Linux commands
- Extensive shell scripting
- Revision control (Git/Subversion)
- Workflow development
- Domain-specific expertise
- Modeling, simulation, analysis and visualization

  Choice of language/toolset depends on a project
- White papers, internal and external publications (LaTeX)

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Keweenaw Climate Science Event #1 of four-part event

The Orpheum Theater

6 – 8 pm on Thursday, 8th September 2016

Subsequent events

6th October 2016

3rd November 2016

1st December 2016

No admission fee

Free pizza and soft drinks

More information

Organized by Keweenaw Climate Community, and sponsored by the local chapter of the American Chemical Society and the Department of Social Sciences at Michigan Tech.

Keweenaw Climate Science Event #2 of four-part event

The Orpheum Theater

6 – 8 pm on Thursday, 6th October 2016

Subsequent events

3rd November 2016

1st December 2016

No admission fee

Free pizza and soft drinks

More information

Organized by Keweenaw Climate Community, and sponsored by the local chapter of the American Chemical Society and the Department of Social Sciences at Michigan Tech.

ICC Distinguished Lecture

CS For All: Considering The Implications Of 'For All'

Dr. Kamau Bobb
Research Scientist, Georgia Tech
Program Officer, CISE, NSF

4th October 2016 1 pm, ME-EM 406

https://www.ceismc.gatech.edu/about/staffdirectory/kamau-bobb

LANL CSCNSI 2017

- Applicant must be a US citizen
- Open to junior and senior undergraduates
- Paid 10-week research internship in Los Alamos, NM
- Introduction to techniques and practices of cluster computing via

  Lectures (seminars from HPC practitioners and researchers) +

  Laboratory (hands-on setup, configuration, administration, testing, monitoring, scheduling, etc. of supercomputer clusters) +

  Technical broadening (research project) +

  Professional development (resume and poster development, verbal and written communication, technical project execution) +

  Tour of the Metropolis Supercomputing Center

Los Alamos National Laboratory | Los Alamos National Laboratory on GitHub
Computer System, Cluster and Networking Summer Institute | Application deadline: 01 December 2016

2016 Distinguished Lecture

Making Research Matter: Democratizing Science And Other Lofty Goals

– Dr. Richelle Winkler
Associate Professor, Social Science

Memorial Union Building (MUB)
Alumni Lounge, 4 – 5:30 pm on Thursday, 13th October 2016

This is a part of the Michigan Tech Research Forum – a university presentation series showcasing the work of Michigan Tech faculty, postdocs, and researchers to strengthen our community.

US DOE Scholars Program Summer 2017

* Applicant must be a US citizen
* Stipend available (up to $650/week)
* Travel to and from appointment site
* Open to undergraduate and graduate students, and post-graduates
* Opportunities to learn from top scientists and subject matter experts, and career possibilities
* Accounting and Finance, Business, Communications, Computer Science and Information Technology, Engineering, Environmental Sciences, Law, Physical and Mathematical Sciences, Policy, Program Management, Safety and Health, and other related areas

US Department of Energy is the nation's leading sponsor for scientific research.
US Department of Energy Scholars Program | Application deadline: 15th December 2016

US DOE Computational Science Graduate Fellowship 2017

- Applicant must be a US citizen
- Open to senior undergraduates and first year graduate students (MS/PhD candidates without MS)
- Fellowship renewable up to 4 years

  $36k of stipend per year +
  Full tuition and other fees +
  $5k academic allowance in first year +
  $1k academic allowance for each renewed year
- Opportunity to attend annual program review
- 12-week research practicum

US Department of Energy is the nation's leading sponsor for scientific research.
US DOE Computational Science Graduate Fellowship | Application deadline: 18th January 2017

US DHS HS-STEM Summer Internship 2017

- Applicant must be a US citizen
- Open to undergraduates and graduate students majoring in homeland security disciplines
- 10-week program with stipend

  $6k for undergraduates / $7k graduate students + Limited travel expenses
- Exposure to and participation in research in DHS mission-relevant research areas
- Networking (w/ scientists & laboratories) and career opportunities

