

UN5390: Scientific Computing I

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Week #14: 2016-12-06 and 2016-12-08

Cross-listed as BE5390, EE5390 and MA5390

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Recap

What we did last week, and what you were supposed to do



<http://dilbert.com/strip/1998-09-14/>

- * Parallel computing examples
 - * Array manipulation
 - * Monte Carlo methods (π ; dart board algorithm)
 - * Numerical integration (π ; trapezoidal rule)
 - * Matrix multiplication
 - * Primes

Week #13 Before We Meet Again

- * Review the syllabus, course material, grade through week #13, notations, active participation, free time exercises, tips, opportunities, mathematical results, videos, and training camps
- * Practice compiling and executing included OpenMP programs
- * Make progress in assignment #12
- * Make progress in the term project
- * Turn in the project status by Friday 4:59 pm
- * Make progress towards Research Marketing III
Send an email to the instructor with the title of your topic by Sunday 5 pm



Parallel Debugging/Profiling

The art of finding and fixing mistakes, and improving the performance



<http://dilbert.com/strip/1995-11-14/>

Commonly Used Techniques

Debugging and profiling serial programs

Taking detailed notes, using `printf()` or equivalent statements, employing smarter text editors/IDEs, understanding various sources of errors and different ways of accomplishing a given task (if/when possible), etc.

Debugging and profiling parallel programs

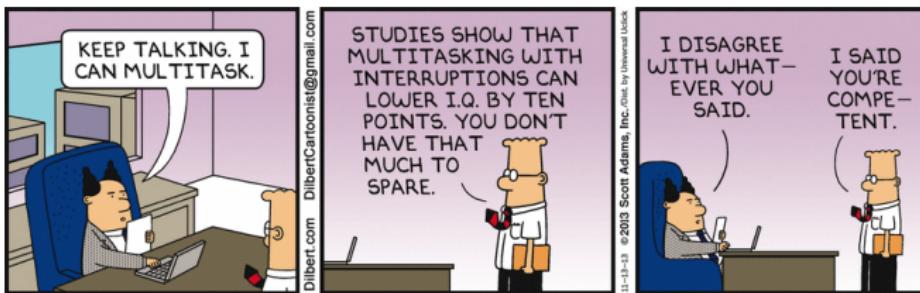
is NOT easy. In addition to the above, understanding race conditions and the under-estimated difficulty of understanding the simultaneous execution of N processes make parallel debugging even more difficult.

Available Tools

- * [HPCToolkit](#) (Rice University)
- * [mpiP](#) | [mpiPView](#) (Lawrence Livermore National Laboratory)
- * [Parallel Application Debugger](#) (Ashley Pittman)
- * [Parallel Tools Platform](#) (Eclipse)
- * [TAU](#) | [PDT](#) | [ParaProf](#) (University of Oregon)
- * \$ Allinea's [DDT](#)
- * \$ Intel's [Trace Analyzer and Collector](#) | [VTune Amplifier](#) | [Inspector](#)
- * \$ PGI's [PGPROF](#)
- * \$ RogueWave's [TotalView](#)

MPICH

Parallel Programming/Message Passing Interface



<http://dilbert.com/strip/2013-11-13/>

Features

- * Often abbreviated/referred to as MPI
- * An explicit and message based parallelism
- * Shared and distributed memory model
- * Programmer is responsible for identifying/implementing parallelism



History of MPICH

Argonne National Laboratory developed early versions as a public domain software. The CH was derived from *Chameleon*, a portable parallel programming library developed by Dr. William Gropp. As of November 2012, MPICH2 project renamed itself to just MPICH.

William Douglas Gropp (1955 – present): American computer scientist. One of the founders of MPICH, he is currently a professor of Computer Science in University of Illinois Urbana-Champaign as well as the acting director of National Center for Supercomputing Applications (NCSA). He served as the General Chair of SC13 in Denver, CO, and is the recipient of [2008 IEEE Computer Society Sidney Fernbach Award](#) and [2016 ACM/IEEE Computer Society Ken Kennedy Award](#).

Components

- * Run-time library routines

- * Used for querying the number of processors (`num_procs`), a processor's unique identifier (`proc_id`), sending/receiving messages, wall time, etc.

Commonly used routines, and the necessary header file

```
#include <mpi.h>

MPI_Init()          # Initialize MPI
MPI_Comm_size()     # Number of processors assigned
MPI_Comm_rank()     # Unique ID of each processor
MPI_Send()          # Send a message
MPI_Recv()          # Receive a message
MPI_Barrier()       # Impose a barrier
MPI_Wtime()         # Wall time
MPI_Finalize()      # Finalize MPI
```

Components

- * Environment variables
 - * Help set the location of MPI wrappers and libraries
 - * Programmer is responsible for initiating the executable with appropriate number of processors

BASH

```
MPICH_CC  
MPICH_CXX  
MPICH_F77  
MPICH_F90  
export PATH=/path/to/mpi/bin  
export LD_LIBRARY_PATH=/path/to/mpi/lib  
export MANPATH=/path/to/mpi/man
```

Download and Installation

MPICH 3.2

MPICH is a freely available and portable implementation of MPI from Argonne National Laboratory. MPICH v3.0 implements the MPI-3.0 standard. One may use `MPICH_CompilerConfigureTest.sh` included in week #11 `AdditionalMaterial` to download and compile MPICH 3.2, and configure `${HOME}/.bash_${USER}` to setup its usage.

Verification (To be performed in `colossus.it`)

```
which mpicc mpicxx  
which mpif77 mpif90  
which mpiexec mpirun
```

One may also check the contents of `*-mpich-* .txt` in
 `${UN5390}/CourseWork/Week_11/${USER}_11/`.

Compilation and Execution

Compilation

```
mpicc -Wall -g -lm PROGRAM.c -o PROGRAM.x  
mpicxx -Wall -g -lm PROGRAM.cpp -o PROGRAM.x
```

Execution

```
# Use processors local to a machine (as in OpenMP)  
mpirun -n NPROCS /path/PROGRAM.x  
  
# Use processors distributed across different machines  
mpirun -n NPROCS -f LIST-OF-MACHINES /path/PROGRAM.x
```

Training Camp: #01, Tasks #07–#09, and #04, Task #21

Necessary for distributed cases to work properly.

NPROCS is the number of processors assigned to run a program. LIST-OF-MACHINES is an ASCII file that contains the one-per-line list of hostnames/machines that are participating in the execution, and should have at least as many entries as NPROCS. -f MACHINES-LIST could be optional if using a single machine. Most queuing systems will generate this file on the fly taking into account the available resources.



Conventions

- * Processor count begins at 0, and ends at (NPROCS-1)
- * Master processor will be identified by `proc_id = 0` (beyond the Hello, World! set of examples) and will perform write operations
- * Worker processors will be identified by `proc_id = 1:(NPROCS-1)`. These will perform read/write operations, and communicate with master and/or other workers iff there is a need
- * Any given parallel program will not allocate/use more processors than physically available

Additional References

- * MPICH MPI (The Official Website)
- * MPICH MPI Guides
- * MPICH Routines
- * Intel MPI Library

Parallel Computing Examples

MPICH (C) programs



<http://dilbert.com/strip/2000-07-11/>

MPICH Sample Programs

In-class activity

To be performed in `colossus.it`

```
cd ${UN5390}  
git pull  
cd CourseWork/Week_11/AdditionalMaterial  
rsync -avhP ./Parallel/ ../${USER}_11/Parallel/  
  
cd ${UN5390}/CourseWork/Week_11/  
git add ${USER}_11  
git commit -m "PM: MPICH samples #14"  
git push origin master
```

Hello, World!

Compilation and execution instructions (parallel; in `colossus.it`)

```
cd ${UN5390}/CourseWork/Week_11/${USER}_11/Parallel
BASENAME="HelloWorld_mpi"
VER="01" # Change this to 02 for version #02
MPICC="mpicc -Wall -g -lm"

# Compile, and run using 1, 2, 4, 8 processors
${MPICC} ${BASENAME}_${VER}.c -o ${BASENAME}_${VER}.x
for x in $(seq 0 1 3)
do
    NPROCS=$(echo "2^$x" | bc)
    mpirun -n ${NPROCS} $(pwd)}/${BASENAME}_${VER}.x
done
```

`HelloWorld_mpi.0*.c` are included in week #11 AdditionalMaterial.



To be performed in `colossus.it`

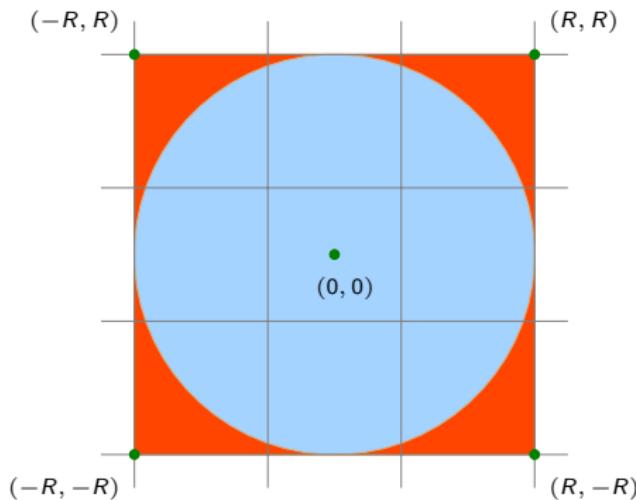
```
cd ${UN5390}/CourseWork/Week_11/${USER}_11/Parallel  
BASENAME="HelloWorld_mpi_01"  
  
# Compilation  
mpicc -Wall -g -lm ${BASENAME}.c -o ${BASENAME}.x  
  
# Execution (local to colossus.it; as in OpenMP)  
mpirun -n 1 $(pwd)}/${BASENAME}.x  
mpirun -n 2 $(pwd)}/${BASENAME}.x  
mpirun -n 4 $(pwd)}/${BASENAME}.x  
  
# Execution (distributed on colossus.it and guardian.it)  
ssh-copy-id ${USER}@guardian.it.mtu.edu  
mpirun -n 2 -f $(pwd)/machines.txt $(pwd)}/${BASENAME}.x  
mpirun -n 8 -f $(pwd)/machines.txt $(pwd)}/${BASENAME}.x
```

Monte Carlo Methods

π evaluation; dart board algorithm

Monte Carlo methods

(Pseudo) Random numbers, seeding the random number generator, statistics, mapping functions, etc.



Monte Carlo Methods

π evaluation; dart board algorithm

Compilation and execution instructions (parallel; in `colossus.it`)

```
cd ${UN5390}/CourseWork/Week_11/${USER}_11/Parallel  
BASENAME="MonteCarloPi_mpi"  
VER="01" # Change this to 02 for version #02  
MPICC="mpicc -Wall -g -lm"  
  
# Compile, and run using 1, 2, 4, 8 processors  
${MPICC} ${BASENAME}_${VER}.c -o ${BASENAME}_${VER}.x  
for x in $(seq 0 1 3)  
do  
    NPROCS=$(echo "2^$x" | bc)  
    mpirun -n ${NPROCS} $(pwd)}/${BASENAME}_${VER}.x  
done
```

`MonteCarloPi_mpi.0*.c` are included in week #11 AdditionalMaterial.

π Evaluation

Dart board algorithm; pseudo-code; MPICH

Define π , π_c , R , N , $n_c = 0$, x , y , ϵ , i

Seed the random number generator

Define n_{c_local} , $NPROCS$, and compute $n_s = N/NPROCS$

LOOP BEGINS: i starts at 0 and does not exceed n_s

Generate x and y randomly, mapped in $(-R, R)$

IF BEGINS: $x^2 + y^2 \leq R^2$

 Set $n_{c_local} = n_{c_local} + 1$

 IF ENDS

 Set $i = i + 1$

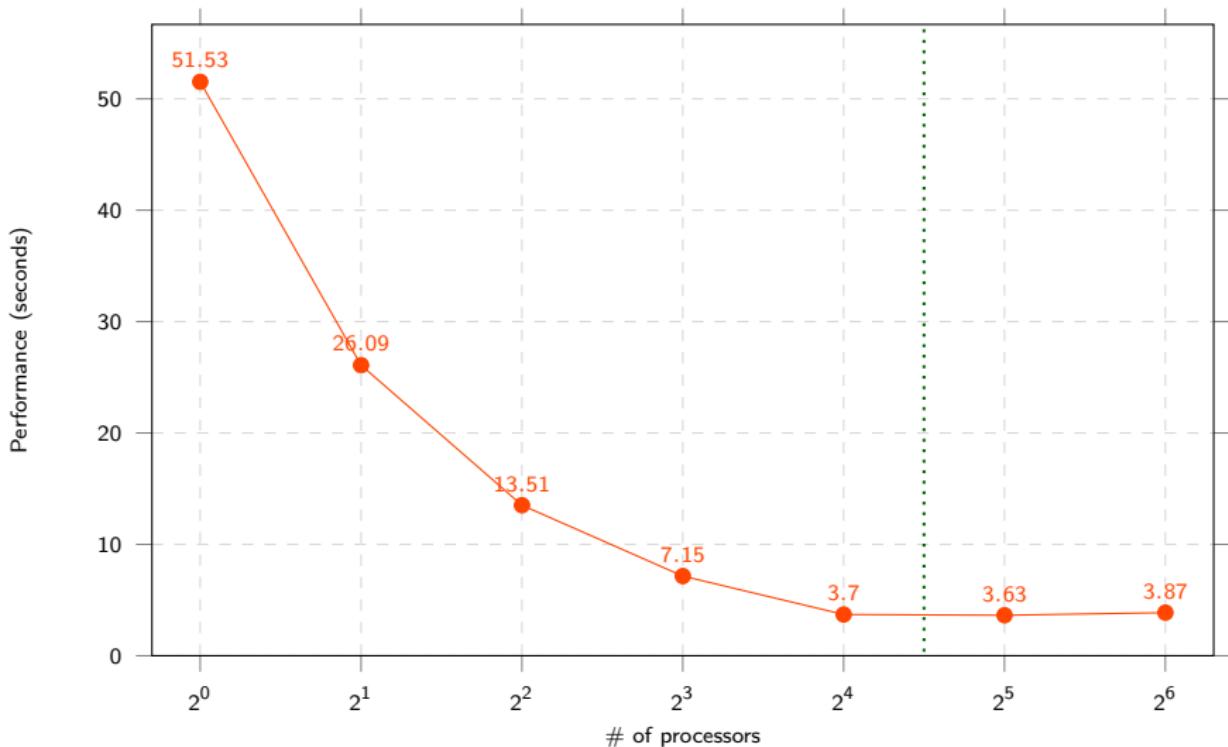
LOOP ENDS

Apply reduction (sum) on n_{c_local} to get n_c

Compute $\pi_c = 4(n_c/n_s)$ and $\epsilon = |\pi - \pi_c|$

π Evaluation

Dart board algorithm; raw performance; MPICH

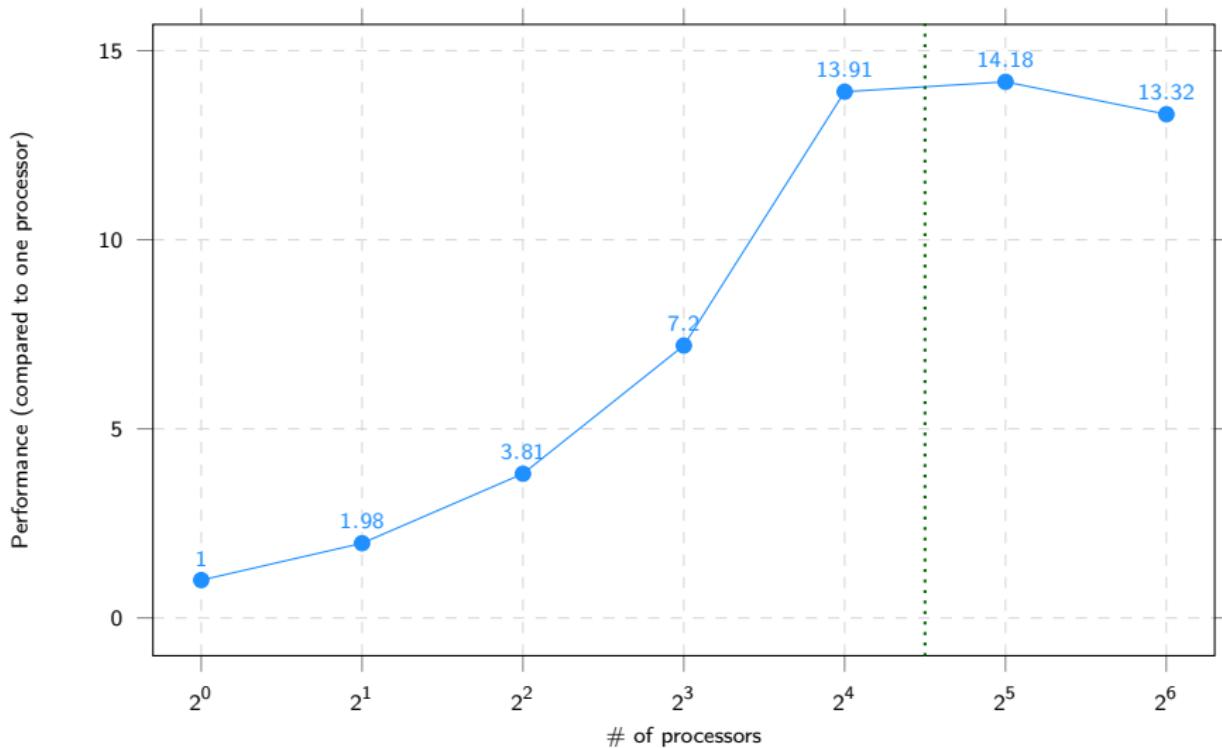


$N = 2^{30}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



π Evaluation

Dart board algorithm; performance scaling; MPICH



$N = 2^{30}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

Journal of Failed Experiments

Input validation, memory pre-allocation, row/column major language, zeros cost space and time, zero is not really zero, order and nature of matrices involved, etc.

$$\begin{pmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \dots & \dots & \dots \\ a_{m1} & \dots & a_{mn} \end{pmatrix} \begin{pmatrix} b_{11} & \dots & b_{1q} \\ b_{21} & \dots & b_{2q} \\ \dots & \dots & \dots \\ b_{p1} & \dots & b_{pq} \end{pmatrix} = \begin{pmatrix} c_{11} & \dots & c_{1q} \\ c_{21} & \dots & c_{2q} \\ \dots & \dots & \dots \\ c_{m1} & \dots & c_{mq} \end{pmatrix}$$

$$a_{ij} = i \times (m - i - 1) \times j \times (n - j - 1)$$

$$b_{ij} = i + j + 2$$

Matrix Multiplication

Compilation and execution instructions (parallel; in `colossus.it`)

```
cd ${UN5390}/CourseWork/Week_11/${USER}_11/Parallel
BASENAME="MatrixMultiplication_mpi"
VER="01" # Change this to 02 for version #02
MPICC="mpicc -Wall -g -lm"

# Compile, and run using 1, 2, 4, 8 processors
${MPICC} ${BASENAME}_${VER}.c -o ${BASENAME}_${VER}.x
for x in $(seq 0 1 3)
do
    NPROCS=$(echo "2^$x" | bc)
    mpirun -n ${NPROCS} $(pwd)}/${BASENAME}_${VER}.x
done
```

`MatrixMultiplication_mpi_0*.c` are included in week #11 AdditionalMaterial.



Matrix Multiplication

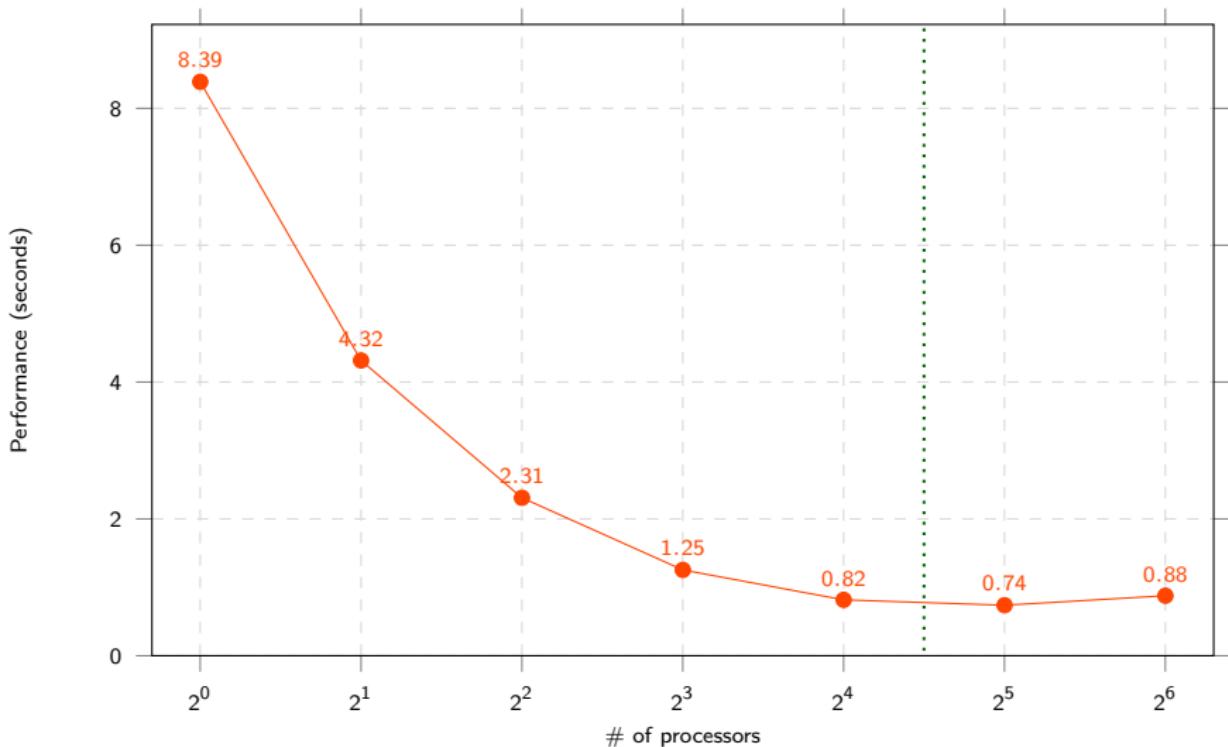
Pseudo-code; MPICH

```
Define  $i, j, k, NRA, NCA, NRB, NCB$ 
Define/Populate  $A[NRA][NCA], B[NRB][NCB], C[NRA][NCB]$ 
Define  $NPROCS, Atmp[NRA][NCA], Ctmp[NRA][NCB]$ 
Send  $B[NRB][NCB]$ , portions of  $A[NRA][NCA]$  to workers
LOOP BEGINS:  $i = 0; i < NRA/NPROCS; i = i + 1$ 
    LOOP BEGINS:  $j = 0; j < NCB; j = j + 1$ 
        Set  $Ctmp[i][j] = 0$ 
        LOOP BEGINS:  $k = 0; k < NCA; k = k + 1$ 
            Compute  $Ctmp[i][j] = Ctmp[i][j] + (Atmp[i][k] \times B[k][j])$ 
        LOOP ENDS
    LOOP ENDS
LOOP ENDS
Collect of  $Ctmp[NRA][NCB]$  from workers
```

A processor's portion of $A[NRA][NCA]$ is $Atmp[NRA][NCA]$.

