

UN5390: Scientific Computing I

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Week #11: 2016/11/08 and 2016/11/10

Cross-listed as BE5390, EE5390 and MA5390

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



Recap

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



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

Week #10 Recap

- * Differential equations
 - * Runge-Kutta methods
- * Matrix methods
 - * LU factorization
 - * Message encryption
 - * Graph theory
 - * Game theory

Week #10 Before we meet again

- * Review the syllabus, course material, grade through week #10, notations, active participation, free time exercises, tips, opportunities, mathematical results, and videos
- * Make progress in assignment #07
- * Discuss the project with the instructor*
- * Make progress in the term project
- * Turn in the project description and status report by Friday 4:59 pm
- * Think parallel, and come prepared to move around the class

* MS course work students.



Parallel computing

An attempt to do (more) work in less time using more processors



<http://dilbert.com/strip/2012-07-31/>

Review

John von Neumann architecture

A description of a design architecture for an electronic digital computer with parts consisting of a processing unit containing an arithmetic logic unit and processor registers, a control unit containing an instruction register and program counter, a memory to store both data and instructions, external mass storage, and input and output mechanisms.

Flynn's taxonomy

A classification of computer architectures that has been used as a tool in design of modern processors and their functionality.

Moore's law (in theory and practice)

The observation/self-fulfilling prophecy that the computing power on a chip doubles approximately every two years.

Review

Performance of a computing infrastructure (FLOPS)

For a computer with one processor,

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

For a computer with N identical/homogeneous processors,

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

Top 500

The list of world's fastest 500 supercomputers, released in June and November each year, based on Linpack benchmark results.

Review

Errors

Journal of Failed Experiments, debuggers and profilers.

Introduction, The Innovators

The Innovators: How A Group Of Hackers, Geniuses, and Geeks
Created The Digital Revolution

W. Isaacson; Simon & Schuster (2014)

Introduction to this book, *How This Book Came To Be*, is available for reading as part of the limited preview from [Google Books](#) (click on the front cover image and scroll down).

W. Isaacson has also authored *American Sketches*, and biographies of Albert Einstein, Benjamin Franklin, Henry Kissinger and Steve Jobs.



Terms to know

Process

Each process has its own complete and private set of run time resources (e.g., memory space, file descriptors, etc.) and provides a self-contained execution environment. Each process has at least one thread.

Thread

Threads exist within a process and provide an execution environment but share the parent process's resources (e.g., memory space, file descriptors, etc.). This often makes for efficient but potentially problematic communication.

A thread is often called a lightweight process (LWP), and creating a new thread requires fewer resources than creating a new process.

Process/Thread is an independent sequence of execution. Inter-Process Communication (IPC) resources facilitate communication between processes – in the same and/or different physical systems (e.g., pipes, sockets, etc.).



Terms to know

Hot spots

Portions of the code where bulk of the work is done. Profilers can help in identifying where the program is spending its time.

Bottlenecks

Portions of the code that cause slowing down or worse, stoppage. I/O operations are a common culprit and can be overcome by a suitable change in algorithm/approach (e.g., vendor-specific compilers).

Terms to know

Latency

Time taken to send a minimal message from point *A* to point *B* (μs).

1 Gb ethernet $50\text{-}125 \mu s$

10 Gb ethernet $5\text{-}50 \mu s$

56 Gb InfiniBand $0.70 \mu s$

Bandwidth

Amount of data that can be communicated per unit time (Gbps).

Communication etiquette

Sending many small messages often causes latency domination.

Combining a suitable number of smaller messages into one larger message increases effective communication bandwidth.

Terms to know

Concurrency

An application makes progress on more than one task at the same time.

In case of a single CPU, the application may not make progress on more than one task at exactly the same time, but more than one task could be processed at a time inside the application – by not completely finishing one task before it begins the next (i.e., time slicing).

Parallelism

An application splits its tasks into smaller sub-tasks which can be processed in parallel at the exact same time.

Terms to know

Fine-grained parallelism

Sub-tasks must/will communicate frequently with each other (e.g., numerous times per second) to stay synchronized.

Coarse-grained parallelism

Sub-tasks must/will communicate less frequently with each other than fine-grained case to stay synchronized.

Embarrassing (or pleasant or perfect) parallelism

Sub-tasks rarely (sometimes, never) communicate with each other to stay synchronized.

Terms to know

Communication overhead

Resources that can be used for computation are used instead to package and transmit data between processors (tasks). Synchronization between processors can often result in some of them waiting rather than doing work. Competing traffic can saturate network bandwidth and degrade performance.

Scalability

Based on time to solution,

1. Weak scaling —> problem size per processor stays fixed as number of processors is increased
2. Strong scaling —> total problem size stays fixed as number of processors is increased



Terms to know

High-Performance Computing

Simulations in this realm are tightly coupled, and require compute nodes connected with high-speed, low latency networks. Such simulations require large amounts of computing power for short periods of time (~ hours or days).

High-Throughput Computing

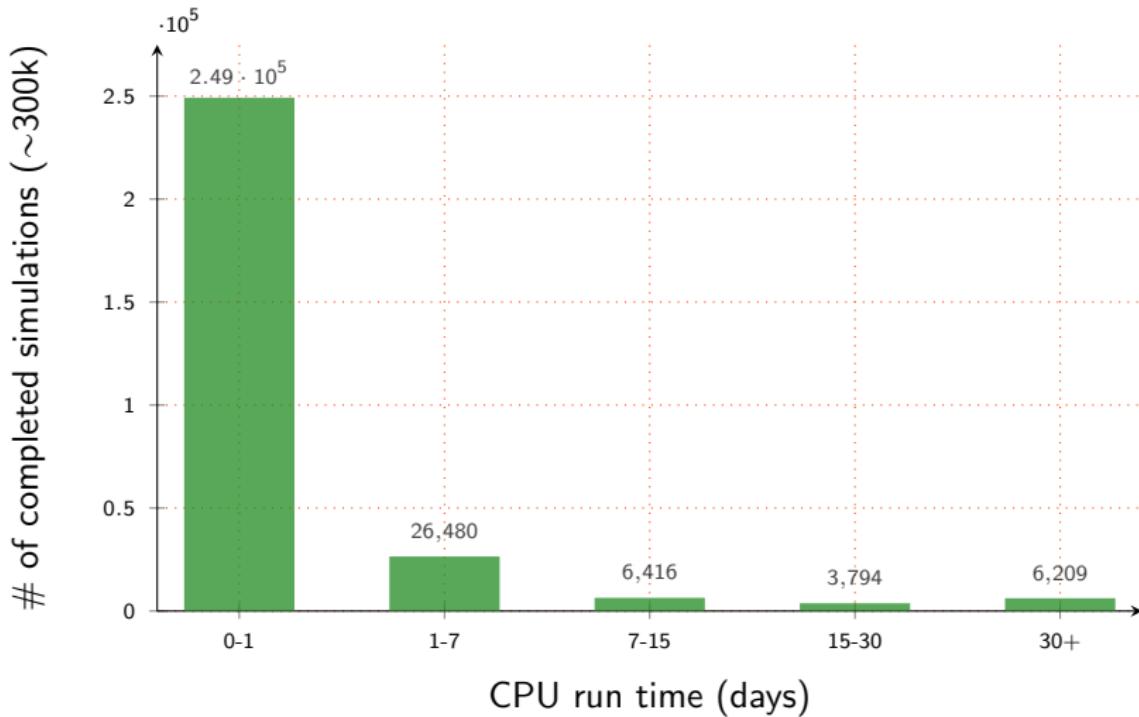
Simulations in this realm require far less communication and synchronization between compute nodes. Loosely coupled parallel programs, often described as *embarrassingly parallel* or *pleasantly parallel*, are a good fit. Such simulations require large amounts of computing power for longer periods of time (~ weeks or months).

At Michigan Tech, HPC and HTC are used interchangeably (and often, former includes the latter).