Oak Ridge Institute for Science and Education (ORISE) administers this internship program through an interagency agreement between the US Department of Energy and the US Department of Homeland Security. ORISE is managed by Oak Ridge Associated Universities (ORAU) for US DOE.
US DHS HS-STEM Summer Internship Program | @GovCareerPaths | Application deadline: 7th December 2016

Keweenaw Climate Science Event #3 of four-part event

The Orpheum Theater

6 – 8 pm on Thursday, 3rd November 2016

Subsequent event

1st December 2016

No admission fee

Free pizza and soft drinks

More information

Robert Handler (1982 – present): Adj. Asst. Professor in Civil and Environmental Engineering and Operations Manager for Sustainable Futures Institute, Michigan Tech; PhD in Environmental Engineering from The University of Iowa (2009)

Stephen Handler (1982 – present): Climate Change Specialist in US Forest Service and Northern Institute of Applied Climate Science (NIACS); MS in Resource Conservation and International Conservation and Development from University of Montana (2007)

Organized by Keweenaw Climate Community, and sponsored by the local chapter of the American Chemical Society and the Department of Social Sciences at Michigan Tech.

41 North Film Festival

Predator/Prey: The Fight For Isle Royale Wolves

Saturday, 5th November 2016, 7:30 pm
Open and free to public

http://hdmzweb.hu.mtu.edu/41north/2016/ | https://www.facebook.com/41northfilmfest/

Before The Flood

Limited free screening on iTunes, National Geographic and YouTube

TechTalks

Memorial Union Building (MUB)

Ballroom B1 and B2, 4 – 5:30 pm on Thursday, 10th November 2016

4:00 – 4:30 pm – Mingling and refreshments
4:30 – 5:00 pm – 2-minute presentations
5:00 – 5:30 pm – Discussions, if interested

Speakers and abstracts

Dress rehearsal for upcoming Research Marketing III

TechTalks are rapid-paced samplings of work from a number of faculty via a two slides in two-minute format. TechTalks showcase both published and unpublished work. These are a part of the Michigan Tech Research Forum – a university presentation series showcasing the work of Michigan Tech faculty, postdocs, and researchers to strengthen our community.

International Education Week

Friday, 11th November 2016, 5:30 pm, Fisher 135
Free admission

Malala Yousafazi (1997 – present): Pakistani activist for female education, and a recipient of the 2014 Nobel Peace Prize.
Sponsored by Michigan Tech Provost Office, International Programs and Services, and Michigan Tech Film Board.

Physics Colloquium

HPC and Simulation

The Third Pillar of Contemporary Science

Dr. Siegfried Hoefinger
Vienna University of Technology

10 am on Friday, 18th November 2016
Fisher Hall 133

https://www.linkedin.com/in/siegfried-hoefinger-a512541

NVIDIA Graduate Fellowship Program 2017-18

- Open to 2nd year PhD students

  Computer Science/Engineering, Systems Architecture, Electrical Engineering or a related area

- Unrestricted funds to further student research

  Up to $50,000 towards tuition, books, living stipend, salary and travel to NVIDIA Research Summit, SIGGRAPH, or relevant conferences

- Re-applicable in subsequent years

NVIDIA | NVIDIA Graduate Fellowship Program
Application deadline: 16th January 2017

Introduction to Python for CS&E (PDF)

Introduction to Python for Computational Science and Engineering
A Beginner's Guide

Hans Fangohr
Professor, Computational Modeling
University of Southampton, UK

Free PDF, and associated materials

Hans Fangohr (1973 – present): German computational scientist (@ProfCompMod)
http://www.southampton.ac.uk/ fangohr/

Mathematical Results

Standing the test of time

Mathematics, rightly viewed, possesses not only truth, but supreme beauty – a beauty cold and austere, like that of sculpture, without appeal to any part of our weaker nature, without the gorgeous trappings of painting or music, yet sublimely pure, and capable of a stern perfection such as only the greatest art can show.

– Bertrand Russell, A History of Western Philosophy (1945)

Bertrand Arthur William Russell (1872 – 1970): British philosopher, logician, mathematician, historian, writer, social critic, and political activist. 1950 Nobel Laureate in Literature.