Matrix Multiplication

Raw performance; MPICH

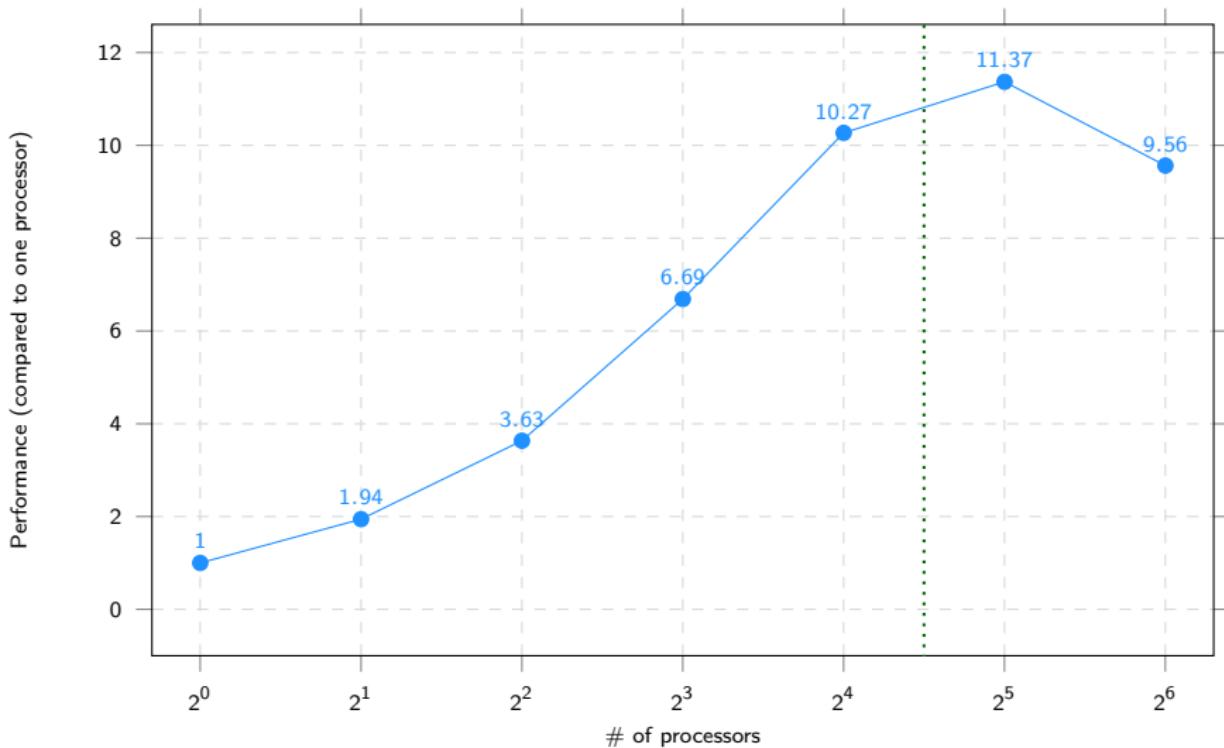


$N = 2^{10}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

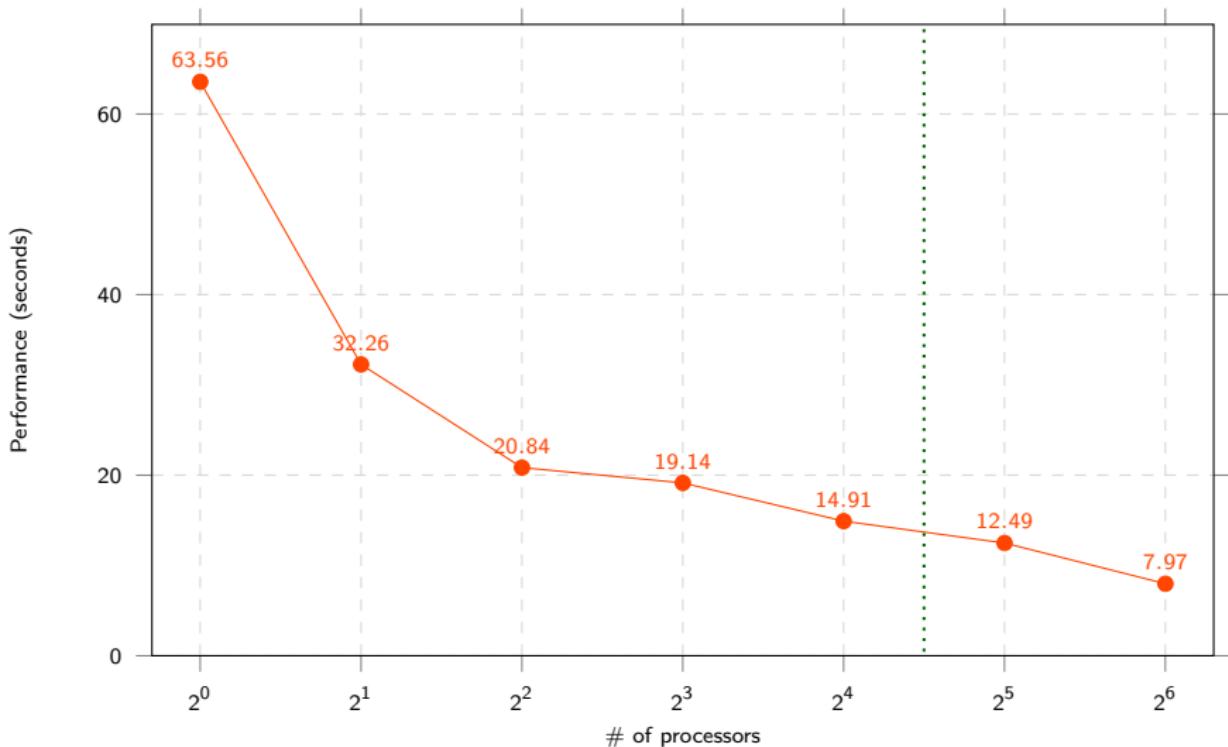
Performance scaling; MPICH



$N = 2^{10}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.

Matrix Multiplication

Raw performance; MPICH

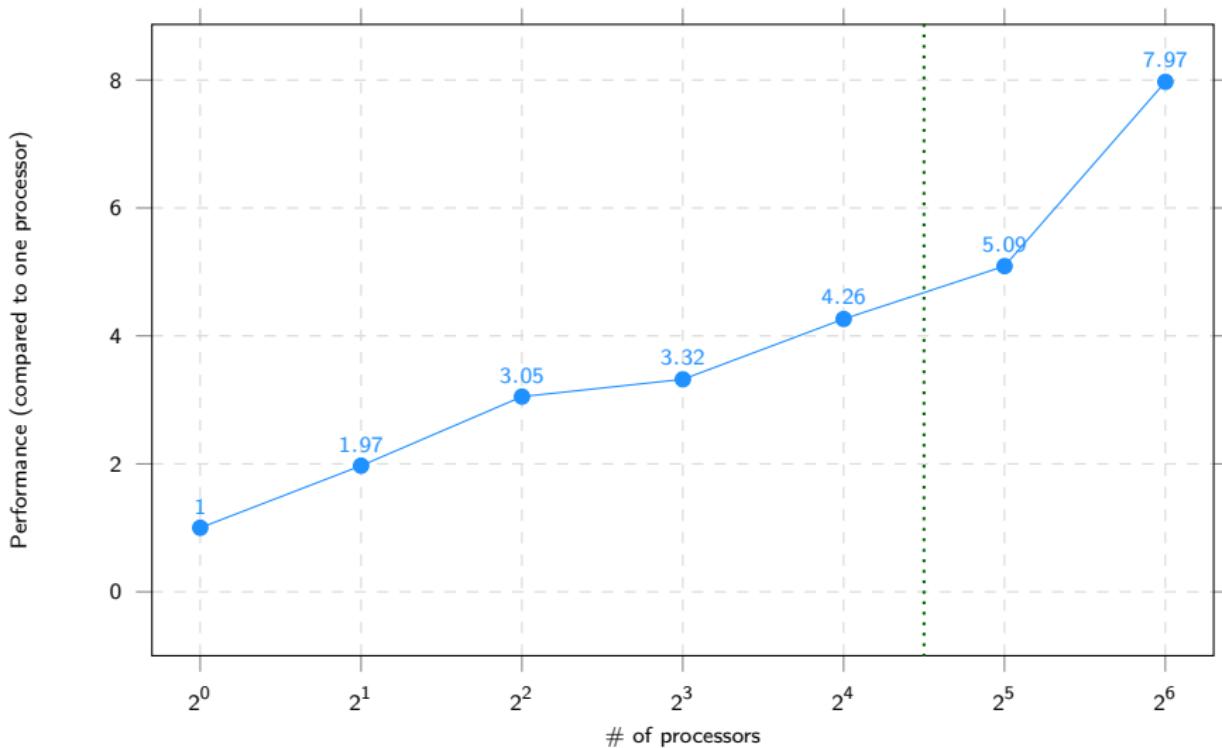


$N = 2^{11}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

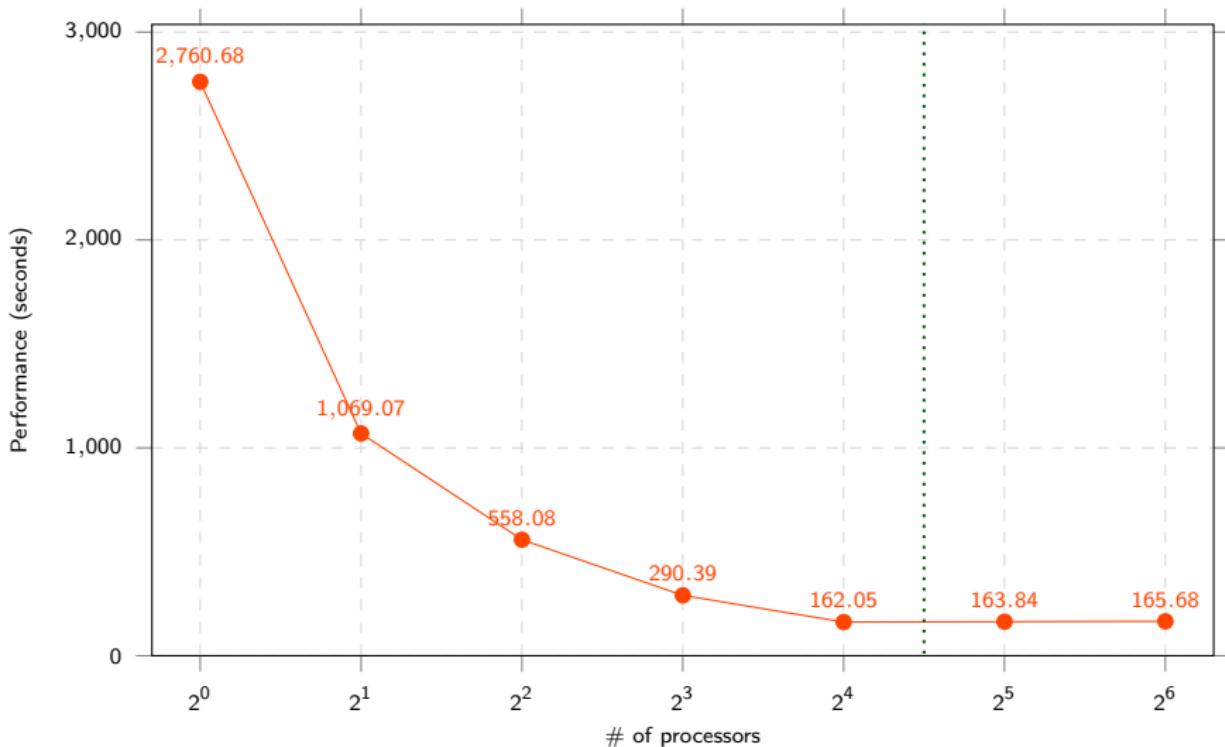
Performance scaling; MPICH



$N = 2^{11}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.

Matrix Multiplication

Raw performance; MPICH

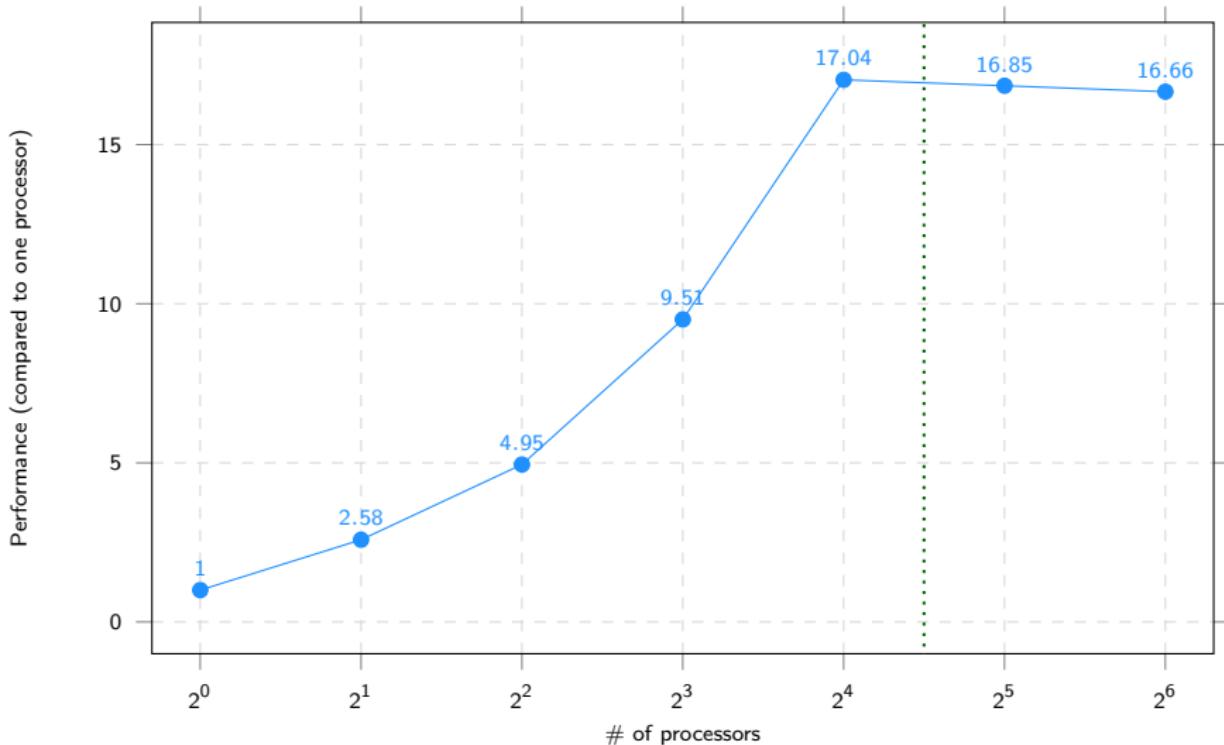


$N = 2^{12}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

Performance scaling; MPICH

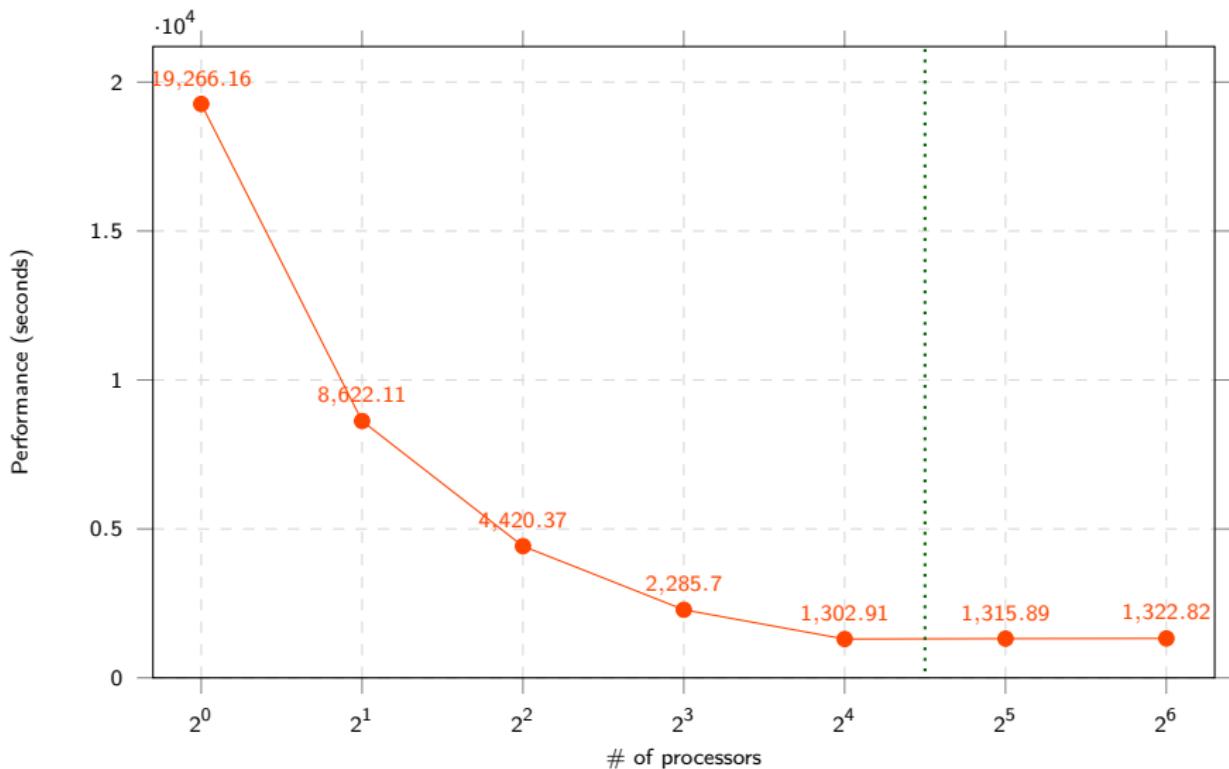


$N = 2^{12}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

Raw performance; MPICH

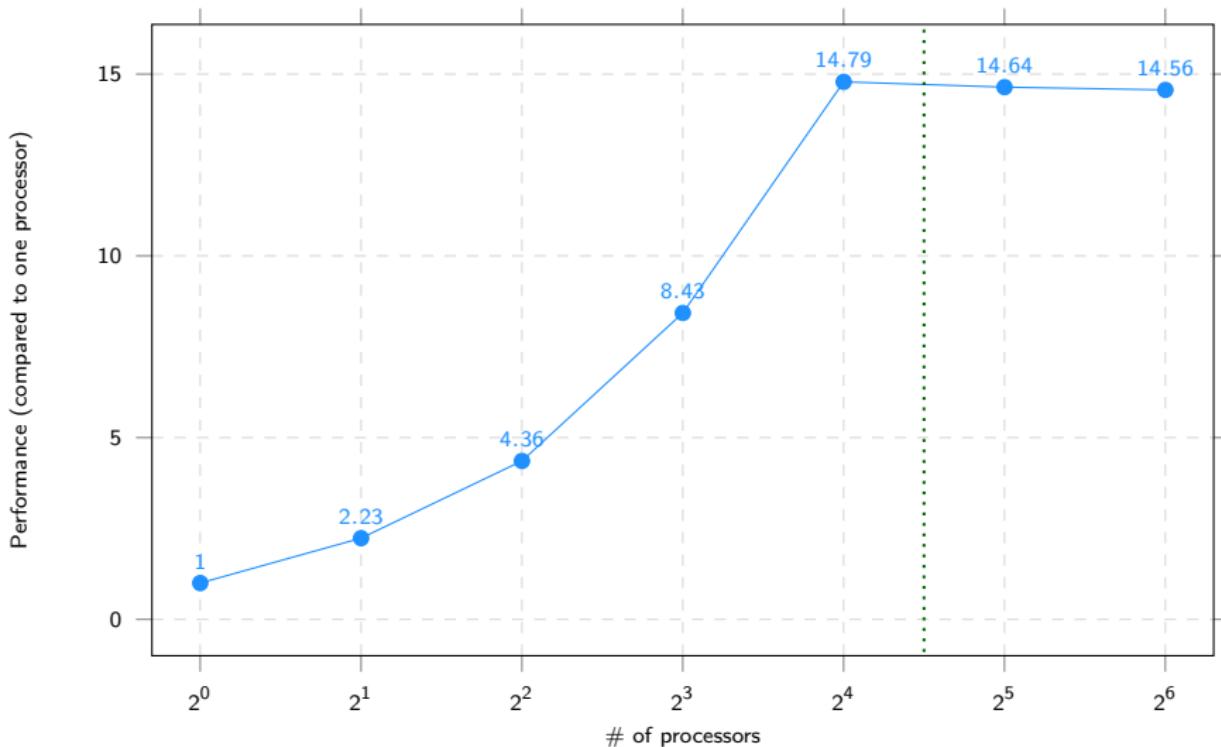


$N = 2^{13}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

Performance scaling; MPICH

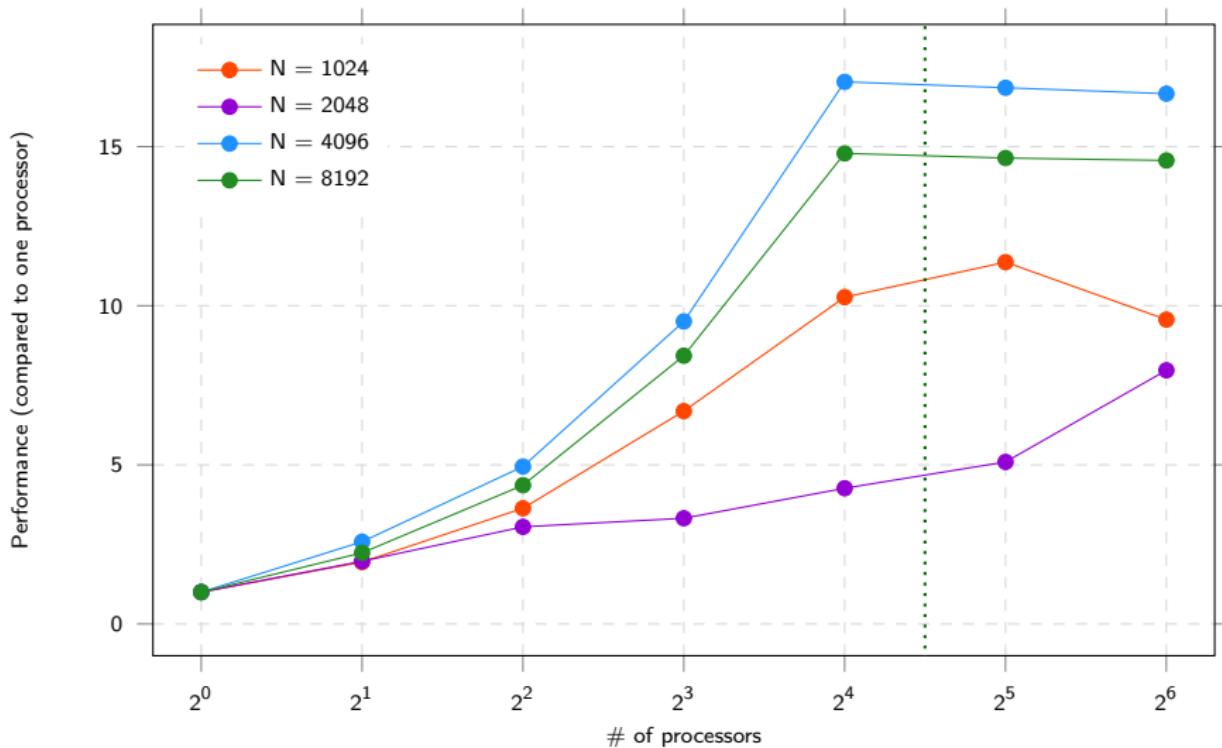


$N = 2^{13}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

Performance scaling (combined)



$N = 2^{10:1:13}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1.