Michigan Tech HPC

Superior, 2013-06-09 – 2016-11-04



<http://superior.research.mtu.edu/analytics/>

Parallel computing

The need

The need for size and speed

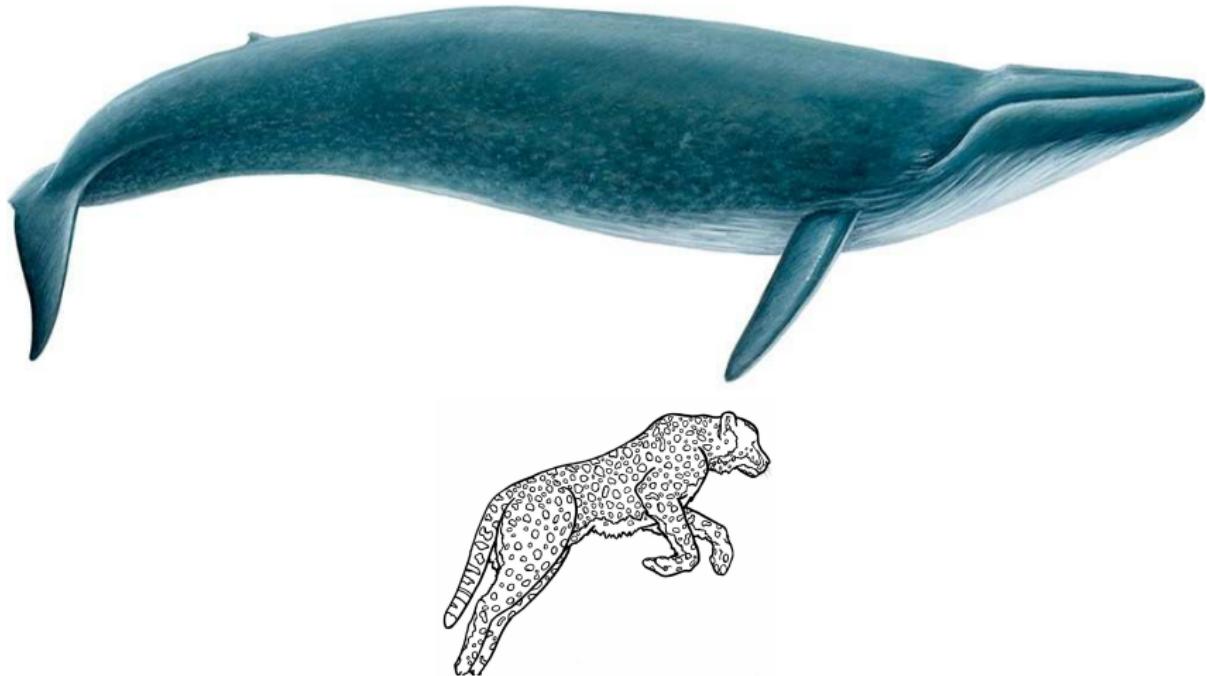
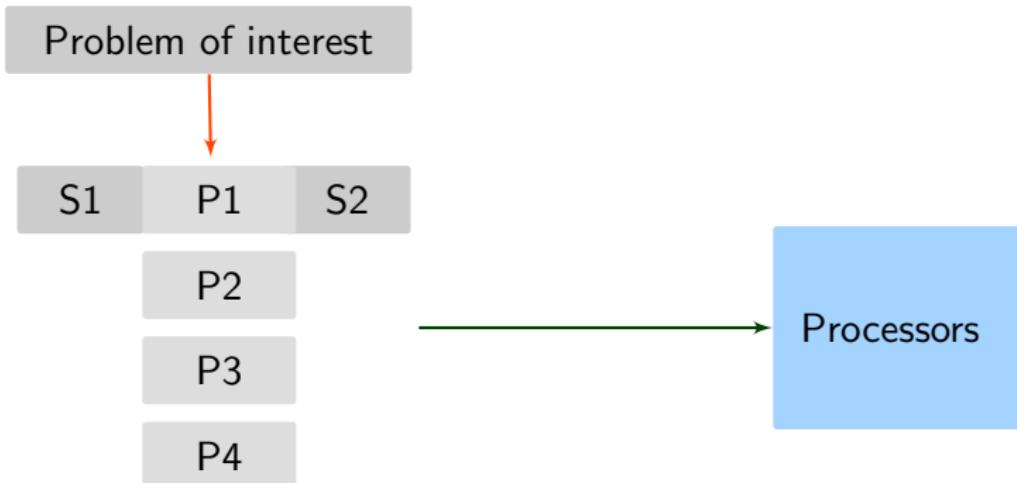


Image courtesy: Google images

The need

- * Task
 - * takes too long to run on a single processor
 - * has parallelizable portions (data and/or tasks)



Parallel computing

Design and development

Design and development

- * Parallel
 - * thinking is not very easy
 - * programming is often complex, time consuming, iterative and error-prone
- * Programmer is responsible for identifying and implementing parallelism

Reflection of our communal/societal logic

Multi-tasking is achieved via time slicing and works pretty well for serial computing. Our inherent intention and ability to work with others to solve complex problems that otherwise can take considerably very long time to do so individually (if at all can be done) is the genesis of parallel computing/programming.



Design and development

The Manhattan Project at Los Alamos National Lab (1940s)

Computations to figure out positioning explosive charges in a cavity to generate a spherical compression wave to start a chain reaction were fairly complex that they had to be done numerically. The IBM Team's computations (using decks of cards, adding machines, sorters, etc.) were very time consuming, and Feynman was put in charge.

Feynman's solution was to assign each problem to a different colored deck of cards, so that the team could work on more than one problem at once. While one deck was using one of the machines for one stage of the computation, another deck could be using a different machine for a different stage (i.e., pipeline parallelism).



Richard Phillips Feynman (1911 – 1988): American theoretical physicist, and 1965 Physics Nobel Laureate

Design and development



The Human Computers, Jet Propulsion Laboratory (1953)

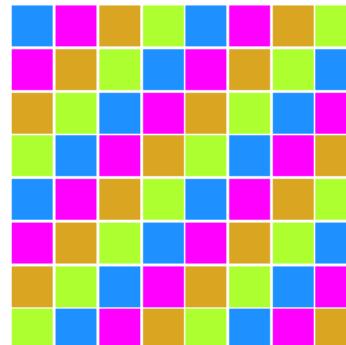
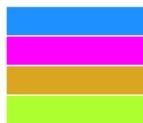
Image courtesy: [National Public Radio](#)

Design and development

- * Fully automatic parallelization
 - * Compiler analyzes the code and identifies parallelism opportunities
 - * Loops (e.g., `for`) are frequent targets
- * Programmer directed parallelization
 - * Programmer directs the compiler, via flags, to parallelize the code
 - * Can be used in conjunction with fully automatic parallelization
- * Decomposition (or parallelization)
 - * Domain (or data)
 - * Functional (or tasks)