Fundamental Theorem of Algebra

Every non-constant single-variable polynomial with complex coefficients has at least one complex root. Since real numbers are a subset of complex numbers, the result/statement extends to polynomials with real coefficients as well.

Alternate statement #1 (proved using successive polynomial division)

Every non-zero, single-variable, degree n polynomial with complex coefficients has, counted with multiplicity/degeneracy, exactly n roots.

Alternate statement #2

The field of complex numbers is algebraically closed.

Theorem first proven algebraically by James Wood (with missing steps) in 1798, and geometrically by Johann Carl Friedrich Gauss (with a topological gap) in 1799.

Fundamental Theorem of Calculus

Suppose that $f(x)$ is defined and continuous on $[a, b]$. Suppose that $y(x)$ is an anti-derivative of $f(x)$. Then

$$\boxed{\int_a^b f(x)\,dx \;=\; y(b) \;-\; y(a)}$$

Changing the notations while retaining the underlying essence,

$$\int_{t_n}^{t_{n+1}} f(y, t)\,dt \;=\; y_{n+1} \;-\; y_n$$

Re-arranging the terms,

$$\boxed{y_{n+1} \;=\; \boxed{y_n} \;+\; \boxed{\int_{t_n}^{t_{n+1}} f(y, t)\,dt}}$$

Intermediate Value Theorem (IVT)

For any function $f(x)$ that is continuous on $[a, b]$, and has values $f(a)$ and $f(b)$ at a and b respectively, then $f(x)$ also takes any value between $f(a)$ and $f(b)$ at some point within the interval.

Lagrange Polynomial Interpolation

Suppose that (x_i, y_i), with $i = 0 : 1 : n$, are a set of $n + 1$ unique points

Joseph-Louis Lagrange (1736 – 1813): Italian mathematician and astronomer
Interpolating Polynomials, L. Shure, MathWorks
Lagrange Interpolating Polynomial, B. Archer, Wolfram

Lagrange Polynomial Interpolation

The general form of Lagrange interpolating polynomial, one that passes through $n+1$ points

$$\boxed{\mathcal{L}_n(x) \;=\; \sum_{i=0}^{n} l_i(x)\, y_i}$$

Lagrange basis polynomials are given by

$$l_i(x) \;=\; \prod_{\substack{m=0 \\ m\neq i}}^{n} \frac{x - x_m}{x_i - x_m}$$

and are built to have the *Kronecker delta* property

$$l_i(x_j) \;=\; \delta_{ij}$$

Lagrange Polynomial Interpolation Linear

Suppose that $(x_\circ, y_\circ)$ and (x_1, y_1) are two known points. The linear interpolant is then a straight line between these two points.

Lagrange Polynomial Interpolation Quadratic

$$\mathcal{L}_2(x) = \frac{(x - x_1)(x - x_2)}{(x_\circ - x_1)(x_\circ - x_2)} y_\circ + \frac{(x - x_\circ)(x - x_2)}{(x_1 - x_\circ)(x_1 - x_2)} y_1 + \frac{(x - x_\circ)(x - x_1)}{(x_2 - x_\circ)(x_2 - x_1)} y_2$$

Lagrange Polynomial Interpolation Error analysis

If $f(x)$ is $n+1$ times continuously differentiable on a closed interval $[a, b]$, and $p_n(x)$ is a polynomial of degree at most n that interpolates $f(x)$ at $n+1$ distinct points x_i, $(i = 0, 1, 2, ..., n)$ in that interval. Then

$$\boxed{\epsilon_n = \int_a^b [f(x) - p_n(x)]\, dx = \int_a^b \frac{f^{(n+1)}}{(n+1)!} \prod_{i=0}^{n} (x - x_i)\, dx}$$

Mean Value Theorem

For any function that is continuous on $[a, b]$ and differentiable on (a, b), there exists a point c in (a, b) such that the line joining $f(a)$ and $f(b)$ (i.e., the secant) is parallel to the tangent at c.