Matrix Multiplication

Performance with and without -L\$MPIP/lib -lmpiP

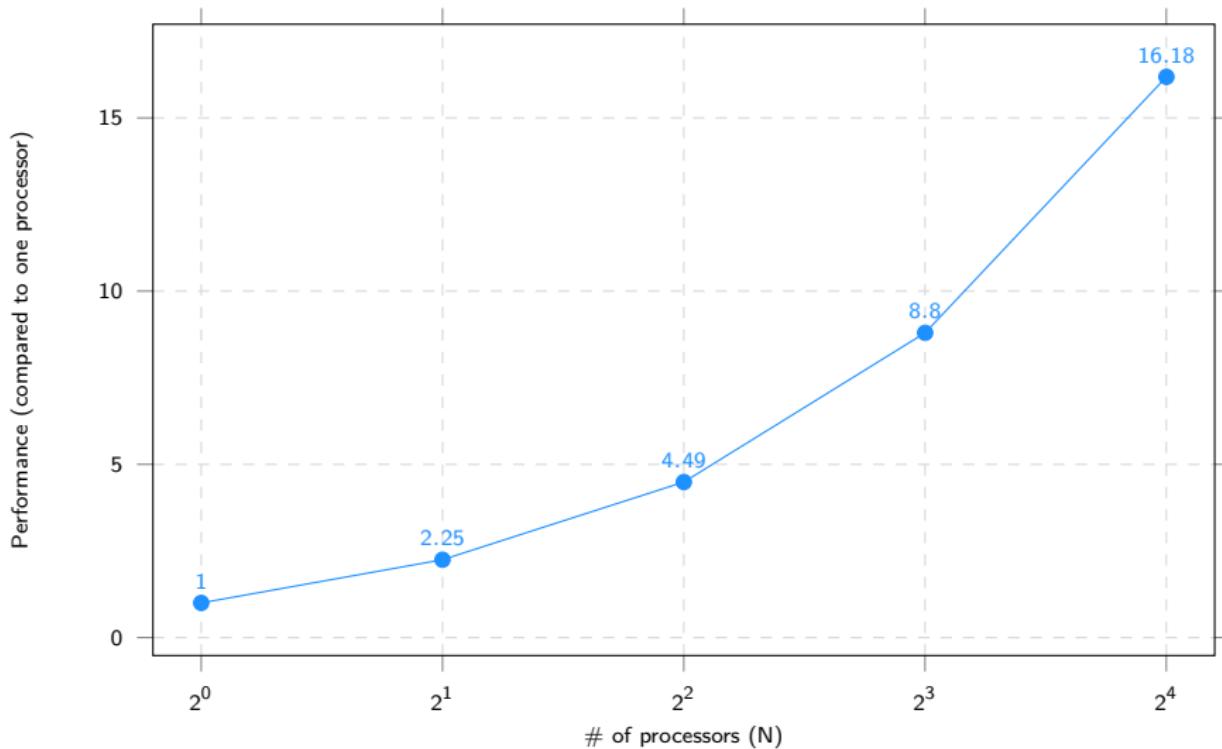
NPROC	N=1024			N=2048		
	with	w/o	Δ	with	w/o	Δ
1	8.39	8.22	0.17	63.56	63.39	0.17
2	4.32	4.84	-0.52	32.26	32.37	-0.11
4	2.31	2.30	0.01	20.84	21.04	-0.21
8	1.25	1.25	0.01	19.14	23.15	-4.01
16	0.82	0.76	0.06	14.91	14.34	0.57

NPROC	N=4096			N=8192		
	with	w/o	Δ	with	w/o	Δ
1	2760.68	2119.53	641.15	19266.16	20218.59	-952.43
2	1069.07	1067.19	1.88	8622.11	8682.60	-60.49
4	558.08	558.43	-0.35	4420.37	4408.65	11.72
8	290.39	285.04	5.35	2285.70	2295.75	-10.06
16	162.05	162.61	-0.56	1302.91	1290.31	12.60

Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; Intel Parallel Studio 2016.1.150, mpiP 3.4.1

Matrix Multiplication

Intel Cluster Studio XE 2013.0.028

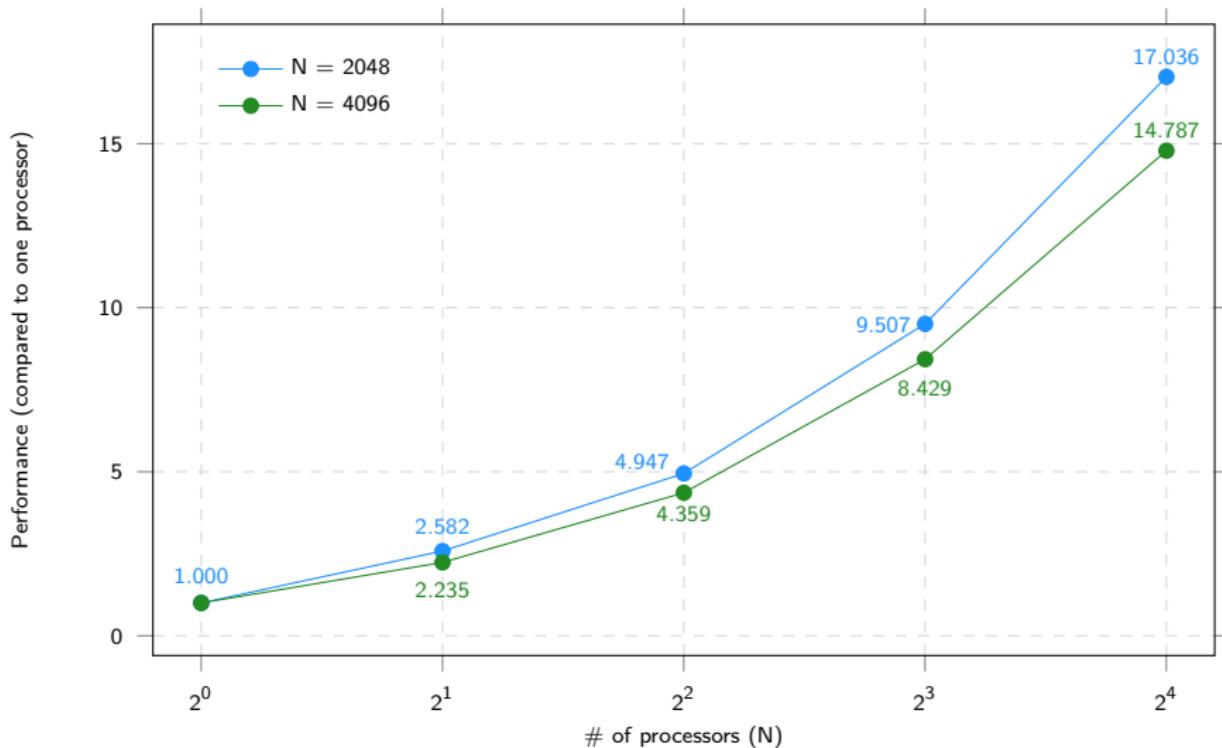


$N = 2^{11}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM.



Matrix Multiplication

Intel Parallel Studio 2016.1.150



$N = 2^{12,13}$; Intel Sandy Bridge E5-2670 2.60 GHz, 16 cores, 64 GB RAM; mpiP 3.4.1.

Matrix Multiplication

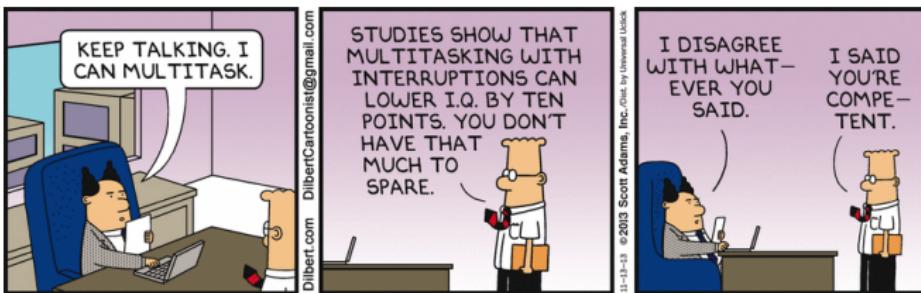
Super-linear scaling

Though rare, one possible reason is the *cache effect* resulting from the different memory hierarchies. In parallel computing, not only do the number of processors change, but so does the size of accumulated caches from different processors.

With the larger accumulated cache size, more or even all of the working set can fit into caches and the memory access time reduces dramatically, which causes the extra speed up in addition to that from the actual computation.

Hybrid MPI+OpenMP

Parallel Programming/Message Passing Interface



<http://dilbert.com/strip/2013-11-13/>

The Need

- * Recent architecture trend
 - * Increase in the processor count per physical machine
 - * Increase in the core count per processor
 - * Multi-level memory hierarchy
 - * Decrease in memory per core
 - * Decrease in memory bandwidth
 - * Decrease in network bandwidth per core

The Need

- * OpenMP
 - * Easy to implement
 - * Implicit communications and dynamic load balancing
 - * Only on shared memory architecture
 - * Does not scale to hundreds of workers
- * MPI
 - * Not easy to implement
 - * Explicit communications
 - * Distributed memory architecture
 - * Portable and scalable (10+k workers)

The Need

- * MPI+OpenMP in homogeneous computing infrastructures
 - * MPI for inter-node work
 - * OpenMP for intra-node work
 - * Prevents additional MPI intra-node communication
 - * Provides better performance than MPI or OpenMP in some cases
 - * Selecting the optimal number of MPI processes and the optimal number of threads per MPI process depends on application and hardware setup
 - NPROCS MPI processes and OMP_NUM_THREADS=NPROCS threads
 - NPROCS MPI processes and OMP_NUM_THREADS=NPROCS/m threads
 - NPROCS MPI processes and OMP_NUM_THREADS=m*NPROCS threads
 - * Class of suitable problems might be very limited

Components

- * Compiler directives

```
#pragma omp parallel shared(VAR1) private(VAR2)
```

- * Run-time library routines

omp.h and mpi.h providing `omp_get_num_threads()`,
`omp_get_thread_num()`, `omp_get_wtime()`, `MPI_Comm_size()`,
`MPI_Comm_rank()`, `MPI_Wtime()`, etc.

- * Environment variables

`OMP_NUM_THREADS`

`MPICH_CC`

`MPICH_CXX`

`MPICH_F77`

`MPICH_F90`



Compilation and Execution

Compilation

```
mpicc -Wall -g -lm -fopenmp PROGRAM.c -o PROGRAM.x  
mpicxx -Wall -g -lm -fopenmp PROGRAM.cpp -o PROGRAM.x
```

Execution

```
OMP_NUM_THREADS=2      # CHANGE TO 1, 2, 4, 8, ETC.  
mpirun -n NPROCS -f LIST-OF-MACHINES /path/PROGRAM.x
```

Training Camp: #01, Tasks #07–#09, and #04, Task #21

Necessary for distributed cases to work properly.

`NPROCS` is the number of processors assigned to run a program. `LIST-OF-MACHINES` is a file that contains the one-per-line list of hostnames/machines that are participating in the execution.

Conventions

- * Processor and thread count begins at 0, and ends at (NPROCS-1) and (OMP_NUM_THREADS-1) respectively. The program will not use more processors/threads than physically available
- * Master processor and master thread will be identified by `proc_id = 0` and `thread_id = 0` respectively, and will perform write operations when necessary
- * Worker processors and threads will be identified by
`proc_id = 1:(NPROCS-1)` and
`thread_id = 1:(OMP_NUM_THREADS-1)` respectively, and will perform read/write operations, and communicate with master and/or other workers iff there is a need

Hello, World!

In-class activity

To be performed in `colossus.it`; uses `guardian.it` as well

```
cd ${UN5390}/CourseWork/Week_11/${USER}_11/Parallel  
BASENAME="HelloWorld_Hybrid"  
MPICC="mpicc -Wall -g -lm -fopenmp"  
  
# Compilation and execution  
${MPICC} ${BASENAME}.c -o ${BASENAME}.x  
ssh-copy-id ${USER}@guardian.it.mtu.edu  
OMP_NUM_THREADS=1  
mpirun -n 1 -f $(pwd)/machines.txt $(pwd)}/${BASENAME}.x  
mpirun -n 2 -f $(pwd)/machines.txt $(pwd)}/${BASENAME}.x  
OMP_NUM_THREADS=2  
mpirun -n 1 -f $(pwd)/machines.txt $(pwd)}/${BASENAME}.x  
mpirun -n 2 -f $(pwd)/machines.txt $(pwd)}/${BASENAME}.x  
mpirun -n 4 -f $(pwd)/machines.txt $(pwd)}/${BASENAME}.x
```

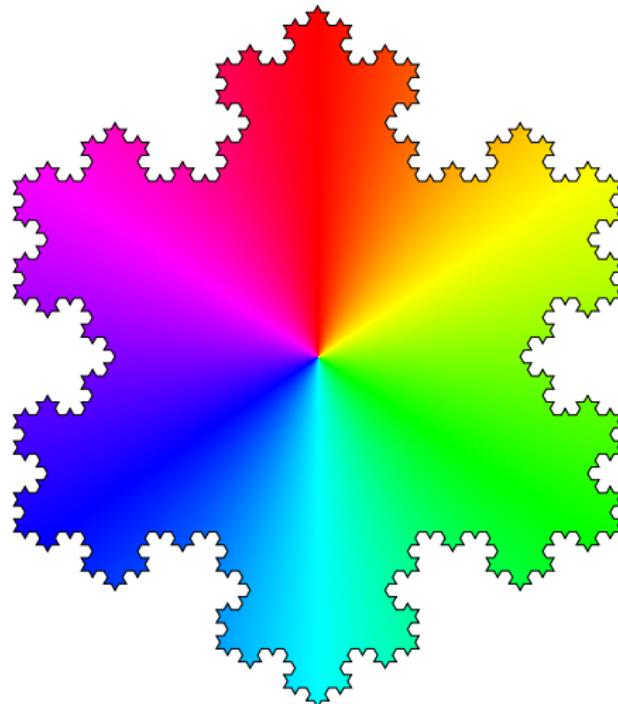


Additional References

- * A Hybrid MPI/OpenMP Parallel Implementation Of NSGA-II For Finding Patterns In Protein Sequences
D. L. Gonzalez-Alvarez, et. al.
Journal of Supercomputing, p. 1 (2016)
- * Massively Parallel And Linear-Scaling Algorithm For Second-Order Moller-Plesset Perturbation Theory Applied To The Study Of Supramolecular Wires
T. Kjaergaard, et. al.
Computer Physics Communications, vol. xxx, p. yyy (2016)
- * Parallel Finite Element Analysis Of Seismic Soil Structure Interaction Using A PC Cluster
B. Zhao, et. al.
Computers and Geotechnics, vol. 80, p. 167 (2016)

Before We Meet Again

- * Review the syllabus, course material, grade through week #14, notations, active participation, free time exercises, tips, opportunities, mathematical results, videos, and training camps
- * Practice compiling and executing included MPICH programs
- * Make progress in assignment #12
- * Make progress in the term project
- * Complete preparations for Research Marketing III



End of Tuesday lecture.

Research Marketing III

Elevator pitch; in-class activity

Title On Time	Time Limit	Clarity	Funding	Total Score
0-3	0-1	0-5	0-1	Row sum

Adam Mitteer, Data Science

Outsourcing Restaurant Polling Solutions

Akhil Kurup, ECE

Hardware Implementation Platforms For Artificial Intelligence

Ashley Kern, Data Science

Data Driven Financials And Success In Higher Education



Research Marketing III

Elevator pitch; in-class activity

Title On Time	Time Limit	Clarity	Funding	Total Score
0-3	0-1	0-5	0-1	Row sum

Avinaash Kovvuri, ECE

Did not provide the necessary information

Cal Riutta, BME

Evaluating Viscosity's Effect On Viscoelasticity Imaging To Aid In Better Lesion Detection

Eisa Hedayati, Physics

Efficient Parallelizing Of Kinetic Monte Carlo Simulation For Crystal Dynamics



Title On Time	Time Limit	Clarity	Funding	Total Score
0-3	0-1	0-5	0-1	Row sum

Hashim Al Mahmud, ME-EM

The Mechanical Properties Of Graphene Nanoplatelet-Carbon Fiber-Epoxy Hybrid Composites Using ReaxFF

Ian Cummings, ECE

The Advantages Of Simultaneous Transmit And Receive In Radar Arrays

Jeff Brookins, MSE

Bioabsorbable Metals And Novel Uses



Research Marketing III

Elevator pitch; in-class activity

Title On Time	Time Limit	Clarity	Funding	Total Score
0-3	0-1	0-5	0-1	Row sum

Paul Roehm, ME-EM

Expanding Molecular Dynamics: Using Finite Elements To Find Geometry And Orientation Effects In Nano-Composites

Prithvi Kambhampati, ECE

Free Education

Qing Guo, Physics

Electric Properties Of Two Dimensional Materials



Research Marketing III

Elevator pitch; in-class activity

Title On Time	Time Limit	Clarity	Funding	Total Score
0-3	0-1	0-5	0-1	Row sum

Sameer Saraf, ECE

Did not provide the necessary information

Sandeep Lanka, ECE

Collab - App/Website For Service Collaboration

Shuo Wang, ECE

Motion Deblurring Of A Plenoptic (Light Field) Camera



Research Marketing III

Elevator pitch; in-class activity

Title On Time	Time Limit	Clarity	Funding	Total Score
0-3	0-1	0-5	0-1	Row sum

Subin Thomas, Physics

Atmospheric Modeling Using SAM

Zhiqiang Zhao, ECE

The Vectorless Voltage Verification Using Current Constraints Without Using Spice Simulator With Exact Current Information

Research Marketing III

Elevator pitch; in-class activity

#	Name	Email	Dept/Program	Score
01	Ashley Kern	ankern	Data Science	136.00
02	Ian Cummings	itcummin	ECE	133.00
03	Cal Riutta *	cdriutta	BME	131.00
04	Paul Roehm	pmroehm	ME-EM	129.00
05	Adam Mitteer	aamittee	Data Science	124.50
06	Jeffrey Brookins *	jmbrooki	MSE	120.00
07	Eisa Hedayati	hedayati	Physics	119.50
08	Hashim Mahmud	hnalmahm	ME-EM	119.00
09	Zhiqiang Zhao	qzzhao	ECE	114.50
10	Sandeep Lanka	slanka	ECE	114.00
11	Subin Thomas	subint	Physics	109.00
12	Prithvi Kambhampati	pkambham	ECE	108.00
13	Shuo Wang	wshuo	ECE	100.00
14	Qing Guo	qinguo	Physics	87.50
15	Akhil Kurup	amkurup	ECE	84.00
16	Avinaash Kovvuri	askovvur	ECE	0.00
17	Sameer Saraf	svsaraf	ECE	0.00

* Undergraduate students; **Score** is the cumulative sum of all individual peer reviews.