Design and development

Domain (data) decomposition



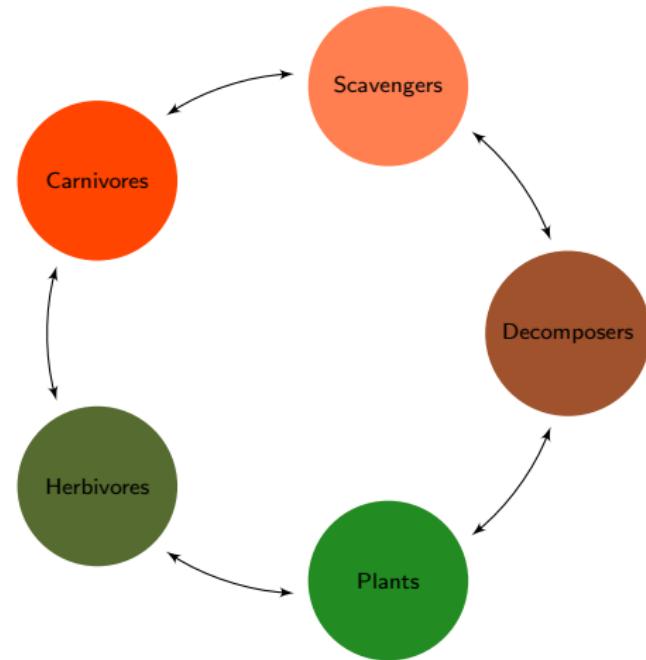
1D: block; cyclic

2D: block,*; *,block; block,block

2D: cyclic,*; *,cyclic; cyclic,cyclic

Design and development

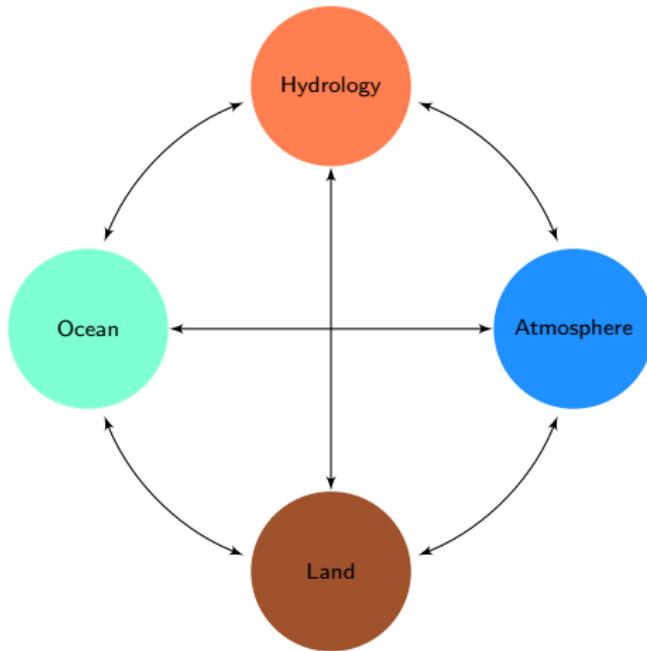
Functional (task) decomposition



Ecosystem modeling: name of the species indicates the model (i.e., task), and arrows indicate data exchange/dependence (extension of predator-prey system).

Design and development

Functional (task) decomposition



Climate modeling: name of the model indicates the task, and arrows indicate data exchange/dependence.

Flynn's taxonomy

Instruction

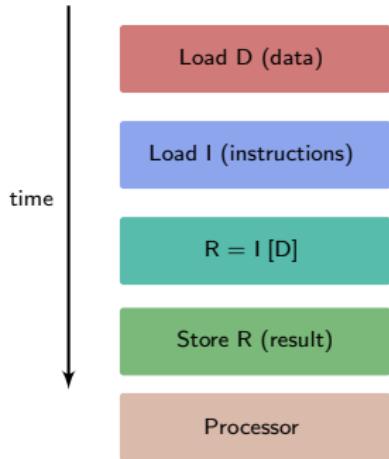
| | | Single | Multiple |
|------|----------|-----------------|-----------------|
| | | SISD (Serial) | MISD (Parallel) |
| Data | Single | SISD (Serial) | MISD (Parallel) |
| | Multiple | SIMD (Parallel) | MIMD (Parallel) |



Michael Flynn (1934 – present): American computer scientist; Professor, Stanford University

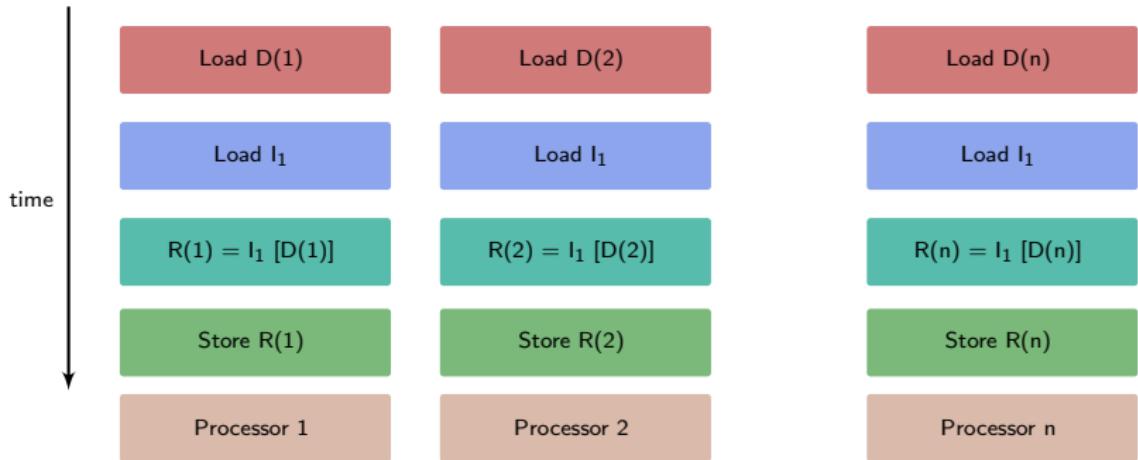
Single instruction, single data (SISD)

- * A problem is split into discrete sequence of instructions
- * Instructions are executed in the given sequence one at a time



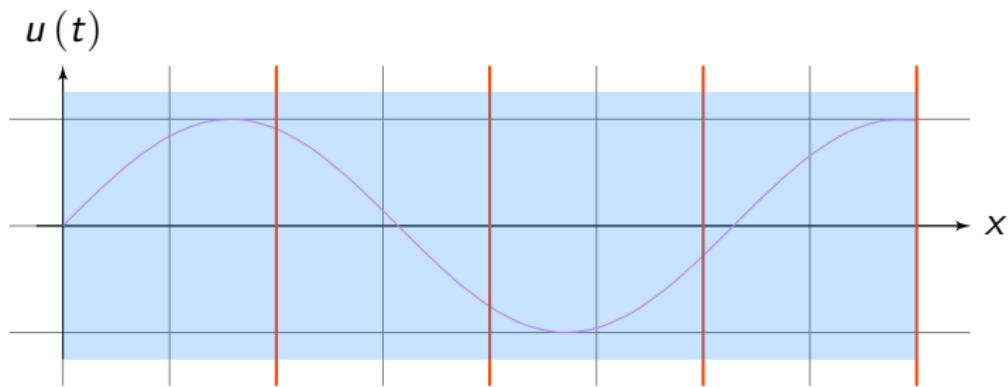
Single instruction, multiple data (SIMD)

- * All processing units execute the same instruction in a given cycle
- * Each processing unit operates on different data



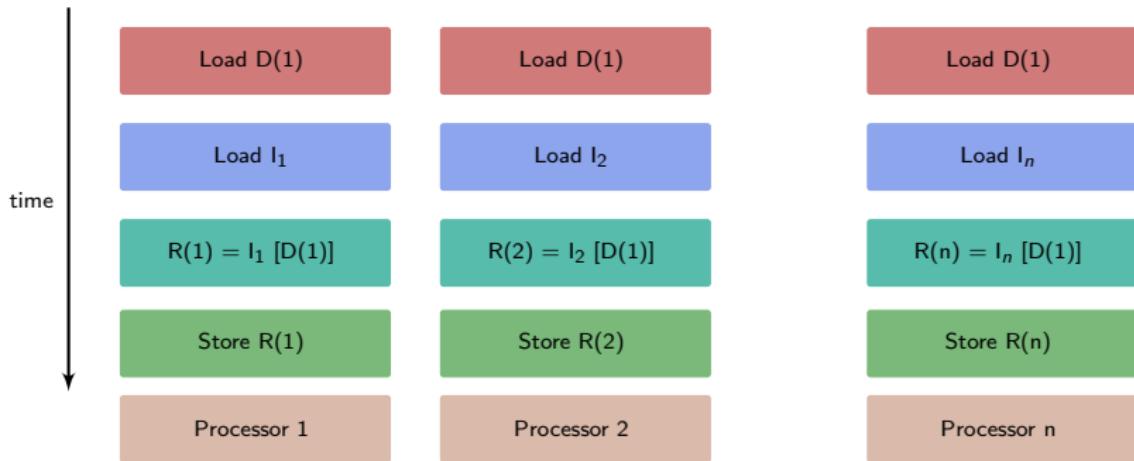
Single instruction, multiple data (SIMD)