Weighted Mean Value Theorem for Integrals

Suppose that $f(x)$ and $g(x)$ are continuous on $[a, b]$. If $g(x)$ never changes sign and is positive, $g(x) \geqslant 0$, in $[a, b]$, then for some c in $[a, b]$

$$\boxed{\int_a^b f(x)\, g(x)\, dx \;=\; f(c) \int_a^b g(x)\, dx}$$

Newton-Cotes Formula

Suppose that $f(x)$ is defined and continuous on $[a, b]$. Consider the integral

$$\boxed{I = \int_a^b f(x)\, dx}$$

If $f(x)$ can be approximated by an nth order polynomial

$$\boxed{p_n(x) = \alpha_\circ + \alpha_1 x + \alpha_2 x^2 + \ldots + \alpha_{n-1} x^{n-1} + \alpha_n x^n}$$

then the integral, I, takes the form

$$\boxed{I = \int_a^b \left[\alpha_\circ + \alpha_1 x + \alpha_2 x^2 + \ldots + \alpha_{n-1} x^{n-1} + \alpha_n x^n\right] dx}$$

Isaac Newton (1642 – 1727): English physicist and mathematician
Roger Cotes (1682 – 1716): English mathematician (no photo)

Taylor Series Expansion

If $f(x)$ is infinitely differentiable at $x_\circ$, then

$$\boxed{f(x) = \sum_{n=0}^{\infty} \frac{(x - x_\circ)^n}{n!} \frac{d^n}{dx^n} f(x)\bigg|_{x=x_\circ}}$$

A more general form that clearly identifies the error term is given by the pth order Taylor series expansion of $f(x)$ with $\tilde{x} \in [x, x + \Delta x]$

$$\boxed{f(x + \Delta x) = \boxed{\sum_{n=0}^{p} \frac{(\Delta x)^n}{n!} \frac{d^n}{dx^n} f(x)} + \boxed{\frac{(\Delta x)^{p+1}}{(p+1)!} \frac{d^{p+1}}{dx^{p+1}} f(\tilde{x})}}$$

Brook Taylor (1685 – 1731): English mathematician

Random Variables and Distributions

The need

Random variables and their distributions provide a basis for developing probabilistic models and describing the behavior of important characteristics of interest (i.e., real data).

Y is a random variable if it is a function that assigns a real numbered value to every possible event in a sample space of interest. Since every possible set of values for a random variable Y corresponds to some event, it has a probability associated with it. A random variable's distribution details the probabilities associated with these sets of values in a meaningful way.

It is a common practice to use an uppercase alphabet to denote the random variable, and the corresponding lowercase alphabet to denote a specific value of this variable. A discrete random variable can assume at most a countable number of values. A continuous random variable can assume an uncountable number of values.

Random Variables and Distributions

PDF and CDF

The probability distribution function (PDF) of some random variable Y is given below. $P(Y = y_i)$ indicates the probability of the random variable Y taking on a given value, y_i. $F(y_i)$ represents the cumulative distribution function (CDF), and is used to model the behavior of Y.

y_i	$P(Y = y_i)$	$F(y) = P(Y \leqslant y_i)$
0	0.10	0.10
1	0.30	0.40
2	0.40	0.80
3	0.20	1.00

All random variables must have a cumulative distribution function.

Uniform Distribution Discrete and continuous

Applicable when

a finite number of values are equally likely to be observed. The probability density function on the interval $[a, b]$ is

$$f(x) = \begin{cases} 0 & x < a \\ 1/(b-a) & a \leqslant x \leqslant b, \text{ and } -\infty < a < b < \infty \\ 0 & x > b \end{cases}$$

Common example(s)

Throwing a fair die with possible values of 1, 2, ..., 6; each face of the die has a probability of 1/6.

Uniform Distribution Probability Distribution Function (PDF)

Bernoulli Distribution Discrete

Applicable when

a random variable takes the value one with success probability of p and the value zero with a failure probability of $1 - p$. Bernoulli distribution is a special case of the Binomial distribution for $n = 1$.

Common example(s)

A coin toss where one and zero could be represented by *head* and *tail* respectively. For a fair coin, $p = 0.50$.

Binomial Distribution Discrete

Applicable when

a number of successes (e.g., a head or a tail) results in a sequence of n independent success/failure-type experiments, each of which yields success with a probability (or fairness factor) p. The probability of getting exactly x successes in n trials for a specified fairness value, p, is

$$\boxed{P = \frac{n!}{x!\ (n-x)!}\, p^x\ (1 - p)^{n-x}}$$

Common example(s); contributed by Fall 2016 students

Throwing a fair die with possible values of 1, 2, ..., 6 (each face of the die has a probability of 1/6); number of times a marksman hits the target after N attempts in a shooting range.