Research Marketing III

Elevator pitch; in-class activity

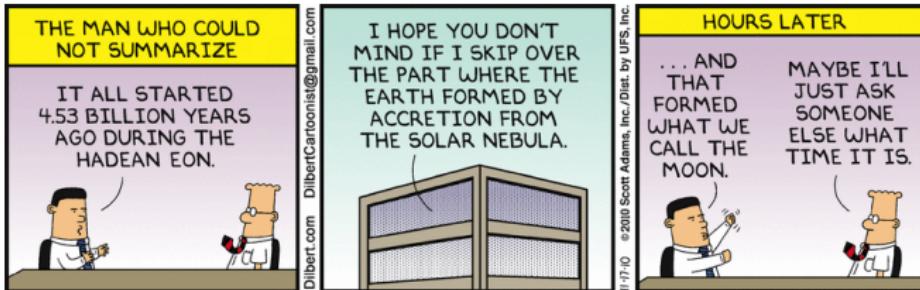


Model B, 16 GB edition, 64 bit quad core CPU, 1 GB RAM,
2.5 A power supply, 6 ft HDMI cable, 2 heat sink

Awarded to the student earning the highest score in peer review of elevator pitch.

Course Summary

What we have accomplished so far, and what lies ahead



<http://dilbert.com/strip/2010-11-17/>

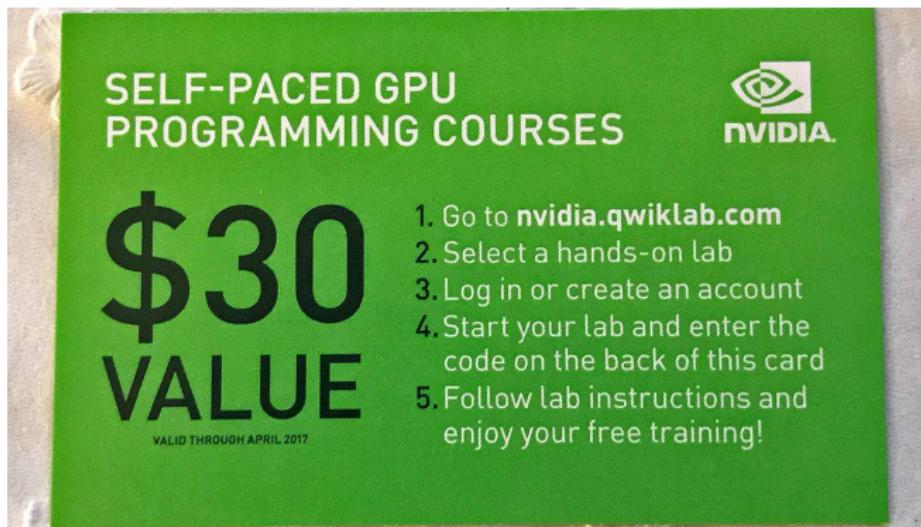
Looking Back



It's like reading a self help book Prior student, now in ORNL



- * An account in Portage, Michigan Tech's educational HPC resource
<http://portage.research.mtu.edu/>
- * Hardware accelerators (Intel MIC | NVIDIA GPU | OpenACC)



- * [Lmod](#) (dynamic modification of environment variables)
- * Data formats and management
 - * [NetCDF](#) | [HDF5](#)
 - * [XML](#) (portable database)
 - * [MariaDB](#) (a drop-in replacement for MySQL)
- * [PHP](#) (web programming language; interacts with XML and MariaDB)
- * [WordPress](#) (content management system; website, blog, etc.)
- * [Bootstrap](#) (framework for developing one's own responsive websites)
- * Visualization: [Google Charts](#) | [Highcharts](#) | [Highstock](#) | [Highmaps](#)



Course Material Distribution

Use the material for your own continuous improvement
but inform the instructor before distributing it



<http://dilbert.com/strip/2004-12-01/>

Course Material Distribution

Fall 2016 material was tailored to meet your specific learning needs – based on the preliminary survey and discussions with your advisor or graduate studies director. Owing to the legality of most PDFs in [AdditionalMaterial](#), distributing them could easily land you on the wrong side of the law.

Feel free to help subsequent students when approached about a problem from this course. But sharing course material or solutions to your assignments or solving problems in their entirety will lead me to form an incorrect opinion of them. This, in turn, will make the reference letter(s) I write for them bloated/dishonest and has a potential to hurt other hard-working students.

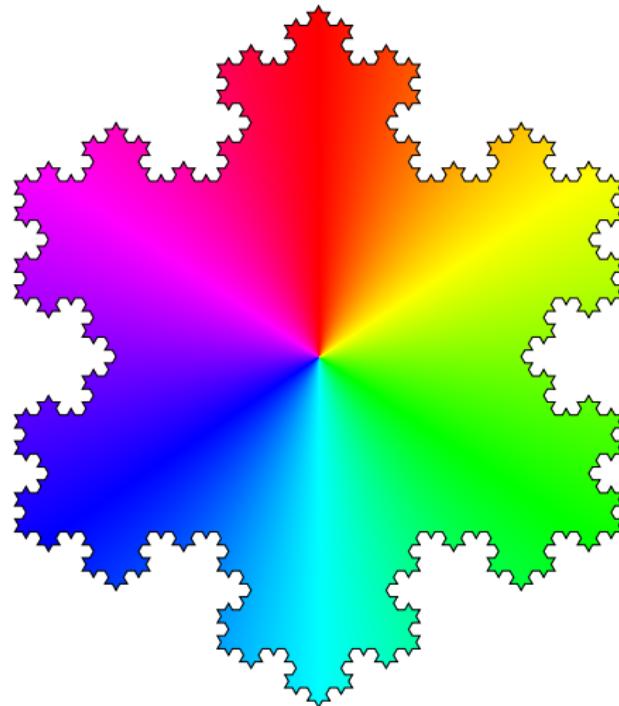
Techniques employed throughout this course are continuously used to (a) write proposals seeking external funding, (b) start/maintain collaborations with industries, academic institutions and supercomputing centers in/outside the US, and (c) publish papers in teaching journals. Help us protect our chances in few and far between opportunities.



Before We Part

- * Review the syllabus, course material, grade through week #14, notations, active participation, free time exercises, tips, opportunities, mathematical results, videos, and training camps
- * Turn in the project status by Friday 4:59 pm on 2016-12-09
- * Complete online course evaluations by 4:59 pm on 2016-12-10
- * Complete assignment #12 and project by 11:59 am on 2016-12-11
- * An email from your advisor by 11:59 am on 2016-12-12
- * Save GitHub repository by 11:59 pm on 2016-12-18

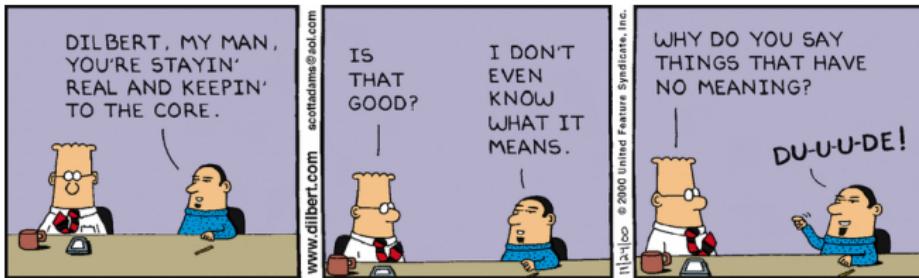
KBC social with your advisors/graduate studies directors
Friday, 9th December 2016, 5 pm ish



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 solution 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.

- * 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



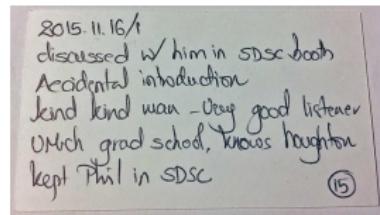
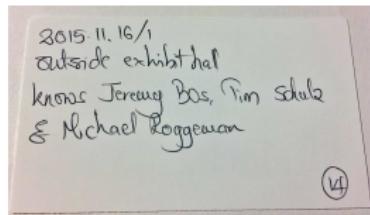
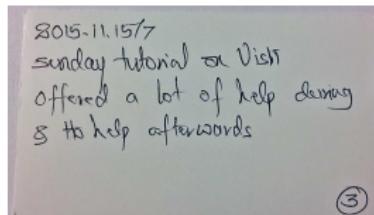
<http://dilbert.com/strip/2011-10-07/>

Research Marketing II

Professional business cards

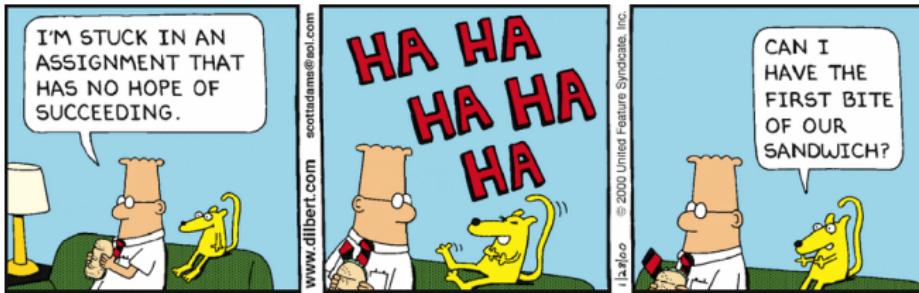
Visit Printing Services in the garden level of the Administration Building (a part of [University Marketing and Communications](#)) and get 100 professional business cards printed with the official Michigan Tech logo.

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
```

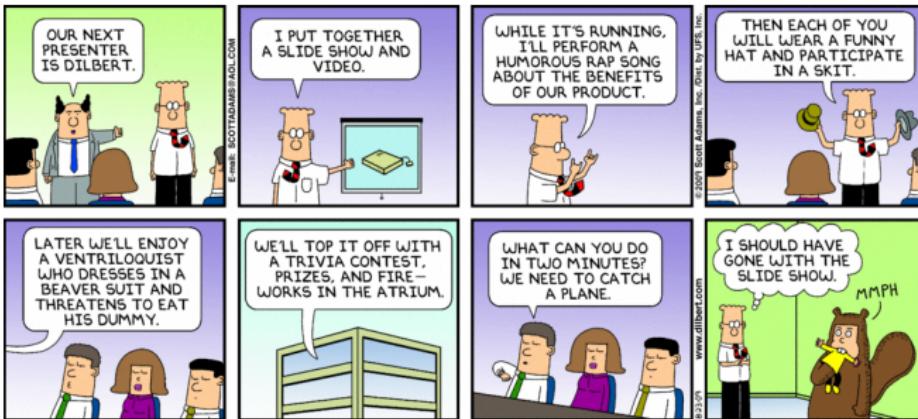


Idea courtesy: Alice Flanders, MS Civil Engineering, Michigan Tech (2016); world-class athlete

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?

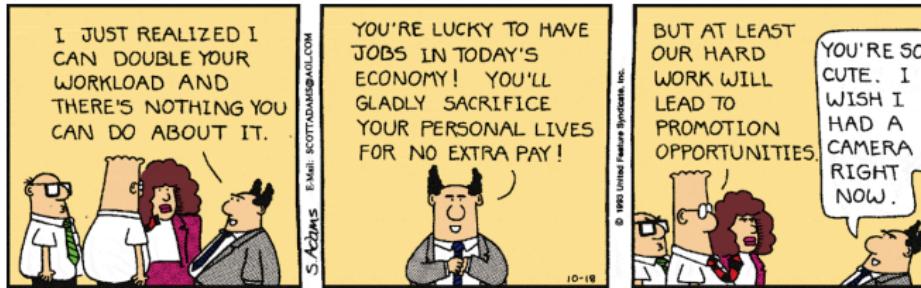
How to craft a winning elevator pitch

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).



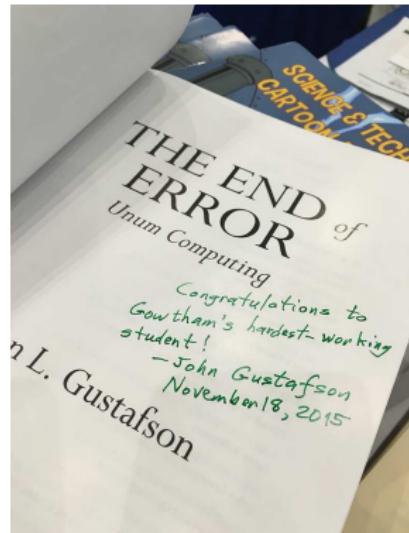
Doing Them All

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.

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,

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

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,

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

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

RAID: Introduction | Standard levels



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 execution. 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 → .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`.

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 [Additional Materials/Profile](#).

Solve by Inspection

Solve for x and y



such that the following expressions hold true

$$\sqrt{x} + y = 7$$

$$x + \sqrt{y} = 11$$

Golden Ratio

Write programs to estimate



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

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

$$x = 1 + \frac{1}{1 + \frac{1}{1 + \frac{1}{1 + \dots}}}$$

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

Roots of a Quadratic Expression

Identify the bugs

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

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

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 $\epsilon_o = |b - a|$, show that the minimum number of iterations necessary to achieve a tolerance δ in successive bisection method is given by

$$n \geq \frac{\ln \epsilon_o - \ln \delta}{\ln 2}$$

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

$$\epsilon_{n+1}^{\text{SB}} \propto \epsilon_n$$

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

What is the value of α in hybrid method?

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

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

Trapezoidal and Simpson's 1/3 rules



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

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, $0.50 \times (1 - e^{-2\pi}) = 0.499063299702889$. How does the error behave?

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

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

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

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

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

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

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

Write a program to estimate the volume of a unit sphere in n D 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



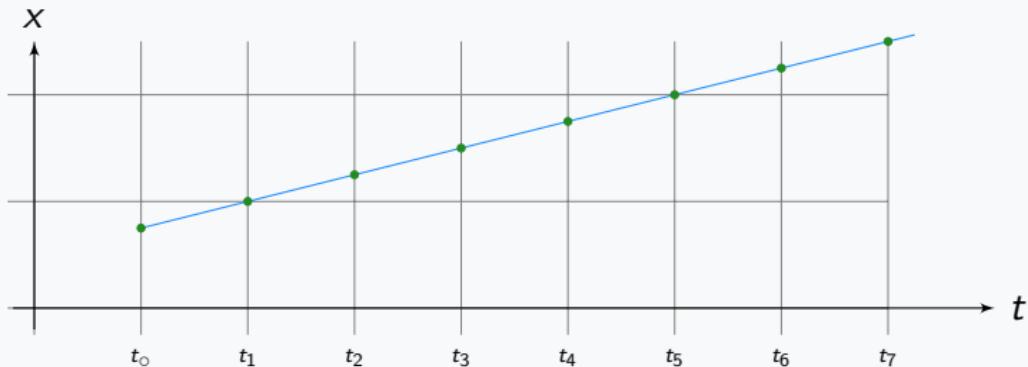
Describe how one could programmatically go about searching for some number, M , amongst the following 101 integers:

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

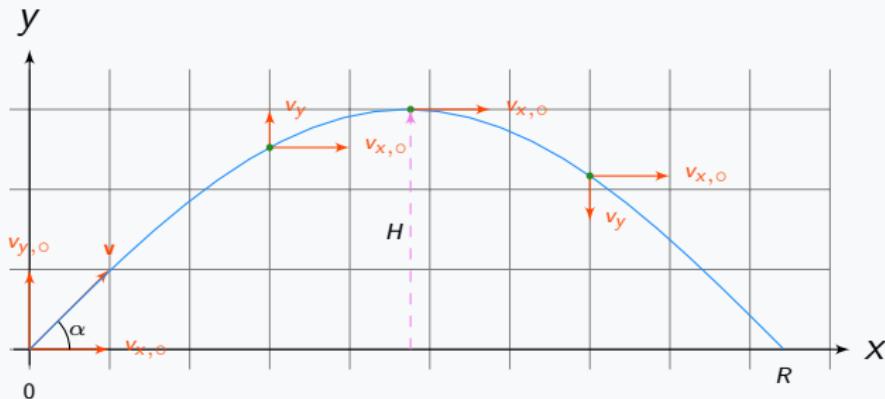
$$f(x_0, t_0) = \left. \frac{dx}{dt} \right|_{t=0} = v_0 ; x(t=0) = x_0$$

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)



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

$$v_{x,n+1} = v_{x,n}$$

$$v_{y,n+1} = v_{y,n} - h g$$

$$x_{n+1} = x_n + h v_{x,n}$$

$$y_{n+1} = y_n + h v_{y,n}$$

With $g = 32.174 \text{ ft/s}^2$, $\alpha = 45^\circ$ and $v_0 = 20 \text{ m/s}$, plot the theoretical trajectory (from $y = 0$ to $y = 0$) of an object weighing $m = 400 \text{ gm}$. 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

$$\epsilon_{\text{local truncation}} = \mathcal{O}(h^3)$$

$$\epsilon_{\text{global truncation}} = \mathcal{O}(h^2)$$

Show that the optimum value of h for ABM2 method is

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

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.

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

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.

$$A_{ij}^T = A_{ji} \quad \Rightarrow \quad (A^T)^T = A$$

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

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

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

$$C_{ij} = (-1)^{i+j} M_{ij}$$

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

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

Determinant



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

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

Matrix Methods: Inversion

Inversion



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

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

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.

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

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^{Nmin} to 2^{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.

Primes: Sieve of Eratosthenes

Time complexity



The algorithm for the sieve of Eratosthenes, as noted in week #13 parallel computing examples discussions, is said to have a time complexity of $\mathcal{O}(N \log \log N)$. Starting with the serial sample program provided by the instructor, [Primes.s.c](#), test this claim for $N = 10^n$ where $n = 0 : 1 : 9$. p is the number of primes between 2 and N , and t_{CPU} is the CPU time taken to find p for a given N .

For each value of N , the modified program should display at least the following information in a pleasant and easy to appreciate fashion. Include plots to represent the tabular data, if possible.

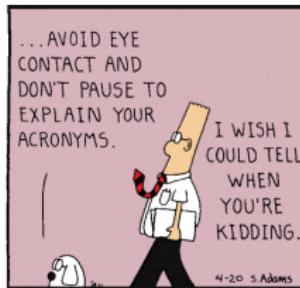
N	t_{CPU}	$N(\log(\log(N)))$	p	$\frac{N}{\ln N}$	$\frac{N}{\ln(N) - 1}$	$\frac{2}{3}$	Δ_{45}	Δ_{46}
-----	------------------	--------------------	-----	-------------------	------------------------	---------------	---------------	---------------

[Primes.s.c](#) is in week #11 [AdditionalMaterial](#).



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.

L^AT_EX 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.



L^AT_EX 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.???.pdf  
rm -f UN5390.sty UN5390_Settings.tex
```

Replace 01 with the appropriate week number.



L^AT_EX 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

L^AT_EX 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.

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  
:sgc:0:1449493098:1449493123:1449499243:0:0:6120:...  
qlogin.q:compute-0-99.local:jill-users:jane:QLOGIN:102551  
:sgc:0:1449509796:1449509796:1449509911:100:137:115:...  
short.q:compute-0-1.local:john-users:amy:test2.sh:102546  
:sgc: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=3.141592653589793238462643383279
```

```
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`.



L^AT_EX 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
```

L^AT_EX 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.???.pdf  
rm -f UN5390.sty UN5390_Settings.tex
```

L^AT_EX 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}.bb1 ${TEXFILE}.blg
rm -f ${TEXFILE}.dvi ${TEXFILE}.log ${TEXFILE}.out
rm -f ${TEXFILE}.ps
```

L^AT_EX 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}.bbt ${TEXFILE}.blg
rm -f ${TEXFILE}.dvi ${TEXFILE}.log ${TEXFILE}.out
```

L^AT_EX 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.



- * 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 -zvxf ${HOME}/tmp/${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"
```

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.

Sort an Array

BASH

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

# Unsorted and sorted arrays
ARRAY_UNSORTED=( simon amy zachary carrie jill henry )
ARRAY_SORTED=( $(
    for tmp in ${ARRAY_UNSORTED[@]}
    do
        echo "${tmp}"
    done | sort) )

# Useful stuff with sorted array
```



Sort Multi-Column Data File

Creating a multi-column data file with *random* information

```
N=10
```

```
touch file.dat
```

```
truncate -s0 file.dat
```

```
for (( i=1; i<=${N}; i++ ))
```

```
do
```

```
    j=$((expr ${i} * ${i} - ${i}))
```

```
    j=$(printf "%03d" "$j")
```

```
    TEXT=$(cat /dev/urandom | tr -dc 'a-zA-Z0-9' | \
          fold -w 32 | head -n 1)
```

```
    echo "${i} ${j} ${N} ${RANDOM} ${TEXT}" >> file.dat
```

```
done
```

Refer to `man fold`, `man sort` and `man tr` for more information.