- * Wave form represents the data
- * Solid, thick vertical lines represents data fragmentation
- * Translucent rectangles represent instruction



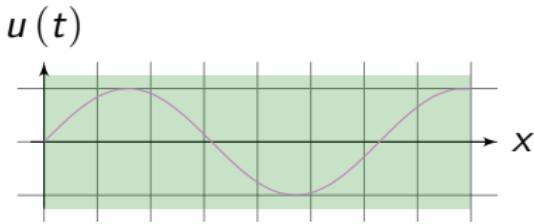
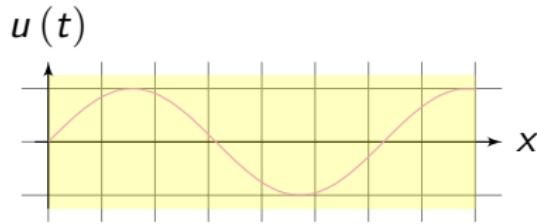
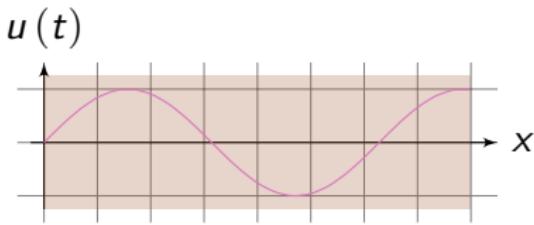
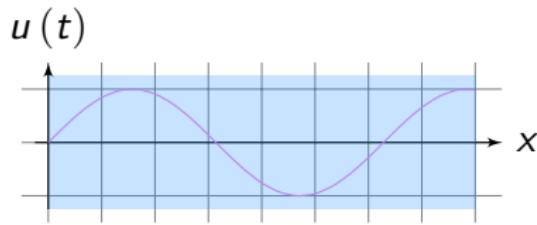
Multiple instruction, single data (MISD)

- * Each processing unit executes different instruction in a given cycle
- * All processing units operate on the same data



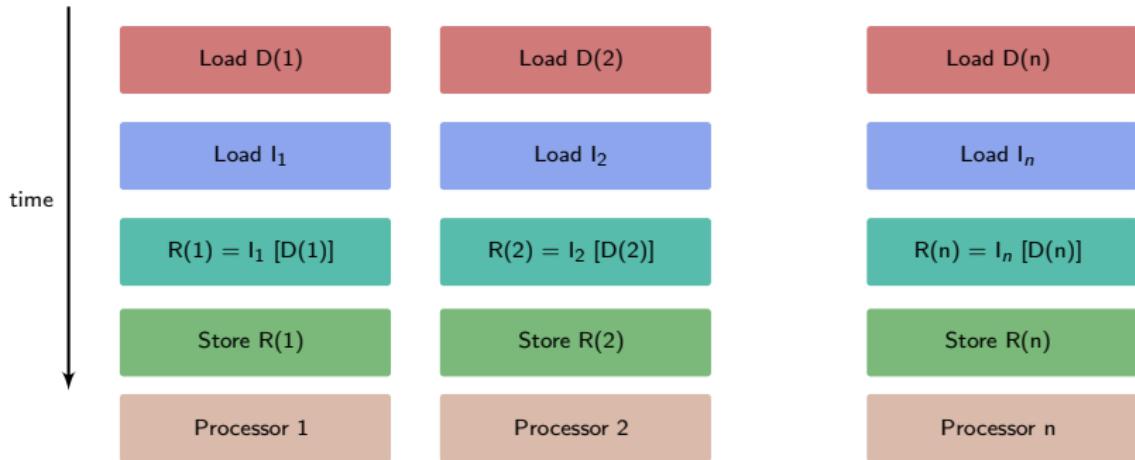
Multiple instruction, single data (MISD)

- * Wave form represents the data
- * Translucent rectangles represent instruction



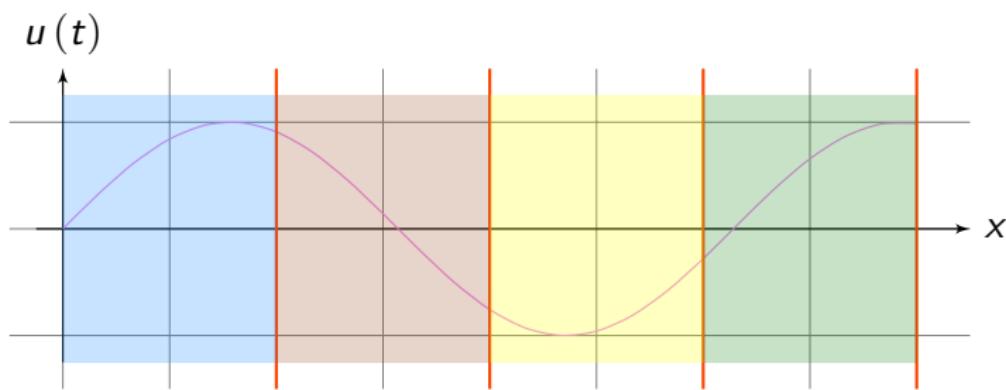
Multiple instruction, multiple data (MIMD)

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Multiple instruction, multiple data (MIMD)

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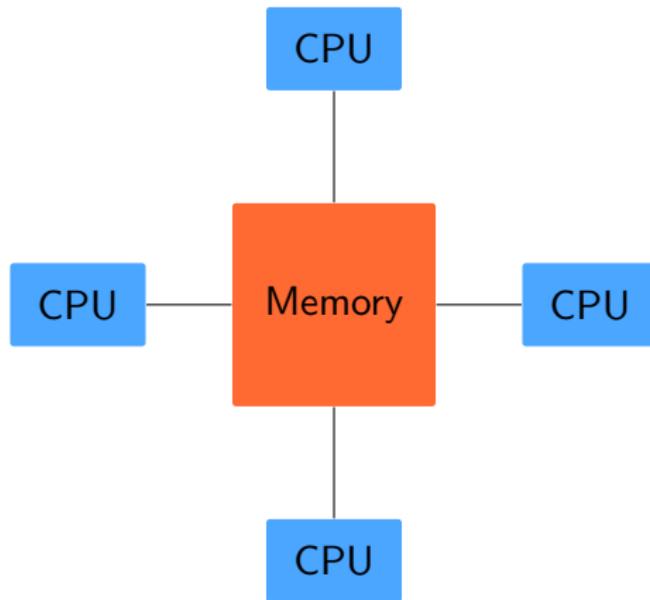


Parallel computing

Memory architecture

Shared memory

- * Uniform Memory Access (UMA)



Shared memory

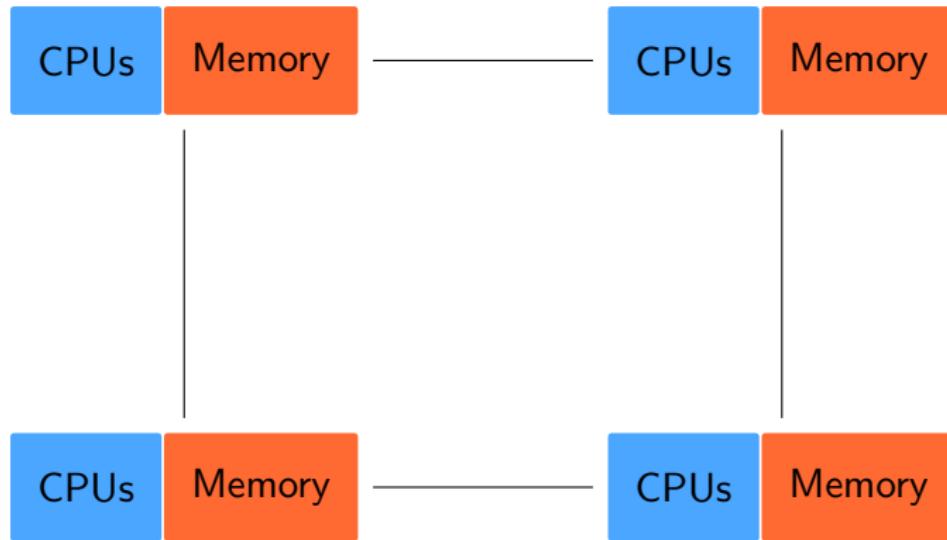
- * Uniform Memory Access (UMA)
 - * CPUs are identical
 - * Equal access and access times to memory (global address space)
 - * Represented by Symmetric Multiprocessor (SMP) machines

Cache coherence

If one CPU updates memory location, then all other CPUs know about it (accomplished at the hardware level).