Binomial Distribution Probability Distribution Function (PDF)

Poisson Distribution Discrete

Applicable when

a given number of events occur in a fixed interval of time if these events occur with a known average rate, independently of time since the last event, and two of them cannot occur at the same time. The probability of observing m events in an interval with the average number of events in an interval designated by λ is

$$\boxed{P(m) = \frac{\lambda^m e^{-\lambda}}{m!}}$$

Common example(s); contributed by Fall 2016 students

Number of machine failures OR accidents (due to snow) OR decaying radioactive atoms OR mutations on a given strand of DNA OR visitors to a website over a time period.

Poisson Distribution Probability Distribution Function (PDF)

Gamma Distribution

Applicable when

the waiting times between Poisson distributed events are relevant. The probability density function with shape parameter α and scale parameter β (inverse of rate parameter) is

$$f(x) = \frac{1}{\Gamma(\alpha)\,\beta^{\alpha}} x^{\alpha-1} \exp\left(-\frac{x}{\beta}\right) \quad x \geqslant 0, \text{ and } \alpha, \beta > 0$$

Common example(s)

The size of insurance claims, amount of rainfall, multipath fading of signal power (wireless communication), interspike intervals (neuroscience), etc.

Gamma Distribution Probability Distribution Function (PDF)

Normal/Gaussian Distribution Continuous

Applicable as

a limiting form of binomial distribution (De Moivre, 1733) and as a plausible distribution for measurement errors (Gauss, 1809). The probability density with mean μ and standard deviation σ is

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \quad -\infty < x, \mu < \infty, \text{ and } \sigma > 0$$

Common example(s); contributed by Fall 2016 students

Mechanical error, students' score, annual income of all people in a given country, etc.

Laplace's Central Limit Theorem: Under very general conditions when n random variables, whatever their distributions, are added together, the distribution of the sum tends towards the normal (i.e., bell shape) as n increases.

Normal/Gaussian Distribution Probability Distribution Function (PDF)

Butcher Tableau

The general form of recursive relation for s-stage Runge-Kutta (RK) method

$$\boxed{y_{n+1} \;=\; y_n + h \sum_{i=1}^{s} b_i \, k_i}$$

$$k_1 \;=\; f\left(y_n, t_n\right)$$

$$k_2 \;=\; f\left(y_n + a_{21}\, k_1, t_n + c_2\, h\right)$$

$$k_3 \;=\; f\left(y_n + a_{31}\, k_1 + a_{32}\, k_2, t_n + c_3\, h\right)$$

$$k_s \;=\; f\left(y_n + a_{s1}\, k_1 + a_{s2}\, k_2 + \ldots + a_{s,s-1}\, k_{s-1}, t_n + c_s\, h\right)$$

John Charles Butcher (1933 – present): New Zealand mathematician

Butcher Tableau

The choice of s (an integer), a_{ij} (the coefficients of $s \times s$ RK matrix), b_i ($i = 1, 2, ..., s$; the weights), c_i ($i = 2, ..., s$; the nodes), and relationship between a_{ij} and c_i uniquely identifies the s-stage RK method and ensures its consistency.

$$
\begin{array}{c|ccccc}
0 & a_{11} & a_{12} & \cdots & a_{1,s-1} & a_{1,s} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2,s-1} & a_{2,s} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & a_{s,s} \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}
$$

$$\boxed{\sum_{j=1}^{i-1} a_{ij} = c_i \quad i = 2, 3, ..., s}$$

Butcher Tableau Explicit RK2 method

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

$[a_{ij}]$ needs to be a lower triangular matrix for explicit methods (i.e., $1 \leqslant j < i \leqslant s$). Drop the explicit mention of zeros

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & 1/2 & 1/2 \end{array}$$

Consistency check is satisfied

$$\sum_{j=1}^{i-1} a_{ij} = c_i \quad i = 2 \qquad \Rightarrow \qquad a_{21} = c_2$$