Sort Multi-Column Data File

Commands

```
# Default; 1st field; use -r for reverse; -n for numeric
sort file.dat
sort -n file.dat

# 4th field; -k 4,4n to force numeric
sort -k 4 file.dat
sort -k 4,4n file.dat

# 3rd field (numeric), then 5th field (to break ties)
sort -k 3,3n -k 5 file.dat

# 3rd field (n), then 5th field, and then 4th field (n)
sort -k 3,3n -k 5 -k 4,4n file.dat
```



mpich_mpi()

A compact function to compile MPICH programs

```
mpich_mpi() {
    if [ $# != 1 ]
    then
        echo " Usage: ${FUNCNAME} PROGRAM.c"
        echo " e.g.: ${FUNCNAME} HelloWorld_mpi_01.c"
    else
        local cbase=$(echo "$1" | awk -F "." '{ print $1 }')
        mpicc -Wall -g -lm $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 `mpich_mpi.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.

mpich_mpi.sh

Template for parent BASH script

- * Accepts two arguments: **FILENAME** and **NPROCS**
- * 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

```
mpicc -Wall -g -lm FILENAME -o BASENAME.x
```

- * Runs **BASENAME.x** using **NPROCS** processors

```
mpirun -n $NPROCS /path/to/BASENAME.x
```

mpiP Download and Installation

Requires completion of MPICH 3.2 (w/ GCC 4.8.5) installation

```
mkdir -p ${HOME}/apps/mpiP/3.4.1/mpich/3.2/gcc/  
cd ${HOME}/apps/mpiP/3.4.1/mpich/3.2/gcc/  
tar -zxvf /tmp/${USER}/src/mpiP-3.4.1.tar.gz  
mv mpiP-3.4.1 4.8.5  
cd 4.8.5  
  
.configure LDFLAGS=-L/usr/lib64 \  
--with-cc=mpicc --with-cxx=mpicxx --with-f77=mpif77 \  
--enable-collective-report-default \  
--enable-demangling=GNU \  
--enable-stackdepth=32 \  
--disable-libunwind \  
--disable-bfd
```

Download `mpiP-3.4.1.tar.gz` from <http://mpip.sourceforge.net/> and save it in `/tmp/${USER}/src/`.

mpiP Download and Installation Continued

Requires completion of MPICH 3.2 (w/ GCC 4.8.5) installation

```
make clean  
make  
make install  
make shared  
  
cd /tmp/  
\rm -r ${USER}
```

Update \${HOME}/.bash_\${USER}

```
# mpiP 3.4.1 (MPICH 3.2 with GCC 4.8.5) settings  
export MPIP="${HOME}/apps/mpiP/3.4.1/mpich/3.2/gcc/4.8.5"  
export LD_LIBRARY_PATH="${LD_LIBRARY_PATH}: ${MPIP}/lib"
```

Run source \${HOME}/.bashrc

mpich_mpiP()

A compact function to compile MPICH programs with mpiP library

```
mpich_mpiP() {
    if [ $# != 1 ]
    then
        echo " Usage: ${FUNCNAME} PROGRAM.c"
        echo " e.g.: ${FUNCNAME} HelloWorld_mpi_01.c"
    else
        local cbase=$(echo "$1" | awk -F "." '{ print $1 }')
        mpicc -Wall -g -lm -L${MPIP}/lib -lmpiP \
            $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 `mpich_mpi.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.

- * Accepts two arguments: **FILENAME** and **NPROCS**
- * 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

```
mpicc -Wall -g -lm -L${MPIP}/lib -lmpiP -lm \
FILENAME -o BASENAME.x
```

- * Runs **BASENAME.x** using **NPROCS** processors

```
mpirun -n $NPROCS /path/to/BASENAME.x
```

Lmod 7.1 compilation (in `colossus.it`)

```
cd /tmp/${USER}/src/
tar -jxvf Lmod-7.1.tar.bz2
cd Lmod-7.1

./configure --prefix=${HOME}/apps/ \
--with-module-root-path=${HOME}/apps/modulefiles \
--with-spiderCacheDir=${HOME}/apps/lmod_data/cacheDir \
--with-updateSystemFn=${HOME}/apps/lmod_data/system.txt
make install

cd /tmp/
\rm -rf ${USER}
```

Download `Lmod-7.1.tar.bz2` from <https://sourceforge.net/projects/lmod/files/> and save it in `/tmp/${USER}/src/`.

Lmod 7.1 configuration (in `colossus.it`)

```
cd ${UN5390}/CourseWork/Week_14/AdditionalMaterial/Lmod  
git pull  
cp profile ${HOME}/apps/lmod/lmod/init/profile  
rsync -avhP ./modulefiles/ ${HOME}/apps/modulefiles/  
# Edit/Use ${HOME}/apps/modulefiles/ as template for more
```

Update \${HOME}/.bash_\${USER} and source \${HOME}/.bashrc

```
# Lmod 7.1 settings  
if [ -d "${HOME}/apps/lmod" ]  
then  
    source "${HOME}/apps/lmod/lmod/init/profile"  
fi
```

Lmod 7.1 sample usage (in `colossus.it`)

```
module list
```

```
module avail
```

```
module load matlab/R2015b
```

```
module list
```

```
echo "${PATH}"
```

```
module load matlab/R2014b
```

```
echo "${PATH}"
```

```
module unload matlab/R2014b
```

```
module load gcc
```

```
module avail
```

```
module load python
```

```
echo "${PATH}"
```

Cleaning Up Local Repository

Workflow (To be performed in `colossus.it` and/or personal machines)

```
cd ${UN5390}  
git pull  
du -sh ./git/  
git repack -a -d --depth=500 --window=500  
du -sh ./git/
```

This workflow is particularly useful when you receive an email from IT indicating that your campus home directory is nearing or has exceeded the limit. It cleans up the `.git` folder, and has been shown to reduce its size by 25-90%. Such an approach should help retain the Git repository through the end of semester OR a project's lifetime without having to explicitly delete project files or folders.

Information courtesy: Prithvi Kambhampati, UN5390 in Fall 2016 ([additional details](#)).

Periodic execution of this workflow is recommended to conserve space (especially in your campus home directory).



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	Eassa Hedayati	hedayati	Physics	John Jaszcak
04	Hashim Mahmud	hnalmahm	ME-EM	Gregory Odegard
05	Jeffrey Brookins *	jmbrooki	MSE	Jaroslaw Drellich
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

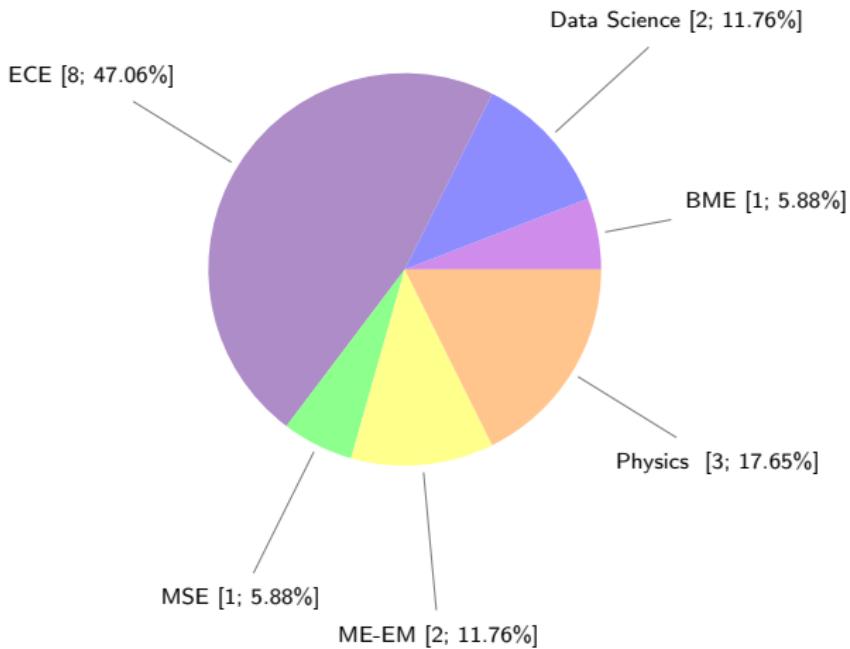
#	Name	Email	Advisor
09	Cal Riutta *	cdriutta	Jinfeng Jiang

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



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\}/\text{LaTeXTemplates}/\text{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.



- * 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)



- * 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)



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>

- * 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



- * 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



Destination Cinema at Michigan Tech
ROZSA CENTER FOR THE PERFORMING ARTS
NOVEMBER 3-6, 2016

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/>

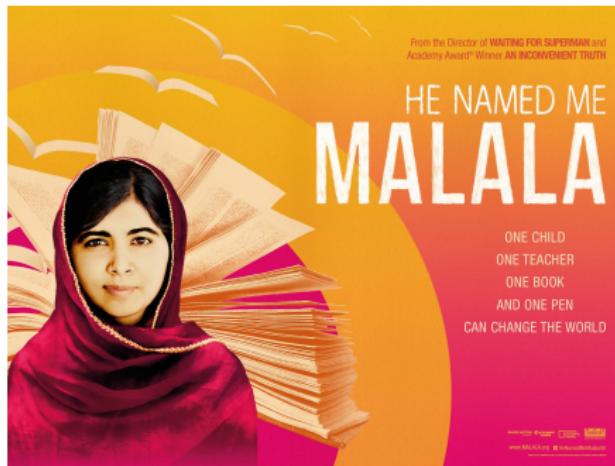


Before The Flood



Limited free screening on [iTunes](#), [National Geographic](#) and [YouTube](#)

International Education Week



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

Malala Yousafzai (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/>

Keweenaw Climate Science Event

#4 of four-part event

The Orpheum Theater

6 – 8 pm on Thursday, 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.



Memorial Union Building (MUB)

Ballroom B, 4 – 5:30 pm on Thursday, 1st December 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.



Blue Waters Graduate Fellowship

- * Applicant must be a US citizen or a permanent resident
- * Graduate students in second or later year
- * \$38k stipend + \$12k tuition allowance
- * 50,000 node-hours of CPU time



<https://bluewaters.ncsa.illinois.edu/fellowships> | Application deadline: 3rd February 2017

Blue Waters Student Internship Program

- * 20 undergraduate research internship
- * \$5k stipend
- * 2 week intensive HPC workshop



GitHub Private Repository (Free)

- * Visit <https://education.github.com/>
- * Click on **Request discount**
- * Select **Student** and **Individual account**
- * School-issued email address: **`${USER}@mtu.edu`**
School name: **Michigan Technological University**
Graduation year: **2018** (or as appropriate)
Intended usage: **Teaching and learning about Git**
- * Click on **Submit request**
- * GitHub folks usually approve the request within 5-7 business days

Saving GitHub Repository

un5390_f2016_\${USER}

- * Create a private repository, un5390_f2016_\${USER}, in your account
- * Click on **Import code**
- * Enter the following for repository's URL
[https://github.com/MichiganTech/un5390_f2016_\\${USER}.git](https://github.com/MichiganTech/un5390_f2016_${USER}.git)
- * Click on **Begin import**. Enter GitHub username and password.
- * Update every local copy (i.e., clone) using the command

```
git remote set-url origin \
git@github.com/johnny/un5390_f2016_${USER}
```
- * Perform the above steps
after 11:59 pm on 2016-12-16 but before 11:59 pm 2016-12-18

Replace johnny with your GitHub username.



HPC-Related Opportunities

<http://hpc.mtu.edu/opportunity/>

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

$$\int_a^b f(x) dx = y(b) - y(a)$$

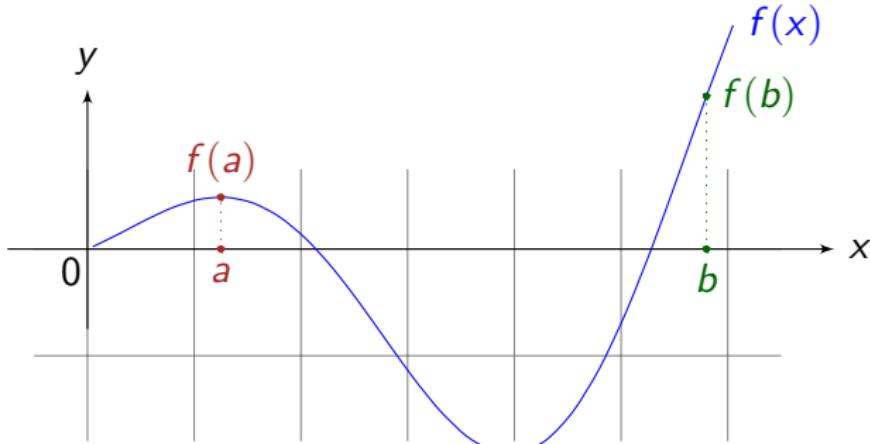
Changing the notations while retaining the underlying essence,

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

Re-arranging the terms,

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

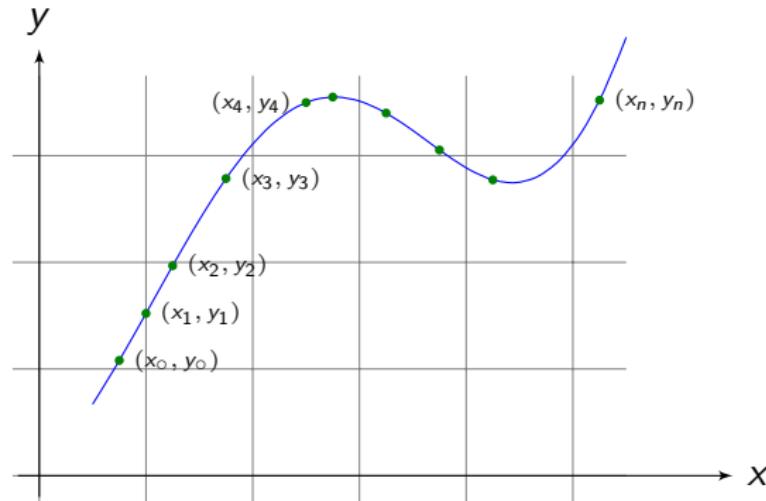
Intermediate Value Theorem (IVT)



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

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

Lagrange basis polynomials are given by

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

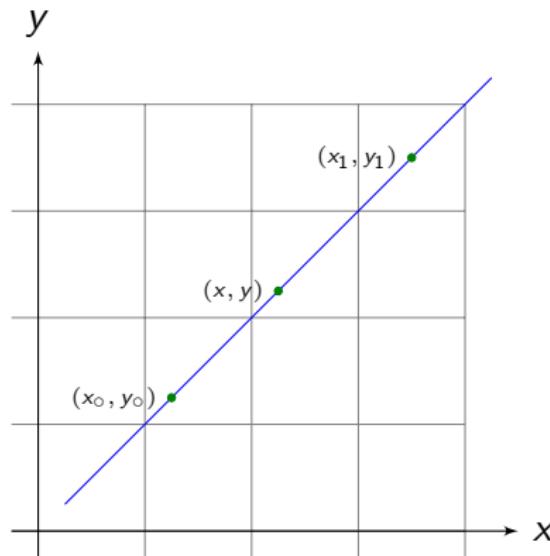
and are built to have the *Kronecker delta* property

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

Lagrange Polynomial Interpolation

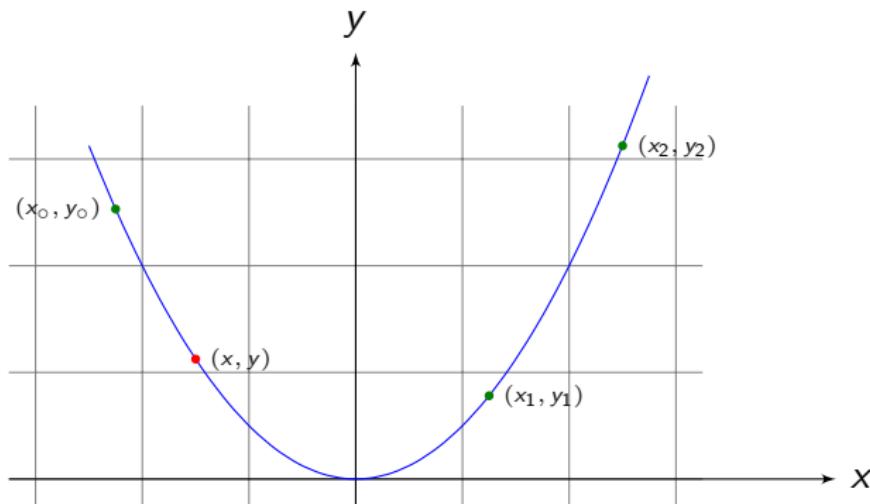
Linear

Suppose that (x_0, y_0) 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



$$\mathcal{L}_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} y_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} y_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} y_2$$

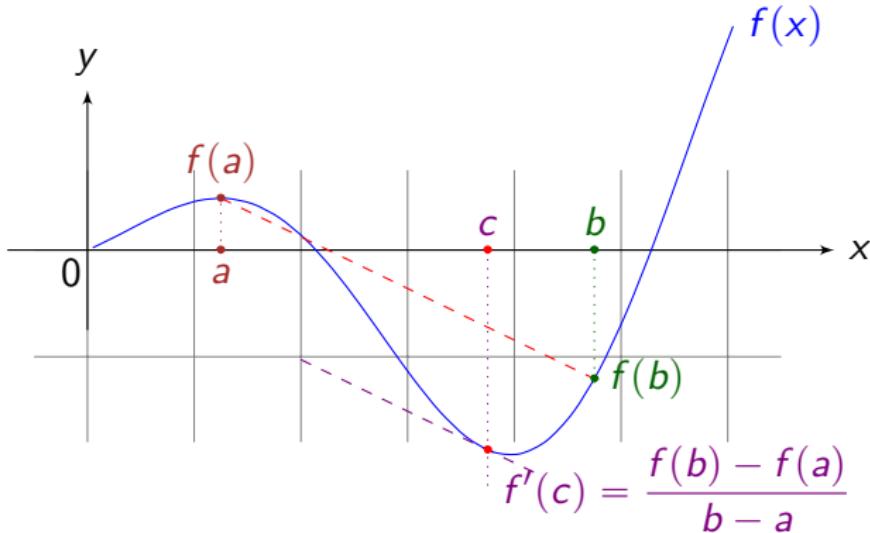
Lagrange Polynomial Interpolation

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 , ($i = 0, 1, 2, \dots, n$) in that interval. Then

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

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, $g(x) \geq 0$, in $[a, b]$, then for some c in $[a, b]$

$$\int_a^b f(x) g(x) dx = f(c) \int_a^b g(x) dx$$

Newton-Cotes Formula

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

Consider the integral

$$I = \int_a^b f(x) dx$$

If $f(x)$ can be approximated by an n^{th} order polynomial

$$p_n(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \dots + \alpha_{n-1} x^{n-1} + \alpha_n x^n$$

then the integral, I , takes the form

$$I = \int_a^b [\alpha_0 + \alpha_1 x + \alpha_2 x^2 + \dots + \alpha_{n-1} x^{n-1} + \alpha_n x^n] dx$$



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_0 , then

$$f(x) = \sum_{n=0}^{\infty} \frac{(x - x_0)^n}{n!} \left. \frac{d^n}{dx^n} f(x) \right|_{x=x_0}$$



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

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

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	$P(Y = y_i)$	$F(y) = P(Y \leq y_i)$
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

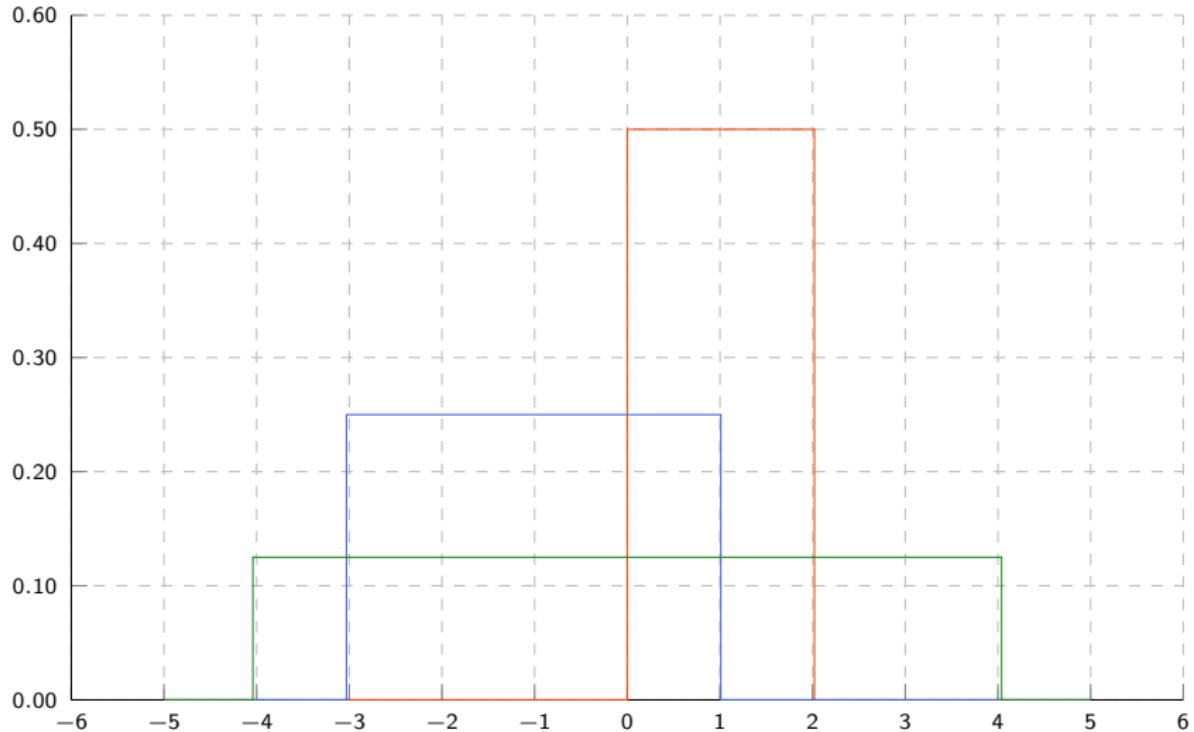
a finite number of values are equally likely to be observed. The probability density function on the interval $[a, b]$ is