Shared memory

- * Non-Uniform Memory Access (NUMA)



Shared memory

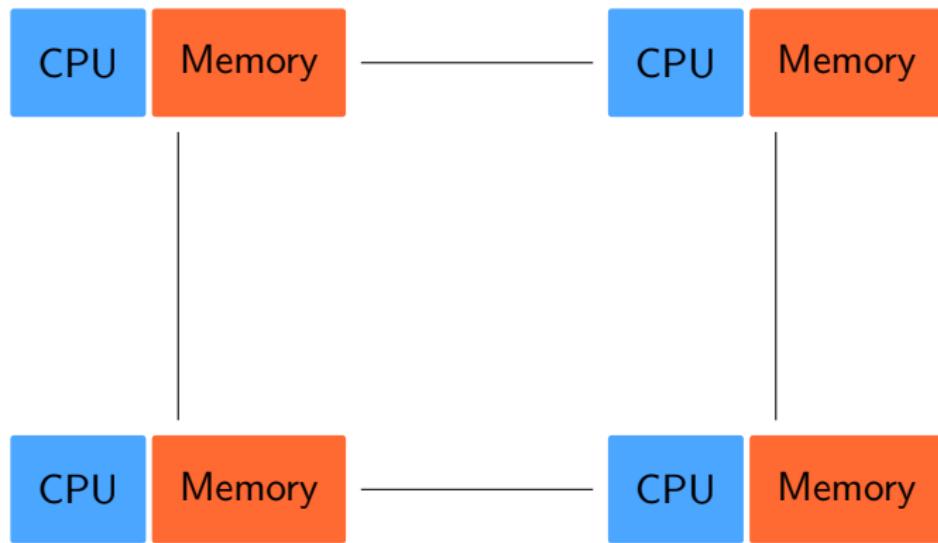
- * Non-Uniform Memory Access (NUMA)
 - * CPUs may be identical
 - * CPU in one SMP can directly access memory in other SMP
 - * Not all CPUs have equal access and access times to all memory
 - * Cache coherence can be achieved
 - * Represented by physical linking of multiple SMPs

Shared memory

Pros and cons

- * Friendly programming perspective
- * Data sharing between tasks can be fast and uniform
- * Adding more CPUs leads to a geometrical increase in traffic
- * Programmer is responsible for task synchronization to ensure appropriate access to memory

Distributed memory



Distributed memory

- * CPUs may be identical
- * Each CPU has its own memory (local address space)
- * Changes to memory by one CPU does not affect that of others
- * A network (e.g., ethernet, InfiniBand, etc.) is necessary for data transfer

Distributed memory

Pros and cons

- * Faster access to local address space
- * Memory scales with an increase in the number of CPUs
- * Longer times to access to data in a non-local address space
- * Programmer is responsible for task and data synchronization

Parallel computing

Costs

Costs

- * Acquiring (access to) suitable computing infrastructure
 - * Powerful CPUs, sufficient RAM, and reliable network system
 - * Fast and reliable scratch space; slow but reliable storage space
 - * Secure data center with reliable racks, power, and cooling
- * Hiring and retaining (well-trained) personnel to manage the infrastructure and port the code, if necessary

Hardware-Software compatibility

The (nearly) state of the art infrastructure helps exploit the features of compilers, libraries and software suites (and vice versa).

Parallel computing

Limitations

Amdahl's Law

Amdahl's Law

Governs and imposes a fundamental limitation on the speed up achieved using parallel processors for a given problem.



Suppose that t_{serial} is the time taken by a serial program and t_{parallel} is the time taken by the same program running in parallel using multiple processors. Observed speed up is

$$S = \frac{t_{\text{serial}}}{t_{\text{parallel}}}$$

Eugene Myron Amdahl (1922 – 2015): American computer scientist/architect and entrepreneur. He was the principal architect of IBM 704 (1955), the first commercial machine with floating-point hardware (~ 5 kFLOPS).

Amdahl's Law

Problem of interest (n total tasks; t time per task)



Serial part ($1 - P$)

Parallel part (P)

In case of serial computing, n tasks can be completed in

$$t_{\text{serial}} = n t$$

Suppose that there are N homogeneous processors and together they can complete a given task in $1/N$ time of just one working alone.

$$t_{\text{parallel}} = (1 - P) n t + \left(\frac{P n}{N} \right) t$$

Amdahl's Law

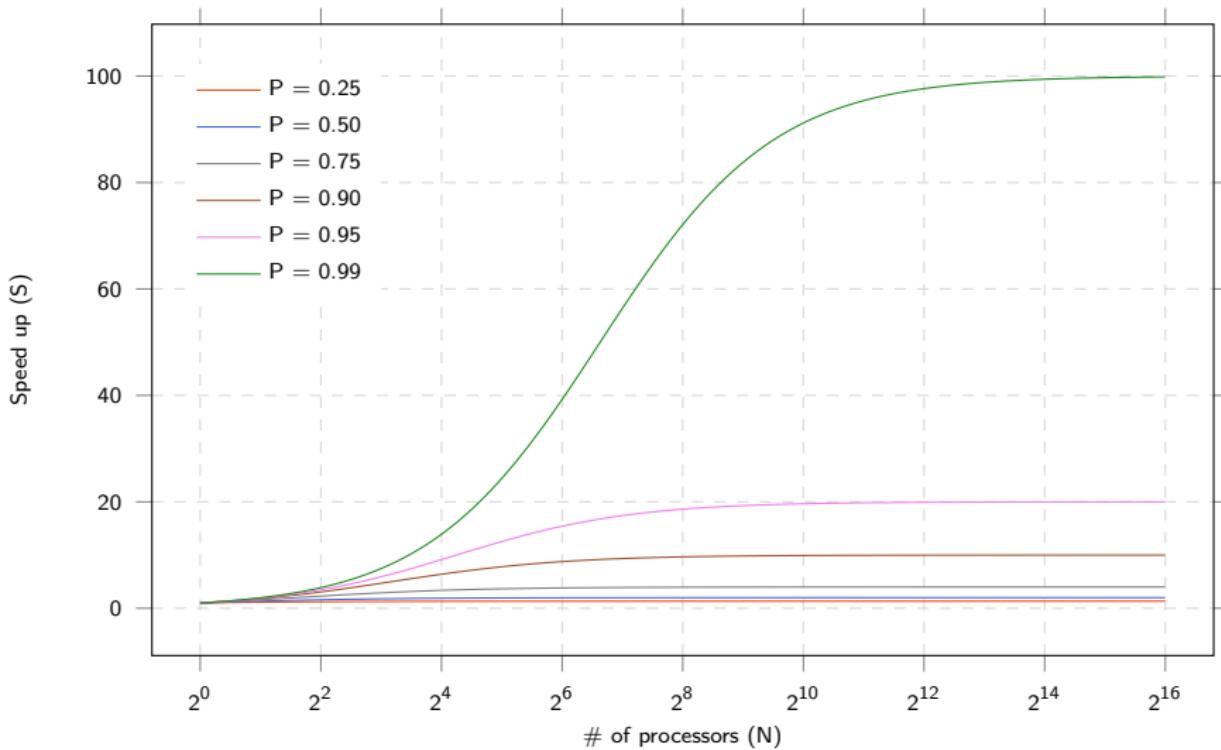
Observed speed up is

$$S = \frac{t_{\text{serial}}}{t_{\text{parallel}}} = \frac{n t}{(1 - P) n t + \left(\frac{P n}{N}\right) t}$$

Simplify

$$S = \frac{1}{(1 - P) + \frac{P}{N}}$$

Amdahl's Law



Gustafson's Law

Gustafson's Law

An observation that researchers scale their problems to match the available computing power, in contrast to Amdahl's assumption that the problem is always the same no matter how capable the computer.