Butcher Tableau Explicit RK2 method

Recursive expression for RK2 (i.e., improved Euler) method

$$y_{n+1} = y_n + h \sum_{i=1}^{2} b_i \, k_i$$

$$y_{n+1} = y_n + h \, b_1 \, k_1 + h \, b_2 \, k_2$$

Use b_i from the Butcher tableau and simplify

$$\boxed{y_{n+1} = y_n + \frac{h}{2} \left(k_1 + k_2 \right)}$$

Butcher Tableau Explicit RK4 method

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1/2 & 1/2 & 0 & 0 & 0 \\
1/2 & 0 & 1/2 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}
$$

Drop the explicit mention of zeros along the diagonal and above

$$
\begin{array}{c|cccc}
0 & & & & \\
1/2 & 1/2 & & & \\
1/2 & 0 & 1/2 & & \\
1 & 0 & 0 & 1 & \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}
$$

Butcher Tableau Explicit RK4 method

Recursive expression for RK4 method

$$y_{n+1} = y_n + h \sum_{i=1}^{4} b_i \, k_i$$

$$y_{n+1} = y_n + h \, b_1 \, k_1 + h \, b_2 \, k_2 + h \, b_3 \, k_3 + h \, b_4 \, k_4$$

Use b_i from the Butcher tableau

$$y_{n+1} = y_n + \frac{h}{6} \, k_1 + \frac{h}{3} \, k_2 + \frac{h}{3} \, k_3 + \frac{h}{6} \, k_4$$

Simplify

$$\boxed{y_{n+1} = y_n + \frac{h}{6} \, (k_1 + 2 \, k_2 + 2 \, k_3 + k_4)}$$

Videos

If a picture is worth a thousand words ...

People and Personalities

and their stories

Richard Phillips Feynman 1918 – 1988

Ada Augusta King, Countess of Lovelace 1815 – 1852

Diagram for the computation by the Engine of the Numbers of Bernoulli. See Note G. (page 722 et seq.)