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

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



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

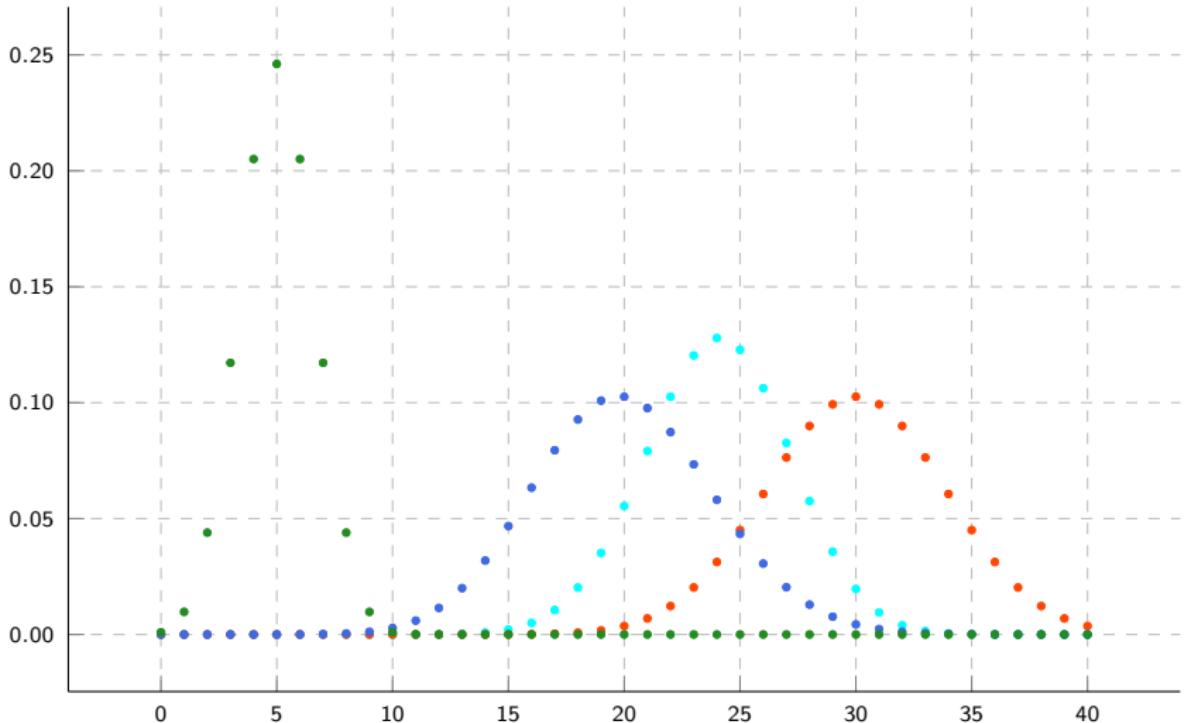
Discrete

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

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

Binomial Distribution



Poisson Distribution

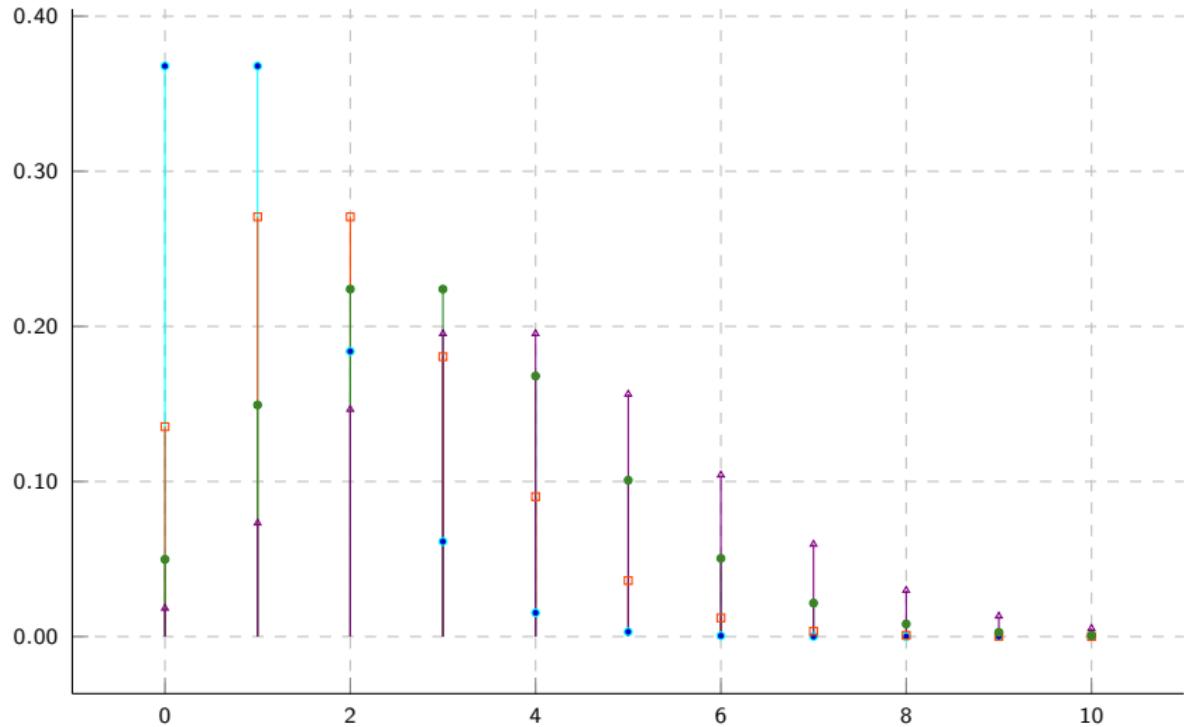
Discrete

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

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

Poisson Distribution



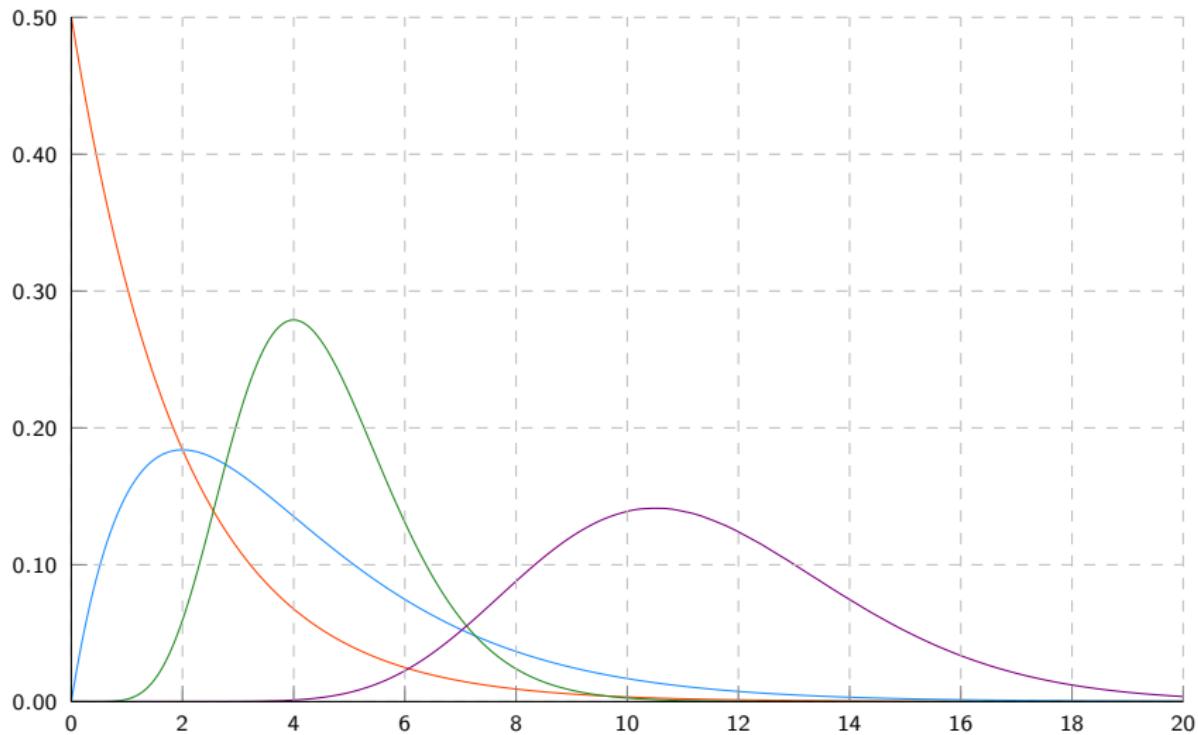
Gamma Distribution

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

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

Gamma Distribution



Normal/Gaussian Distribution

Continuous

Applicable as

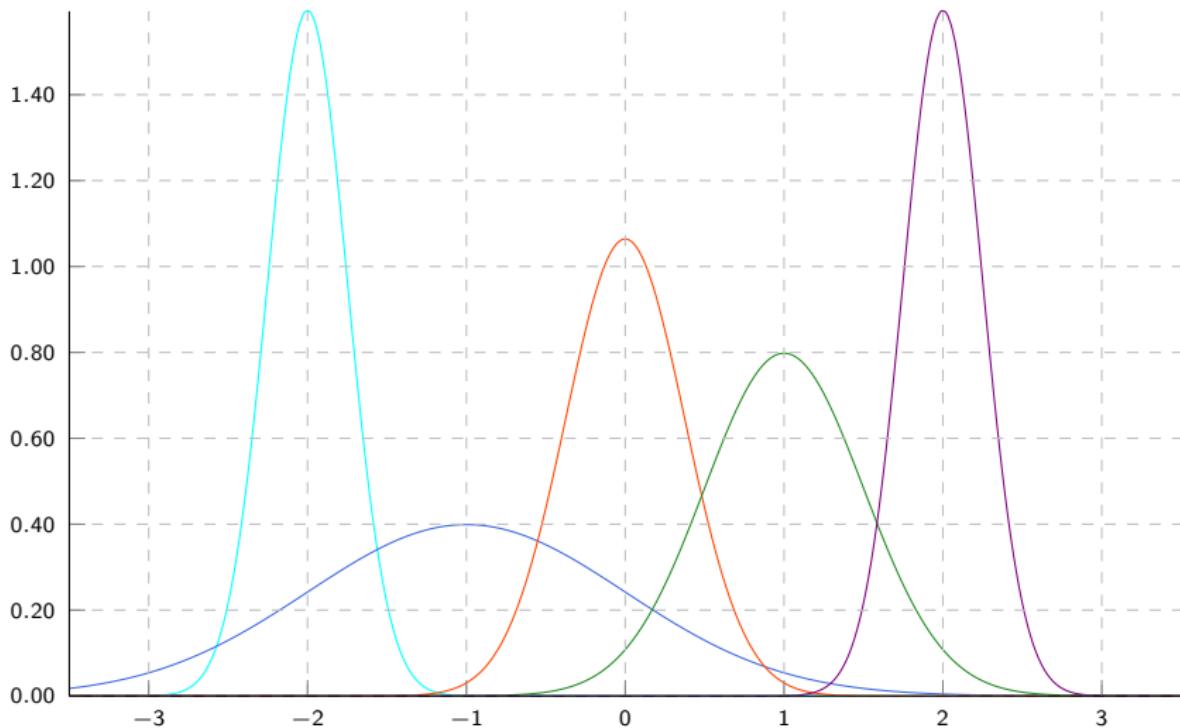
a limiting form of binomial distribution (De Moivre, 1733) and as a plausible distribution for measurement errors (Gauss, 1809). The probability density with mean μ and standard deviation σ is

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

Central limit theorem (Laplace)

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



Butcher Tableau

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



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

$$k_1 = f(y_n, t_n)$$

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

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

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

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 ($i = 1, 2, \dots, s$; the weights), c_i ($i = 2, \dots, s$; the nodes), and relationship between a_{ij} and c_i uniquely identifies the s -stage RK method and ensures its consistency.

0	a_{11}	a_{12}	\dots	$a_{1,s-1}$	$a_{1,s}$
c_2	a_{21}	a_{22}	\dots	$a_{2,s-1}$	$a_{2,s}$
\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
c_s	a_{s1}	a_{s2}	\cdots	$a_{s,s-1}$	$a_{s,s}$
	b_1	b_2	\cdots	b_{s-1}	b_s

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

Butcher Tableau

Explicit RK2 method

0	0	0
1	1	0
	1/2	1/2

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

0		
1	1	
	1/2	1/2

Consistency check is satisfied

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



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

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

Butcher Tableau

Explicit RK4 method

0	0	0	0	0
1/2	1/2	0	0	0
1/2	0	1/2	0	0
1	0	0	1	0
	1/6	1/3	1/3	1/6

Drop the explicit mention of zeros along the diagonal and above

0				
1/2	1/2			
1/2	0	1/2		
1	0	0	1	
	1/6	1/3	1/3	1/6



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

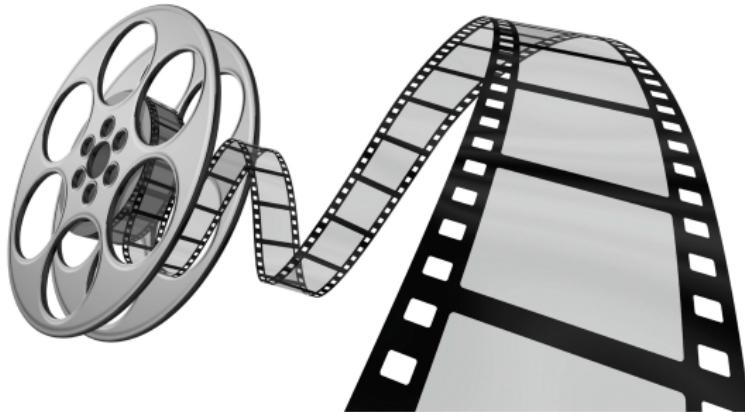
$$y_{n+1} = y_n + \frac{h}{6} k_1 + \frac{h}{3} k_2 + \frac{h}{3} k_3 + \frac{h}{6} k_4$$

Simplify

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

Videos

If a picture is worth a thousand words ...

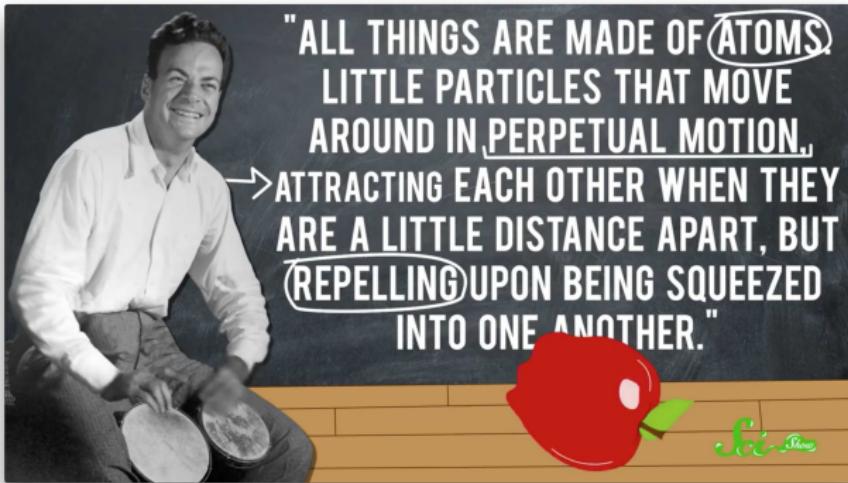


People and Personalities

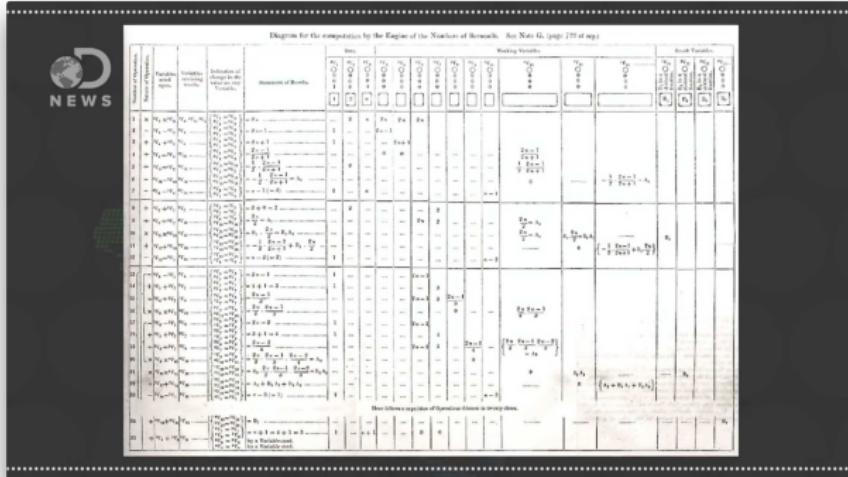


and their stories

Richard Phillips Feynman 1918 – 1988



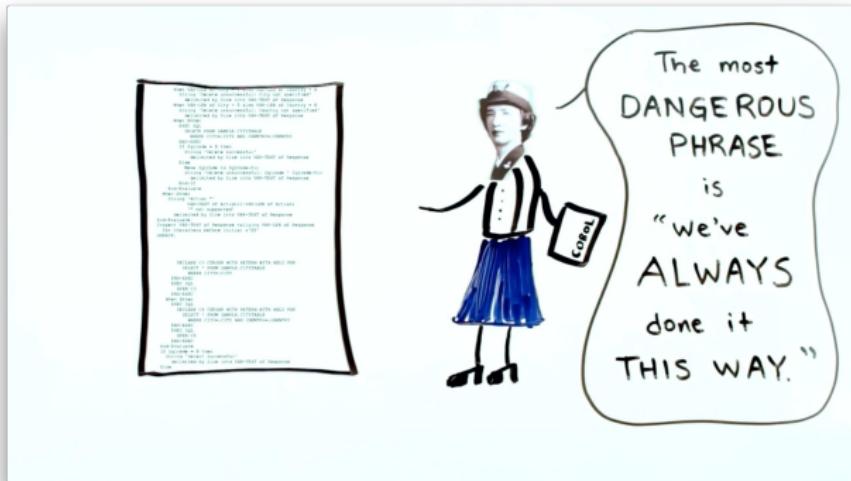
Ada Augusta King, Countess of Lovelace 1815 – 1852