Suppose that t_{serial} is the time taken by a serial program and t_{parallel} is the time taken by the same program running in parallel using multiple processors. Observed speed up is

$$S = \frac{t_{\text{serial}}}{t_{\text{parallel}}}$$

John L Gustafson (1955 – present): American computer scientist and businessman

Gustafson's Law

Problem of interest (n total tasks; t time per task)



Serial part ($1 - P$)

Parallel part (P)

The time required to perform a given task using N processors

$$t_{\text{parallel}} = (1 - P) n t + P n t$$

The time required to perform a given task using a single processor

$$t_{\text{serial}} = (1 - P) n t + N P n t$$

Gustafson's Law

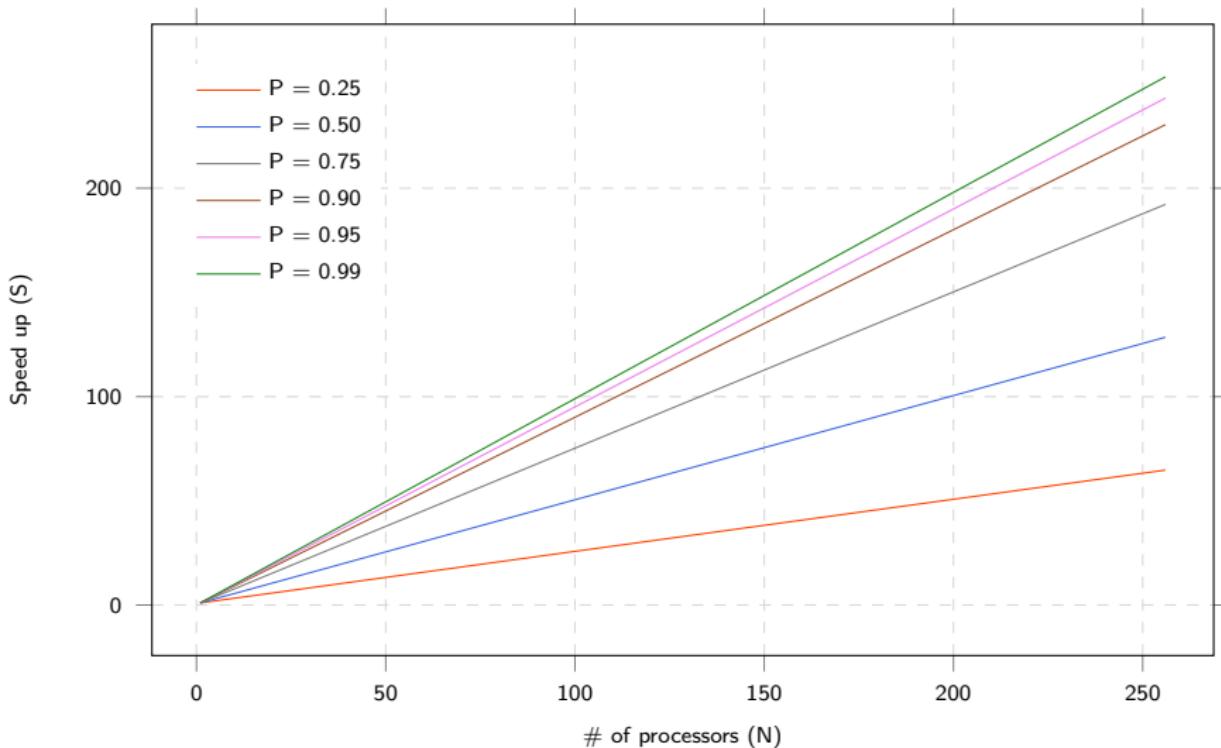
Observed speed up is

$$S = \frac{t_{\text{serial}}}{t_{\text{parallel}}} = \frac{(1 - P) n t + N P n t}{(1 - P) n t + P n t}$$

Simplify, add and subtract N from RHS, and further simplify

$$S = N - (1 - P)(N - 1)$$

Gustafson's Law



Parallel computing

Infrastructure design, operations and management

Components

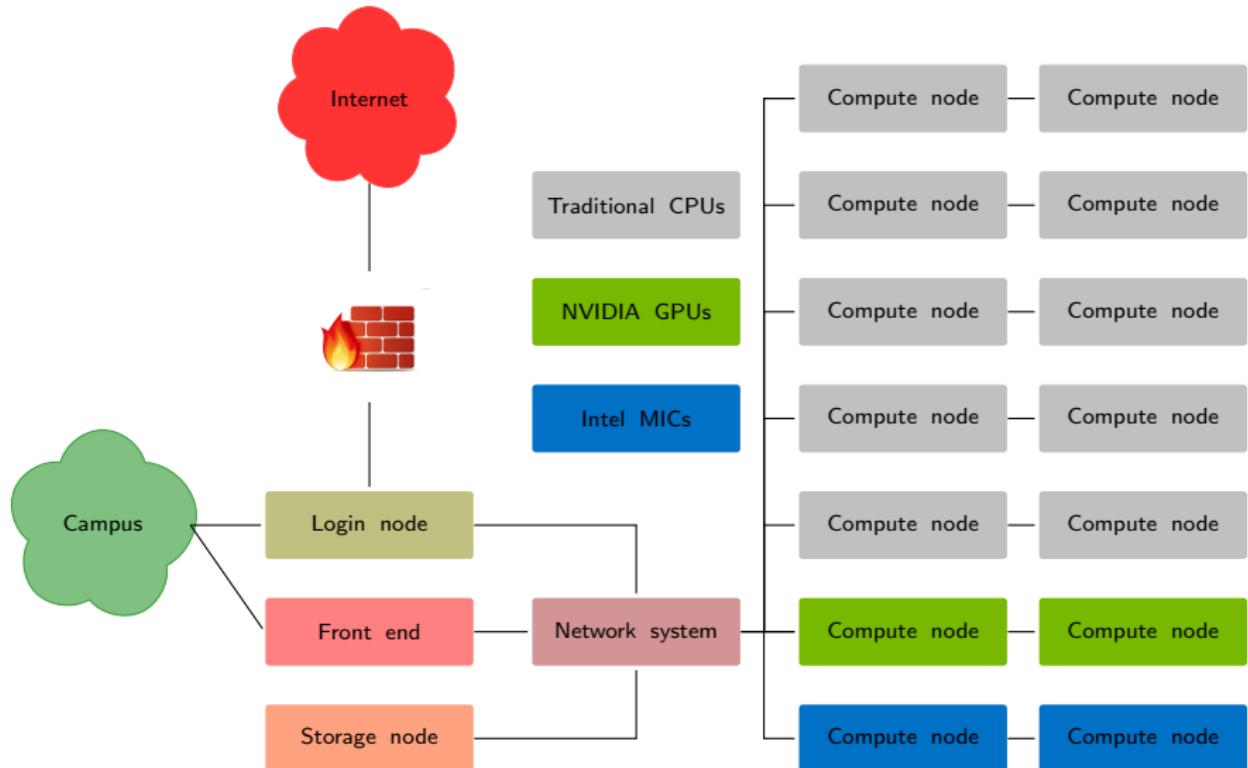
- * Front end (i.e., master/head node)
- * Login node[†]
- * Compute nodes (i.e., worker nodes)
 - * Traditional CPUs
 - * Hardware accelerators (NVIDIA GPUs and/or Intel MIC)[†]
- * Network/Switching system (Ethernet, InfiniBand[†], etc.)
- * Storage node[†]
- * Racks, power, cooling

[†] Optional component.