Number of Operation.	Nature of Operation.	Variables acted upon.	Variables receiving results.	Indication of change in the value on any Variable.	Statement of Results.	Data. V_1 = 0 0 1 [1]	Data. V_2 = 0 0 2 [2]	Data. V_3 = 0 0 1 [n]	Working Variables. V_4 = 0 0 0	V_5 = 0 0 0	V_6 = 0 0 0	V_7 = 0 0 0	V_8 = 0 0 0	V_9 = 0 0 0	V_{10} = 0 0 0	V_{11} = 0 0 0 0	V_{12} = 0 0 0	V_{13} = 0 0 0 0	Result Variables. V_{14} = 0 0 0 [B_1]	V_{15} = 0 0 0 [B_2]	V_{16} = 0 0 0 [B_3]	V_{17} = 0 0 0 [B_7]
1	×	$V_2 \times V_3$	V_4, V_5, V_6	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 2n$	...	2	n	2n	2n	2n											
2	−	$V_4 - V_1$	V_4	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 2n - 1$	1	...	...	2n − 1													
3	+	$V_4 + V_1$	V_4	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 2n + 1$	1	...	...	...	2n+1												
4	+	$V_4 + V_1$	V_{11}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$\frac{2n-1}{2n+1}$	...	...	...	0	0	...	...	...	...	...	$\frac{2n-1}{2n+1}$						
5	+	$V_{11} + V_2$	V_{11}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_{11}, V_5 = V_5, V_6 = V_6\}$	$= \frac{1}{2} \cdot \frac{2n-1}{2n+1}$	...	2	...	...	...	...	...	...	...	...	$\frac{1}{2} \cdot \frac{2n-1}{2n+1}$						
6	−	$V_{12} - V_{11}$	V_{12}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_{11}, V_5 = V_{12}, V_6 = V_6\}$	$= -\frac{1}{2} \cdot \frac{2n-1}{2n+1} = A_2$	...	...	...	...	...	...	...	...	...	...	0	.....	$-\frac{1}{2} \cdot \frac{2n-1}{2n+1} = A_2$				
7	−	$V_8 - V_1$	V_{13}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_{12}, V_5 = V_5, V_6 = V_6\}$	$= n - 1\ (= 3)$	1	...	n	...	...	...	...	...	...	n − 1							
8	+	$V_2 + V_2$	V_2	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 2 + 0 = 2$	...	2	...	...	...	...	2	...	...	...							
9	+	$V_8 + V_2$	V_{13}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{13}\}$	$= \frac{2n}{2} = A_1$	...	...	...	...	...	2n	2	...	...	...	$\frac{2n}{2} = A_1$						
10	×	$V_{13} \times V_{10}$	V_{12}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{12}\}$	$= B_1 \cdot \frac{2n}{2} = B_1 A_1$	...	...	...	...	...	...	...	...	...	...	$\frac{2n}{2} = A_1$	$B_1 \cdot \frac{2n}{2} = B_1 A_1$	.....	B_1			
11	+	$V_{12} + V_{10}$	V_{13}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{13}\}$	$= -\frac{1}{2} \cdot \frac{2n-1}{2n+1} + B_1 \cdot \frac{2n}{2}$	...	...	...	...	...	...	...	...	...	...	.....	0	$\left\{-\frac{1}{2} \cdot \frac{2n-1}{2n+1} + B_1 \cdot \frac{2n}{2}\right\}$				
12	−	$V_{13} - V_1$	V_{14}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= n - 2\ (= 2)$	1	...	...	...	...	...	...	...	...	n − 2							
13		$V_4 - V_1$	V_4	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 2n - 1$	1	...	...	...	...	2n − 1											
14	+	$V_1 + V_2$	V_2	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 2 + 1 = 3$	1	...	...	...	...	...	3										
15	+	$V_4 + V_2$	V_4	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$\frac{2n-1}{3}$	...	...	...	...	...	2n − 1	3	$\frac{2n-1}{3}$									
16	×	$V_4 \times V_{12}$	V_{11}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$\frac{2n}{2} \cdot \frac{2n-1}{3}$	...	...	...	...	...	...	...	0	...	...	$\frac{2n}{2} \cdot \frac{2n-1}{3}$							
17		$V_6 - V_1$	V_4	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 2n - 2$	1	...	...	...	...	2n − 2											
18	+	$V_1 + V_2$	V_2	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= 3 + 1 = 4$	1	...	...	...	...	...	4										
19	+	$V_6 + V_2$	V_6	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_6\}$	$= \frac{2n-2}{4}$	...	...	...	...	...	2n − 2	4	...	$\frac{2n-2}{4}$	...	$\left\{\frac{2n}{2} \cdot \frac{2n-1}{3} \cdot \frac{2n-2}{3}\right\} = A_3$							
20	×	$V_6 \times V_{12}$	V_{13}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{13}\}$	$= \frac{2n}{2} \cdot \frac{2n-1}{3} \cdot \frac{2n-2}{4} = A_3$	...	...	...	...	...	...	...	...	0								
21	×	$V_{10} \times V_{13}$	V_{12}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{12}\}$	$= B_3 \cdot \frac{2n}{2} \cdot \frac{2n-1}{3} \cdot \frac{2n-2}{3} = B_3 A_3$	...	...	...	...	...	...	...	...	...	...	0	$B_3 A_3$	.....	.....	B_3		
22	+	$V_{12} + V_{13}$	V_{13}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{13}\}$	$= A_3 + B_1 A_1 + B_3 A_3$	...	...	...	...	...	...	...	...	...	...	.....	0	$\{A_3 + B_1 A_1 + B_3 A_3\}$				
23	−	$V_{13} - V_1$	V_{14}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{14}\}$	$= n - 3\ (= 1)$	1	...	...	...	...	...	...	...	...	n − 3							
Here follows a repetition of Operations thirteen to twenty-three.																						
24	+	$V_{14} + V_2$	V_{14}	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_{14}\}$	$= B_7$	...	...	...	...	...	...	...	...	...	...	.....		.....	.....	.....	.....	B_7
25	+	$V_1 + V_2$	V_1	$\{V_2 = V_2, V_3 = V_3, V_4 = V_4, V_5 = V_5, V_6 = V_1\}$ by a Variable-card. by a Variable card.	$= n + 1 = 4 + 1 = 5$	1	...	n + 1	...	...	0	0										