Alan Mathison Turing 1912 – 1954



Grace Brewster Murray Hopper 1906 – 1992



Margaret Heafield Hamilton 1936 – present

SHE BECAME
THE HEAD OF THE
APOLLO FLIGHT
SOFTWARE
DEVELOPMENT
TEAM

Credit: NASA



Sci

Computer History Museum

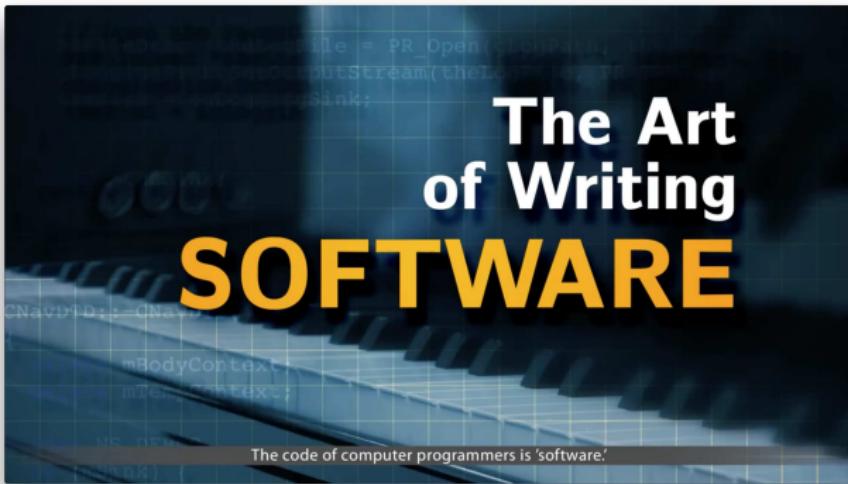


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The Fairchild Notes



The Art of Writing Software

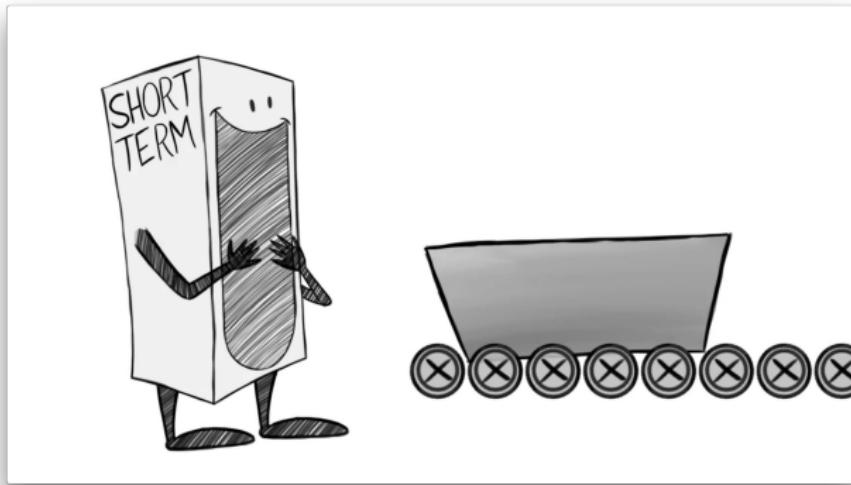


TED Ed

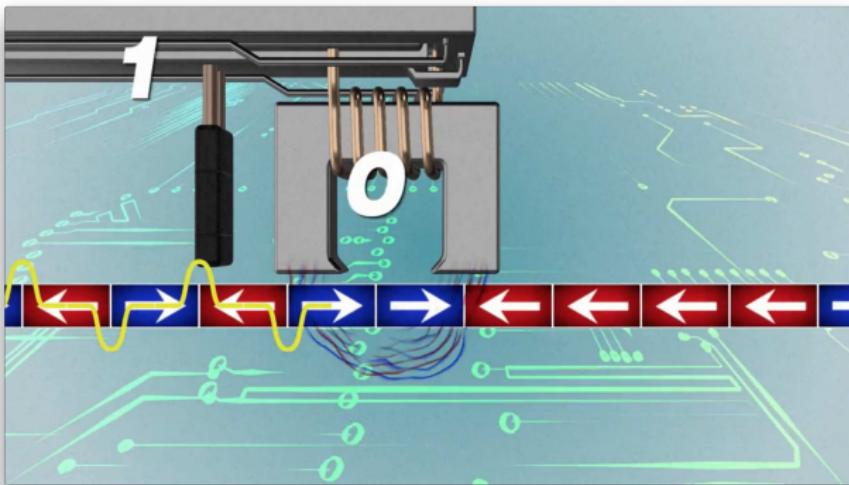
LESSONS WORTH SHARING



Computer Memory



Hard Drives



Turing Test



Algorithm

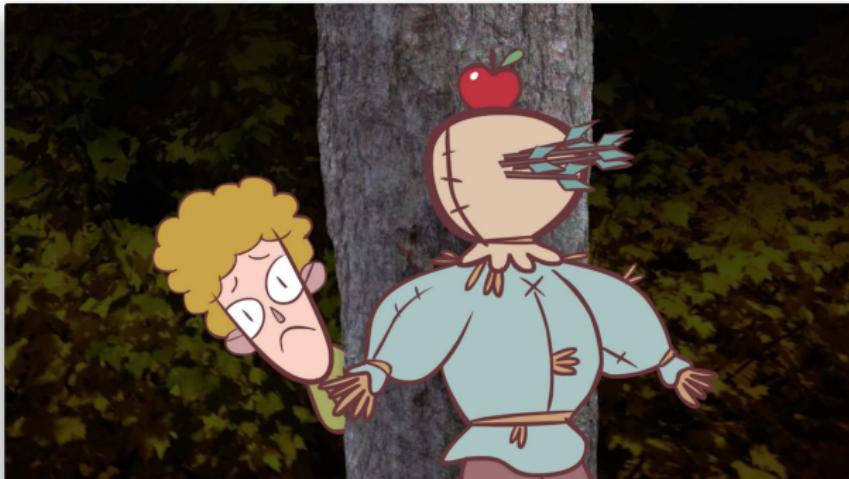
Pseudocode

let **N** = 0

For each person in room

Set **N** = **N** + 1

Accuracy vs Precision



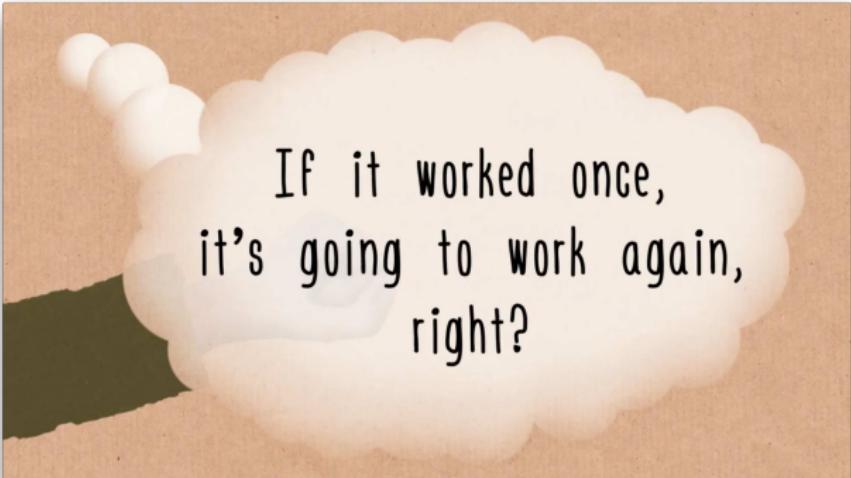
Big Data



Graph Theory

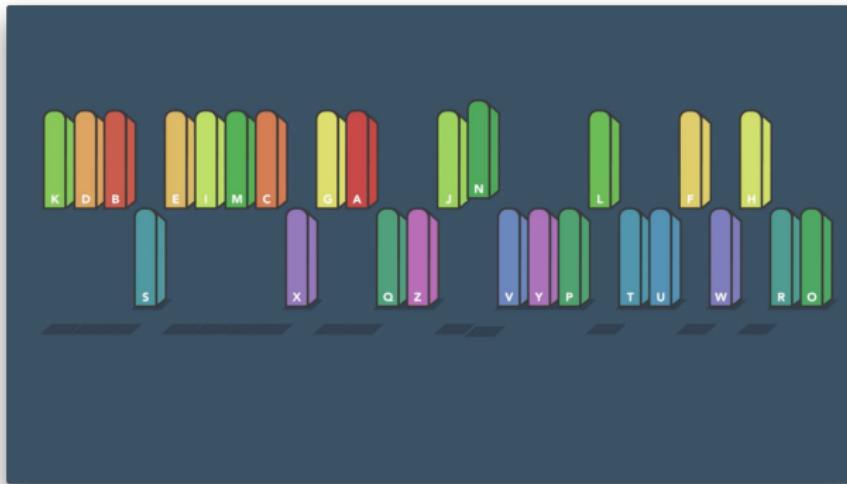


Game Theory



If it worked once,
it's going to work again,
right?

Sorting Books

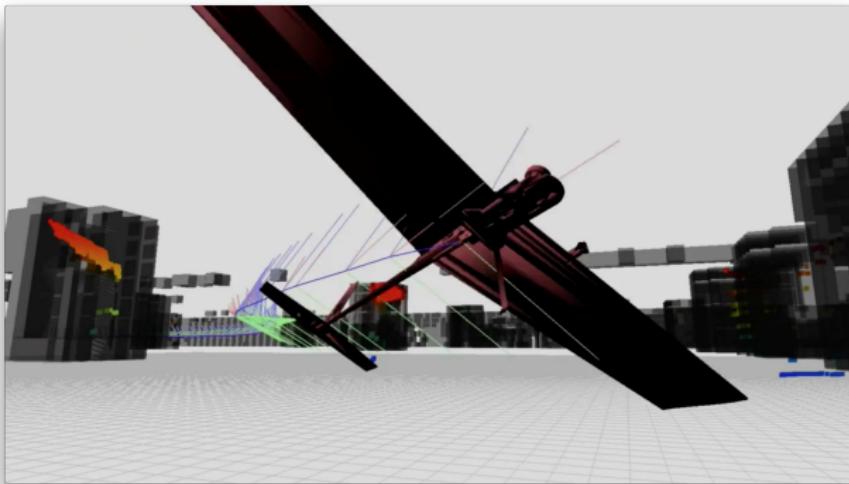




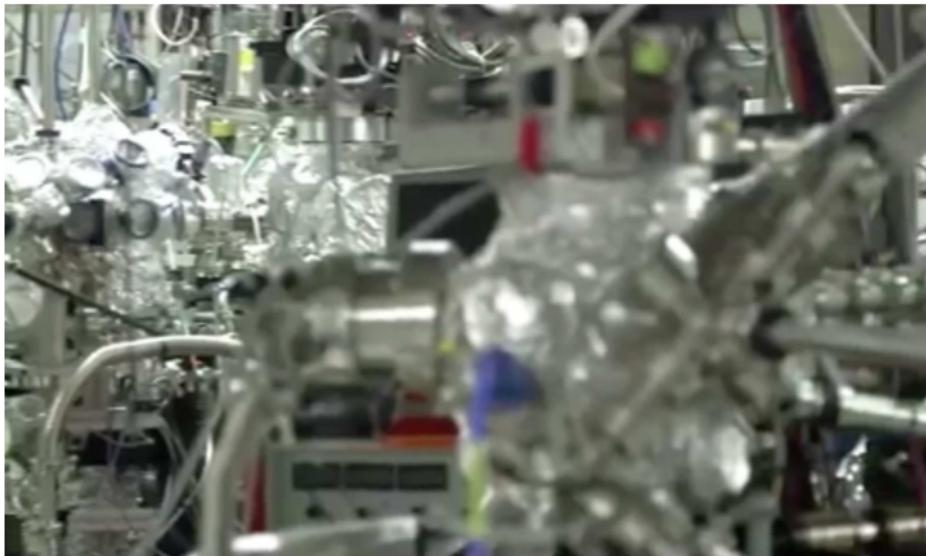
The International Conference for High Performance Computing,
Networking, Storage and Analysis

What is HPC?

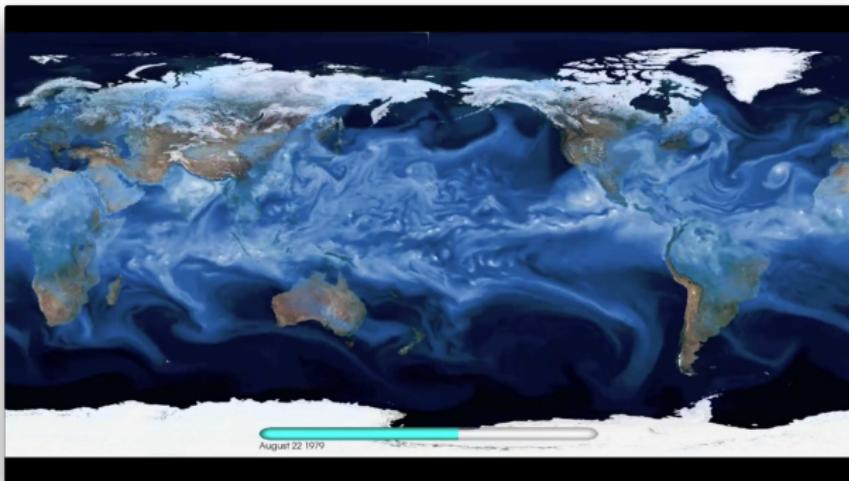
Aerospace



Batteries



Climate Modeling



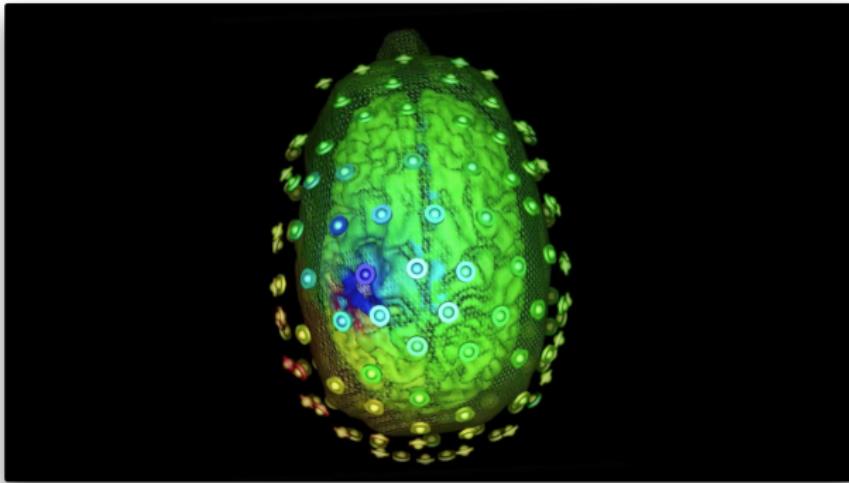
Diapers, Detergents, Shampoo



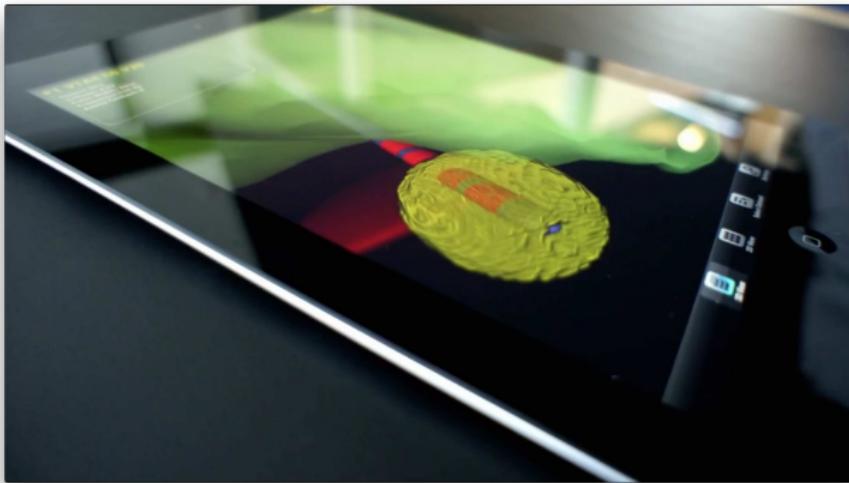
Entertainment



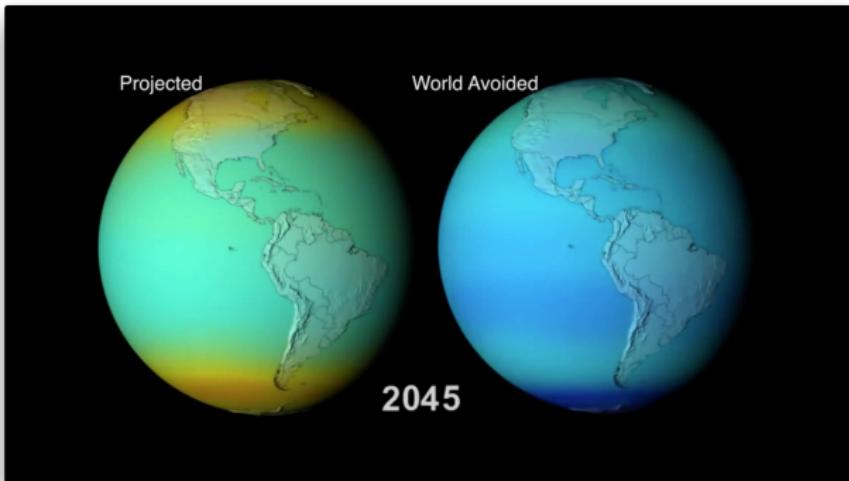
Epilepsy Treatments



Parkinson's Treatments



Human-Induced Climate Change



Missing Plane, MH370

Malaysia Airliner MH370: Water of an Airliner

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

On March 8, 2014, Malaysia Airlines Flight MH370 disappeared from a flight path at least 1 hour after take-off on a flight from Kuala Lumpur to Beijing. The Boeing 777-200ER carried twelve crew members and 227 passengers. The search and rescue team announced that "it is believed that the aircraft crashed" and "it is therefore with deep sadness and regret that I must inform you that there has been a crash in the Southern Indian Ocean." Though the exact fate of the aircraft is still unknown, the available evidence indicates a crash into the ocean. However, theorizing as this is, no all-emergency survival procedures were followed as the crew are compelled, end in tragedy. In the "Wreck on the Southern Ocean," Gowtham Chen, Cong Gu, Philip J. Morris, Yi-Ching Wang, and Tomasz Wierzbicki, the "Sudsy" indispensable and his crew successfully ditched US Airways Flight 1549, an Airbus A320-232, into the Hudson River in New York City after a bird strike on take-off from LaGuardia Airport. These two cases are similar.

Figure 12 and the video animation referenced on the second page of this article show our "trip reconstruction" of a crash into the Southern Indian Ocean. (TOMS) and Texas A&M University at Qatar (TAUQ) are also a member of the Institute for Space Science Research (ISSR) and TAUQ is a member of ISSR's graduate committee. TAUQ, aka,

Cong Gu is currently a Ph.D. candidate in the mathematics department of TAUQ. His email address is cgu@qf.edu.qa.
Philip J. Morris is a Boeing 737 Walkin Professor of Aerospace Engineering and Mechanics from University. His email address is pjm@tamu.edu.

(a) nose dive water entry

(b) pressure distribution and mesh

Time: 0.500

5e+05
4e+05
3e+05
2e+05
1e+05
1e+04

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.

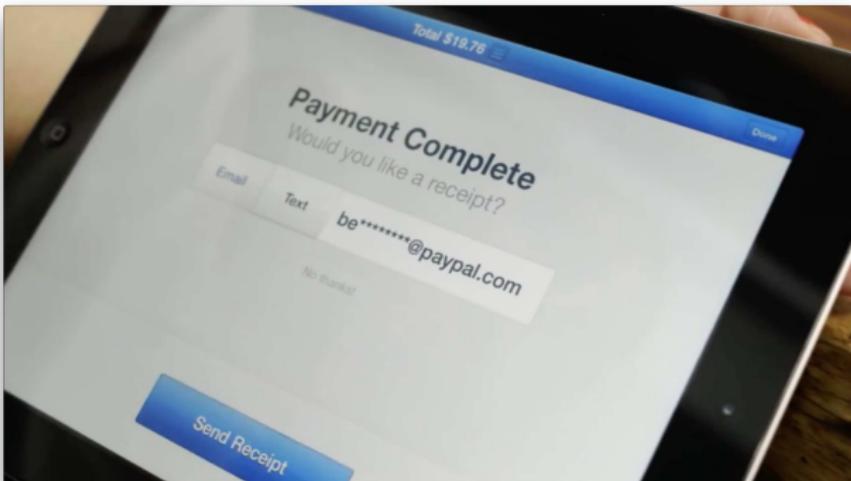
failure modes occur at low impact velocities, as has been demonstrated with a real model of a retired aircraft in DYCAST (Dynamic Crash Analysis of Structures) by NASA [FW86]. These findings were published nearly three decades ago but remain valid today.

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UN5390: Scientific Computing I · Week # 14 · Slide # 282

1889

PayPal



Storm Prediction



Precision Medicine



Preview of SC11



Preview of SC12



Preview of SC13



SCinet is a high-performance network that is built, once a year, in support of the annual International Conference for High Performance Computing, Networking, Storage and Analysis (SC). It is the primary network for the conference and is used by attendees to demonstrate and test high-performance distributed applications. Originated in 1991 as an initiative within the SC center.

Preview of SC14



Preview of SC15

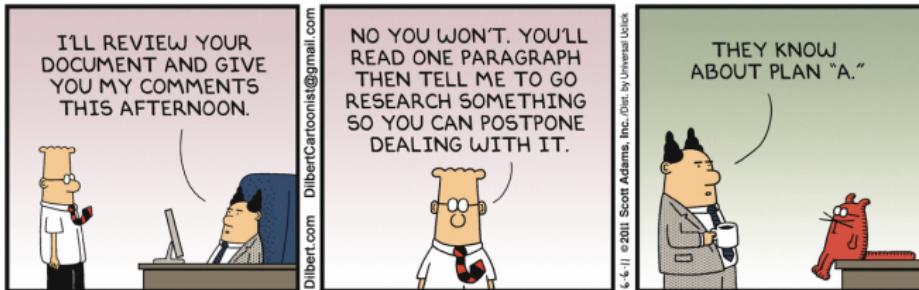


Preview of SC17

we cry. we rejoice. we reflect.

Review of Performance

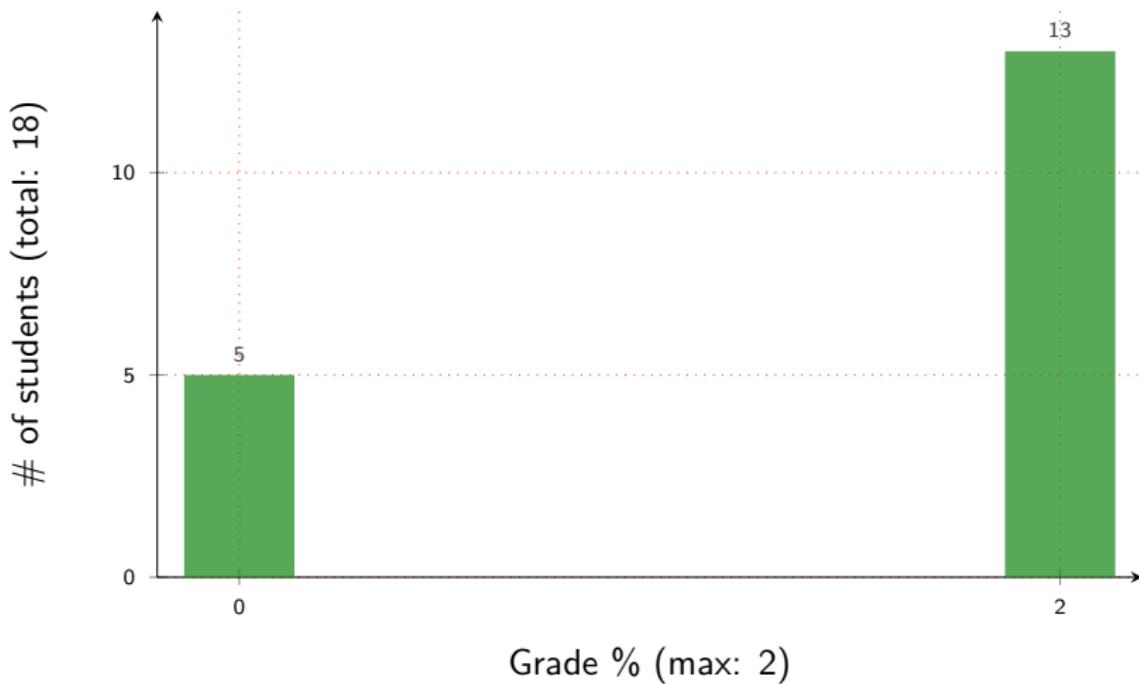
How well have we been performing?