Front end can also serve as a storage node in smaller clusters. In larger clusters, a high-speed network (e.g., InfiniBand) and a separate storage node are often a requirement. Network usually accounts for 15-20% of the overall cost. The cost of storage node depends on physical size, level of redundancy, desired performance, and is non-trivial.



Schematic representation



Build philosophy

Is building the infrastructure in itself the end goal?

OR

Is the infrastructure a platform for accomplishing other goals?

Pros and cons

In the first case, one can achieve very high performance (95+%) often at the expense of very short life for the infrastructure (\sim hours). Process of fine tuning could often result in rebuilding the infrastructure multiple times per day.

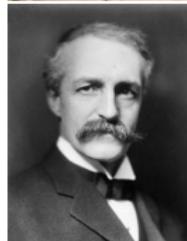
In the second case, one settles for a slightly lower performance (\sim 90%) but the infrastructure stays up and running to support very long production quality simulations (several hours to days to months).



Usage philosophy

Greatest good for the greatest number

– Warren Perger and Gifford Pinchot



Much is said of the questions of this kind, about greatest good for the greatest number. But the greatest number too often is found to be one. It is never the greatest number in the common meaning of the term that makes the greatest noise and stir on questions mixed with money ...

– John Muir



This is the philosophy in use at Michigan Tech, at least since 2013.

Warren Perger (1950 – present): American electrical engineer and physicist; Professor, Michigan Tech

Gifford Pinchot (1865 – 1946): American forester and politician

John Muir (1838 – 1914): Scottish-American naturalist

CPU time vs Wall time

Why should anyone care?

If a serial program runs for an hour of real time, then t_{CPU} and t_{Wall} wall time should be approximately equal (i.e., an hour). If t_{CPU} is much smaller than t_{Wall} , then it's an indication of bottlenecks in the program.

If a parallel program using N processors runs for an hour of real time, then t_{CPU} should be approximately N hours while t_{Wall} is one hour. If the ratio, t_{CPU}/t_{Wall} , is not approximately equal to N , then it's an indication of unbalanced work distribution.

Most computing infrastructures – including Amazon Web Services, Google Cloud Platform, XSEDE supercomputers – bill/charge users by t_{CPU} (usually in terms of a Service Unit that has 1,000 CPU hours).

Additional references

- * Validity Of The Single Processor Approach To Achieving Large Scale Computing Capabilities
G. M. Amdahl
Proceedings of the Spring Joint Computer Conference, p. 483 (1967)
- * Reevaluating Amdahl's Law
J. L. Gustafson
Communications of the ACM, vol. 31, p. 532 (1988)
- * Extending Amdahl's Law And Gustafson's Law By Evaluating Interconnections On Multi-Core Processors
T. Huang, Y. Zhu, M. Qiu, X. Yin, X. Wang
Journal of Supercomputing, vol. 66, p. 305 (2013)
- * Human Computers | The Age Of Female Computers

PDF in [AdditionalMaterial](#) folder.



Additional references

- * Feynman Lectures On Computation
R. P. Feynman, A. J. G. Hey; Westview Press (2000)
- * Feynman And Computation
A. J. G. Hey; Westview Press (2002)
- * The Innovators
W. Isaacson; Simon & Schuster (2014)
- * Hidden Figures
M. L. Shetterly; HarperCollins (2016)
- * Rise of Rocket Girls
N. Holt; Little, Brown and Co. (2016)
- * Rocks Cluster Distribution

PDF in [AdditionalMaterial](#) folder.



Message Passing Interface

As applicable to parallel programming



Definition and implementations

A language-independent communications protocol (i.e., neither a language nor an implementation but an agreed upon library specification) used to program parallel computers with support for both point-to-point and collective communication.

- * OpenMP (previously known as LAM/MPI)
- * MPICH from Argonne National Laboratory
- * Bindings are available for Java, Perl, Python, R and Ruby

Initial release of MPI in early 1990s was a result of about 80 researchers from 40 organizations in the US and Europe. The preliminary proposal was designed by J. Dongarra, R. Hempel, T. Hey and D. W. Walker in a 1992 workshop on Standards for Message Passing in a Distributed Memory Environment.

Common workflow

- * Initialization
- * Process/Task identification
- * Number of processors/tasks/teams
- * Division of labor
- * Sending and receiving messages as necessary
 - * Point-to-point communication
 - * Collective communication
- * Synchronization and collection of results
- * Finalization

Types of communication

Packing slip in real life

Order # 1011

From

John Sanderson
123 Lost Souls Ave
Hell, MI 48169 USA

To

Dr. Jane Jameson
666 Enlightenment Blvd
Paradise, MI 49768 USA

| Item # | Description | Qty |
|--------|-------------|-----|
| 001 | Samples | 5 |
| 002 | Report | 1 |

Sender _____

Receiver _____



Types of communication

Packing slip in parallel processing

Message ID i + 10

From

Processor i

To

Processor j

| Item # | Description | Qty |
|--------|--|-----|
| 1 | N, long integer variable | 1 |
| 2 | radius, double-precision variable | 1 |
| 3 | x _i , double-precision variable | 2 |
| 4 | A, 2D double-precision array of size N x N | 1 |
| 5 | B, 1D double-precision array of size N x 1 | 1 |
| 6 | C, 1D double-precision array of size N x 1 | 1 |

Sender _____

Receiver _____



Point-to-point communication

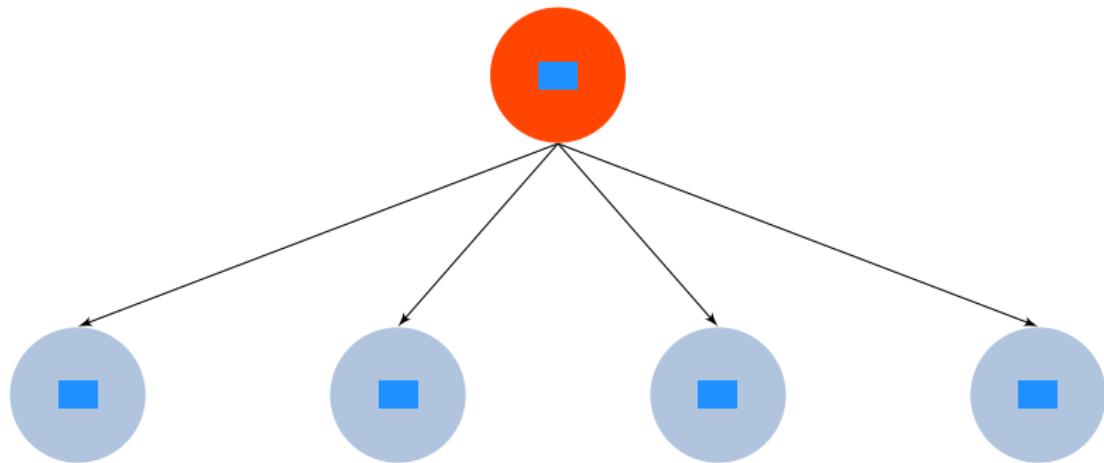
- * Sender pauses after the `send` statement
- * Message goes into a buffer on the receiver
- * Receiver receives the message when it has reached corresponding `recv` statement
- * Receiver pauses `recv` until the message has been received
- * Sender and receiver resume execution after the message has been received by the receiver

Communications overhead

Idle time (i.e., waiting to receive a message OR to get the confirmation that the message was received) often affects the performance.