Alan Mathison Turing 1912 – 1954

Grace Brewster Murray Hopper 1906 – 1992

Margaret Heafield Hamilton 1936 – present

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Missing Plane, MH370

Malaysia Airlin
MH370: Water
of an Airliner

Goong Chen, Cong Gu, Philip J. Morris, Er
Yi-Ching Wang, and Tomasz Wierzbicki

On March 8, 2014 Malaysia Airlines Flight MH370 disappeared less than an hour after take-off on a flight from Kuala Lumpur to Beijing. The Boeing 777-200ER carried twelve crew members and 227 passengers. On March 24 the Malaysian Prime Minister announced that "It is therefore with deep sadness and regret that I must inform you that ...Flight MH370 ended in the Southern Indian Ocean." Though the exact fate of Flight MH370 remains undetermined, the available evidence indicates a crash into the ocean. However, disturbing as this is, not all emergency water landings, referred to as *"ditching"* when they are controlled, end in tragedy. In the "Miracle on the Hudson," on January 15, 2009, Capt. Chelsey B. "Sully" Sullenberger and his crew successfully ditched US Airways Flight 1549, an Airbus A320-200, in the Hudson River after a loss of power due to a bird strike on take-off from La Guardia Airport. There was no loss of life.

Figure 1 and the video animation referenced on the second page of this article show our "representation" of a commercial airliner, a Boeing

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(a) nose-dive water entry

(b) pressure distribution and mesh

Figure 12. Pitch angle = −90°, angle of approach = 93°. This corresponds to Case 4. A video animation can be viewed at https://www.dropbox.com/s/vaf0qenjw0lk5yz/comb-90.mp4.

Figure 13. Schematics for nose-diving. The ocean current pushes the aircraft to the right, causing it possibly to finish belly-up on the ocean floor. This corresponds to Case 4.

failure modes occur at *low impact velocities*, as has been demonstrated with a real model of a retired aircraft in DYCAST (Dynamic Crash Analysis of Structures) by NASA [FWR87]. These findings were published nearly three decades ago but remain valid today.

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Storm Prediction

Precision Medicine

Preview of SC11

Preview of SC12

Preview of SC13

Preview of SC14

Preview of SC15

Preview of SC17

we cry. we rejoice. we reflect.

Review of Performance

How well have we been performing?

http://dilbert.com/strip/2011-06-06/

Active Participation #01 Research Marketing I: Twitter

Assignment #01

Active Participation #02 PB&J Sandwich Recipe

Active Participation #03 Research Marketing II: Professional/University Business Cards

Assignment #04

Assignment #07

Superior and Top 500

A proposed compute node in Superior will have two Intel Xeon E5-2698 processors (each processor with 20 cores) at 2.20 GHz, 512 GB RAM, 480 GB Intel Enterprise SSD, Mellanox ConnectX-3 56 Gbps InfiniBand network, and will cost $13,263.13.

Ignoring the cost of physical space, racks, network, storage, electricity and labor, estimate the cost to build a #500 supercomputer (∼405 TFLOPS) with homogeneous compute nodes as the ones described above.

For a computer with N identical/homogeneous processors,

$$\boxed{\text{FLOPS} = \text{N} \times \text{CPU speed} \times \frac{\text{FLOPs}}{\text{CPU cycle}}}$$

You and The Board Week #02: Sameer Saraf

Celsius $\longleftrightarrow$ Fahrenheit

Convert temperature between Celsius and Fahrenheit scales.

Is there a well-known technique to verify the conversion scheme?

Matrix elements

How many elements in a square matrix of order N? How will this number change if the matrix is upper (or lower) triangular?

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} \qquad \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1n} \\ 0 & b_{22} & \dots & b_{2n} \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & b_{nn} \end{pmatrix}$$

You and The Board Week #04: Sandeep Lanka

The impact and limitations of Moore's Law

Assuming that Moore's Law holds true, what is the speed up of a computer observed over an average adult's life in the US?

Drawing queens

Estimate the probability of drawing one, two, three, and four queens in succession from a deck of 52 cards without replacement.

Got Questions?

If you do, find a way to contact me; and do so sooner than later

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