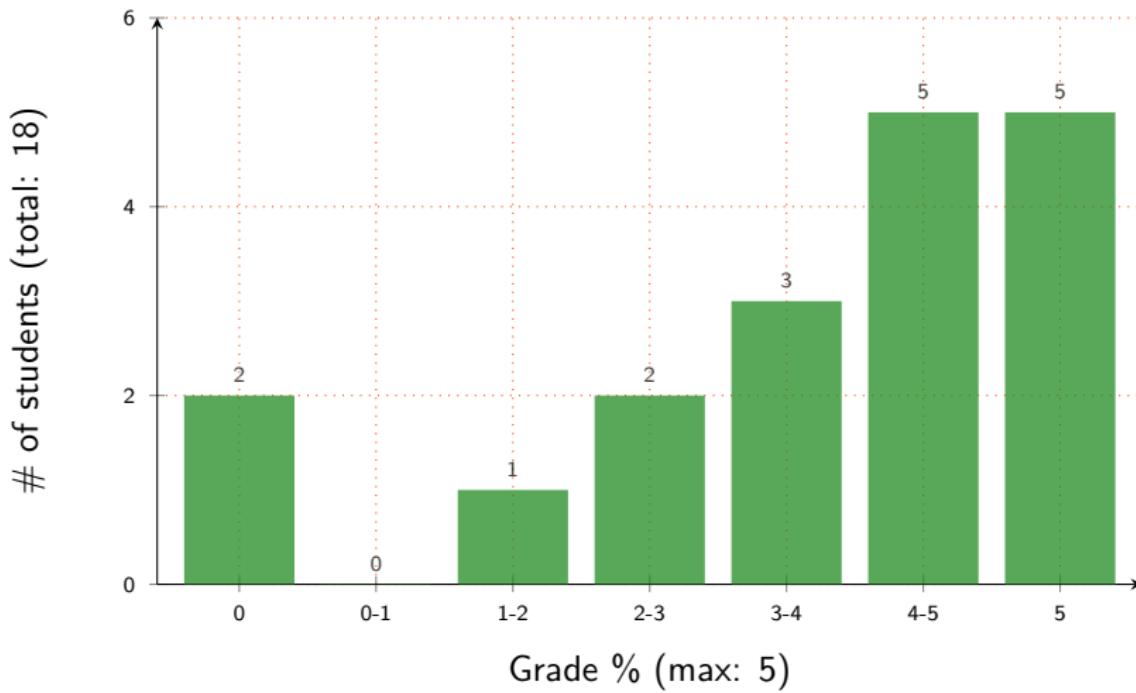
<http://dilbert.com/strip/2011-06-06/>

Active Participation #01

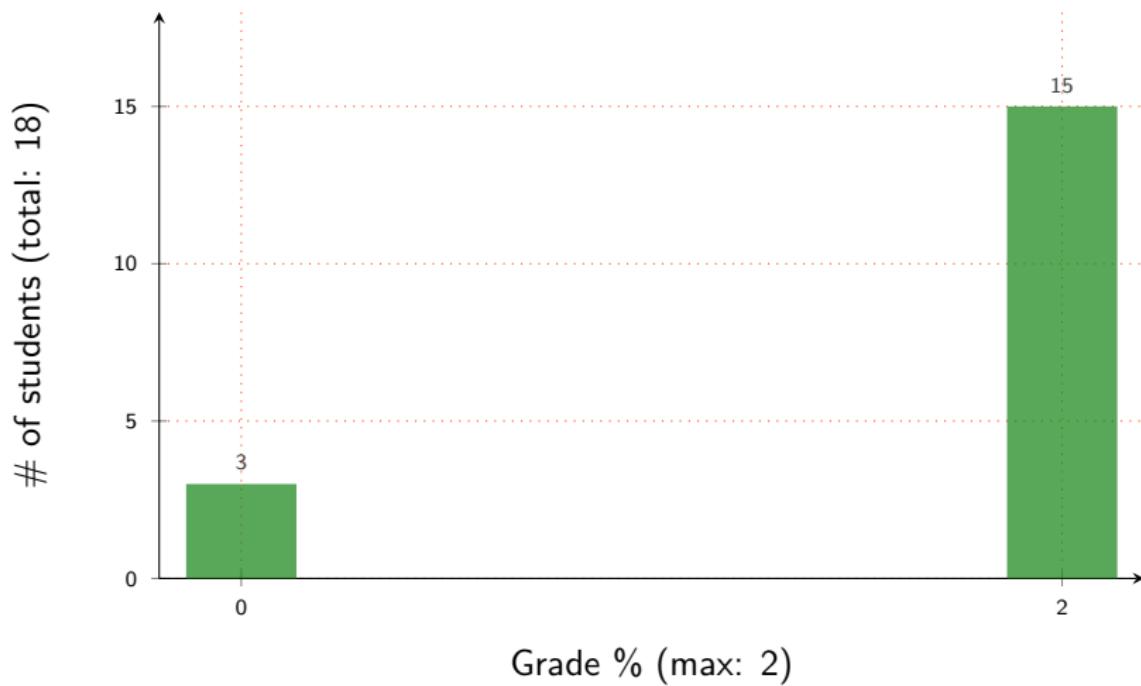
Research Marketing I: Twitter



Assignment #01

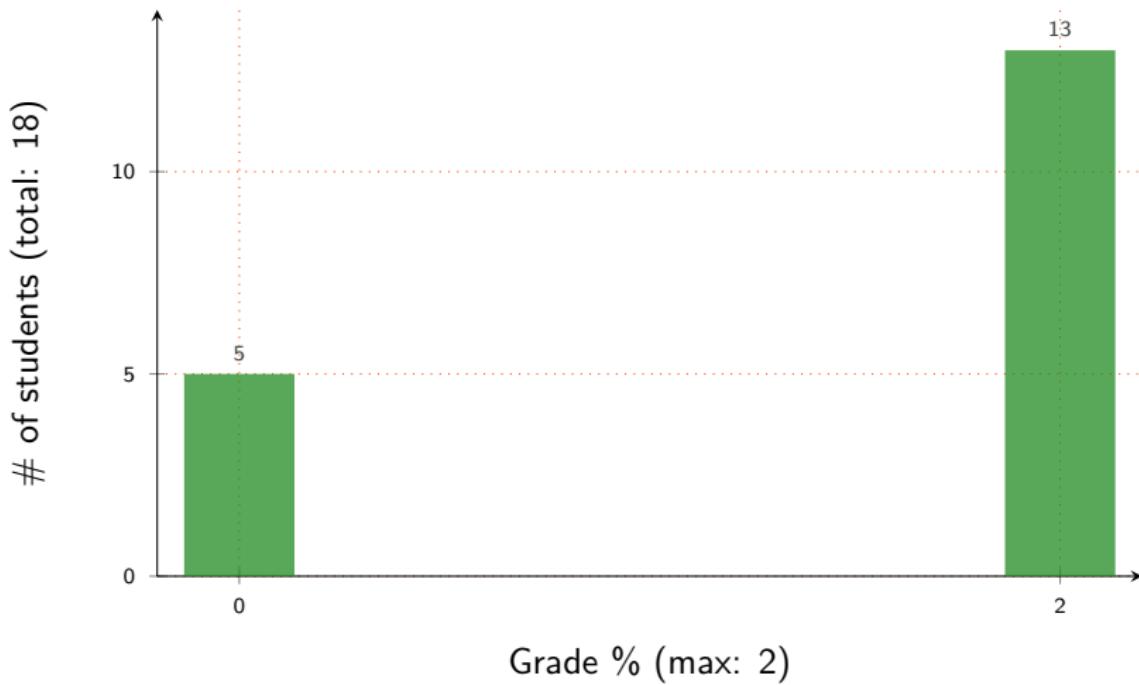


Active Participation #02 PB&J Sandwich Recipe

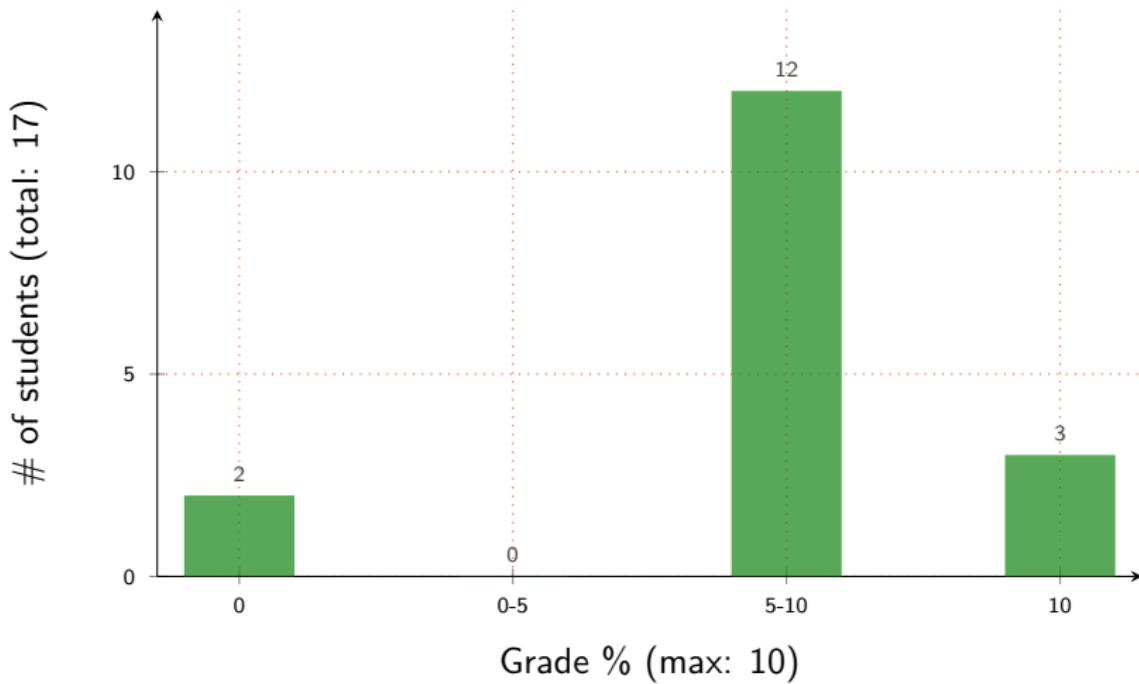


Active Participation #03

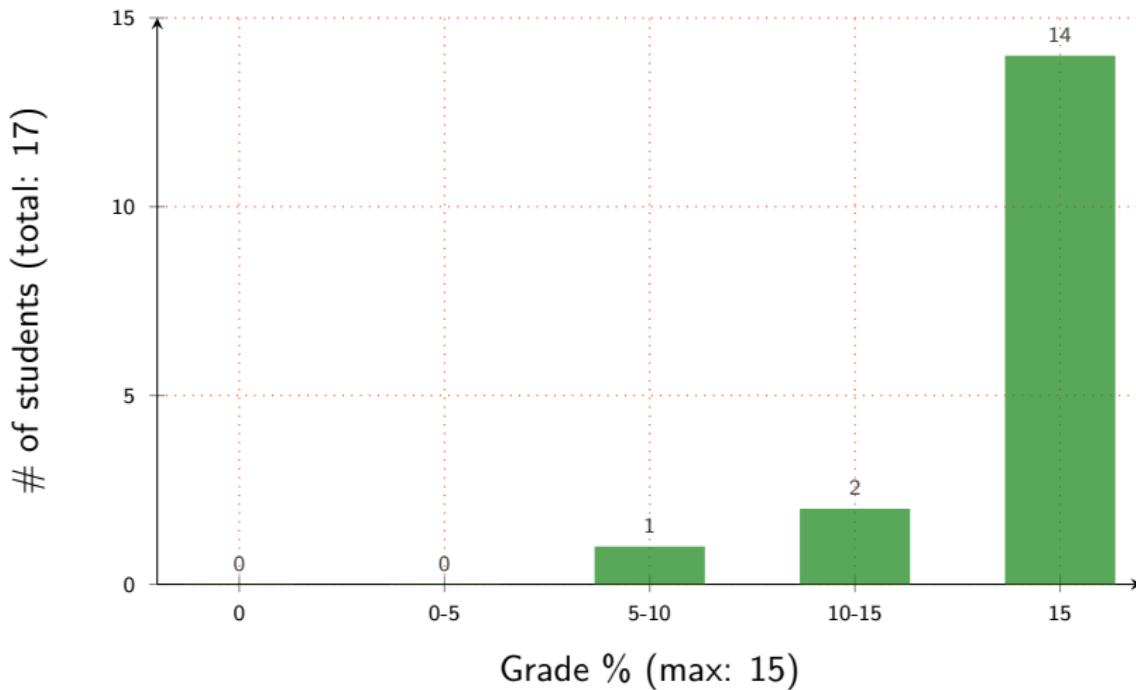
Research Marketing II: Professional/University Business Cards



Assignment #04

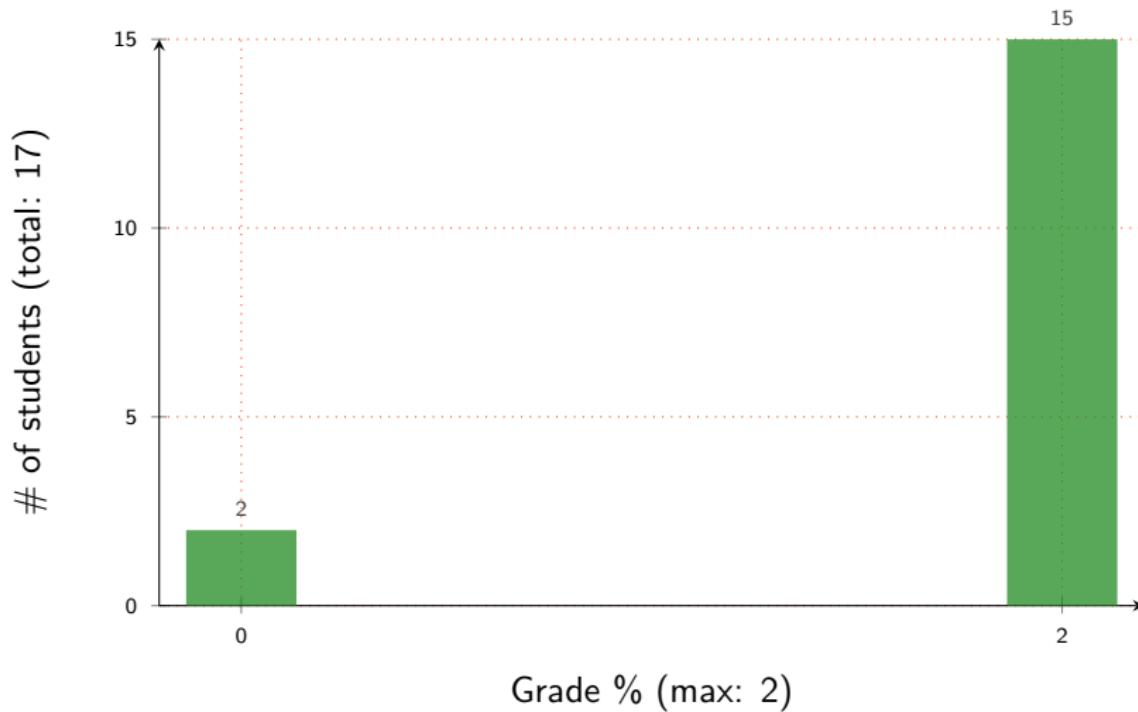


Assignment #07

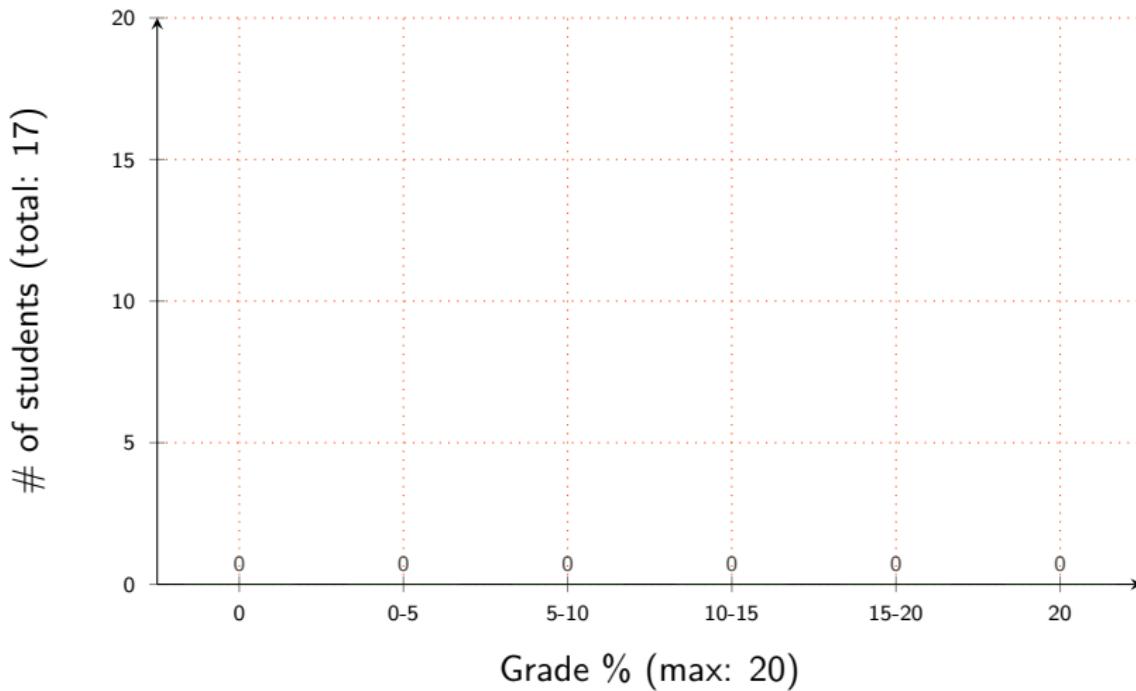


Active Participation #04

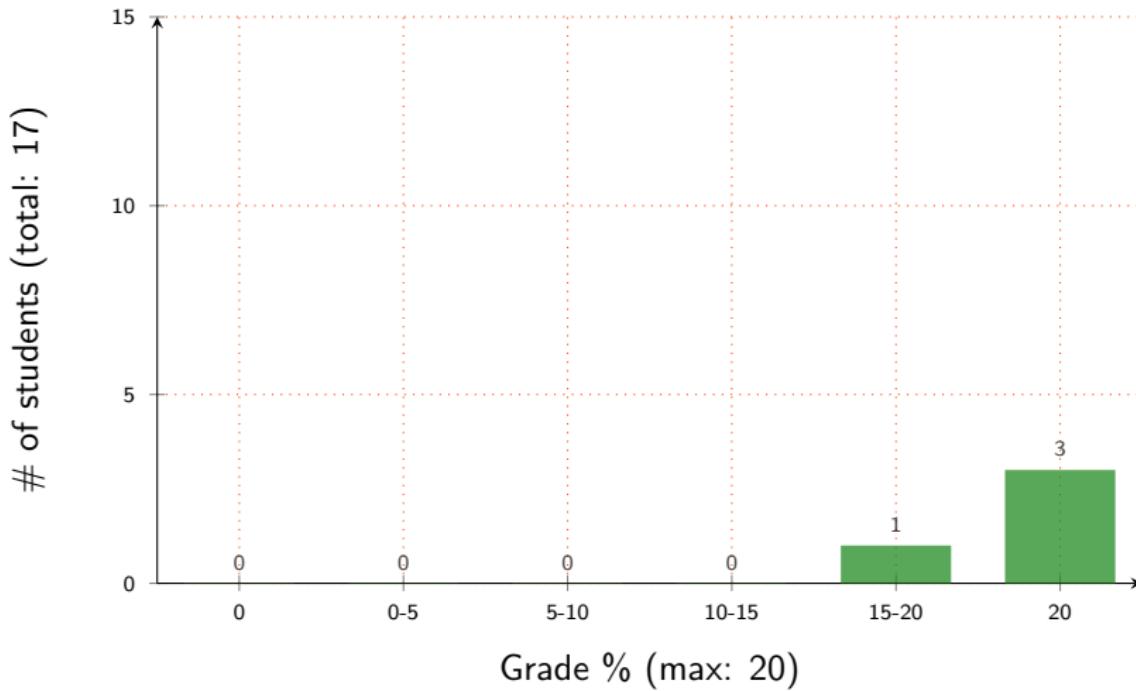
Research Marketing III: Elevator Pitch



Assignment #12

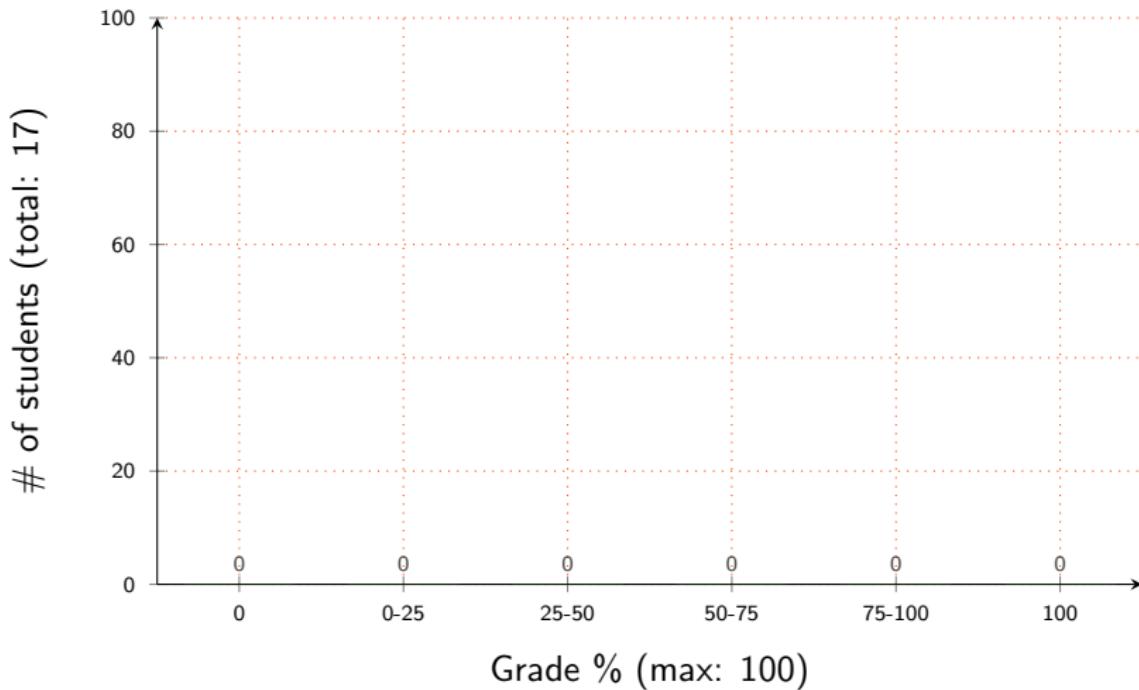


Term Project



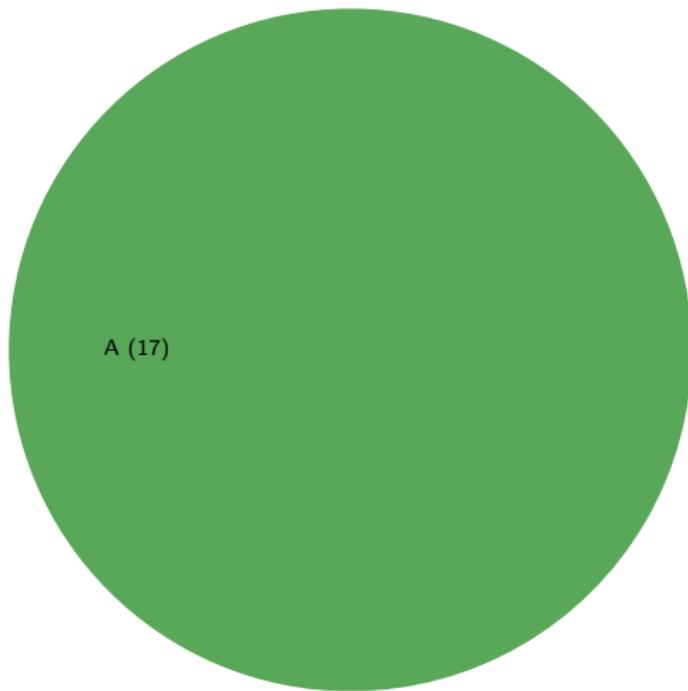
Overall Performance

Score distribution



Overall Performance

Letter grade distribution



17 registered students.



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,

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

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?

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

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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