Collective communication

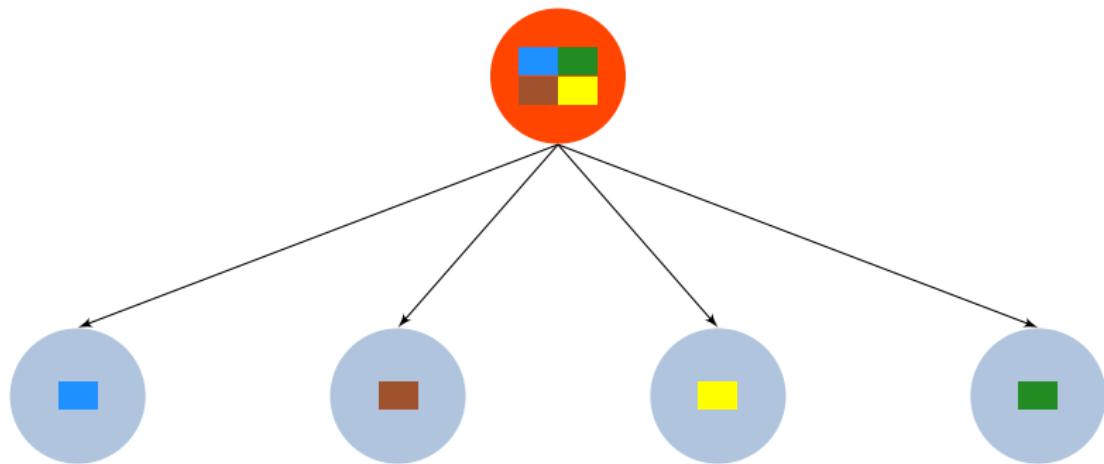
Broadcast



Broadcast function sends the exact same message to all participating processors.

Collective communication

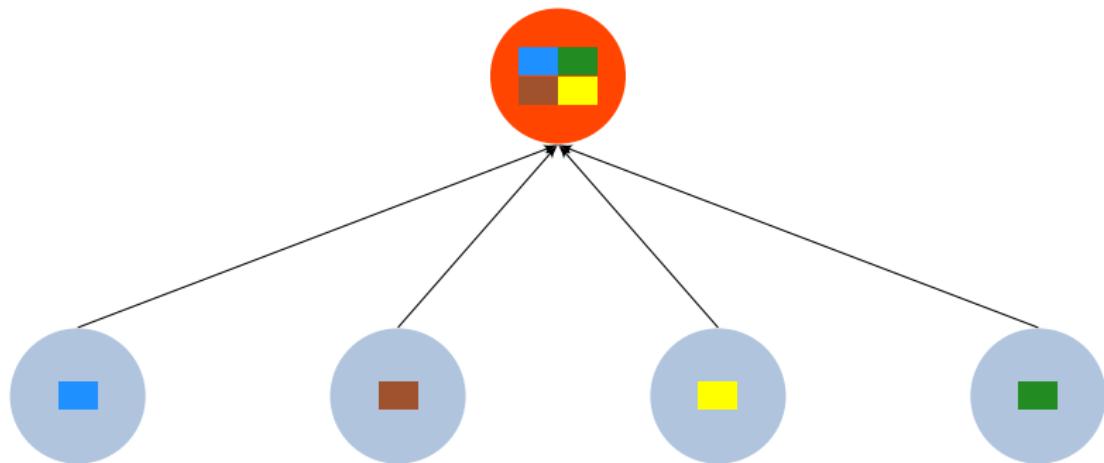
Scatter



Scatter function sends distinct messages from one processor to all other participating processors.

Collective communication

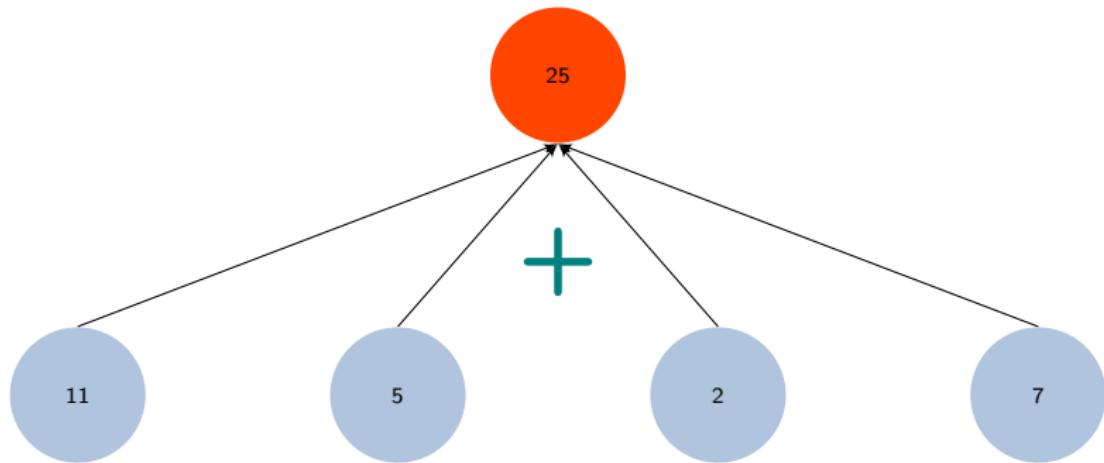
Gather



Gather function collects distinct messages from all participating processors to a single processor.

Collective communication

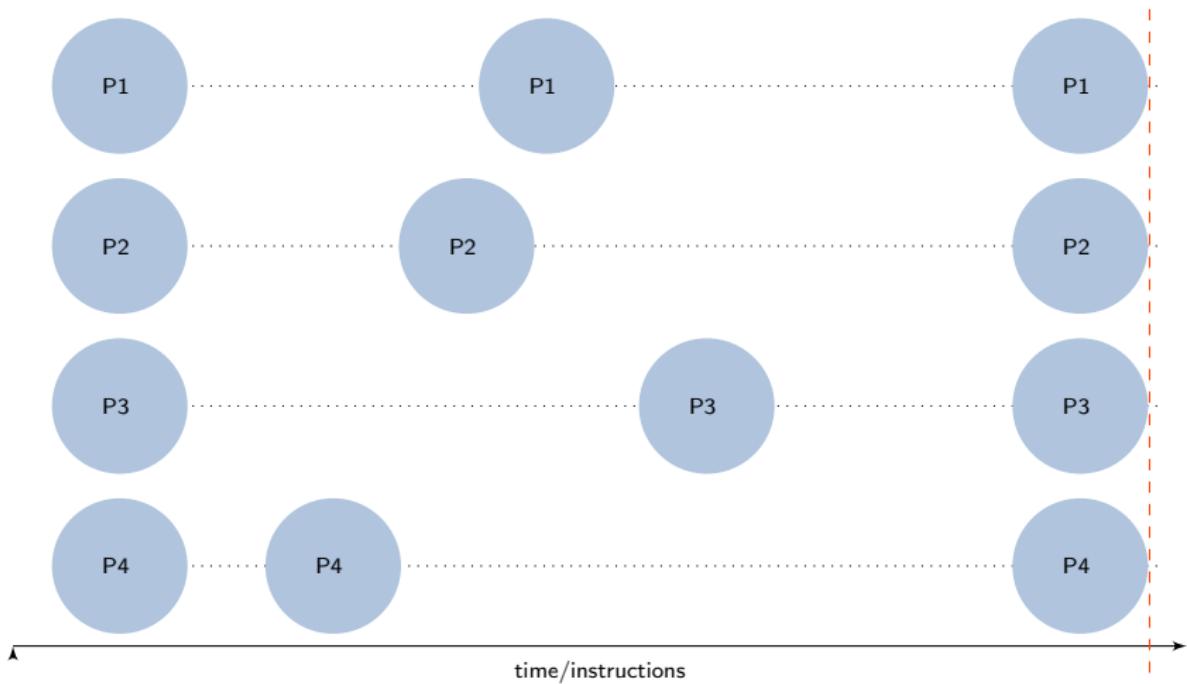
Reduce



Reduce function performs reduction operation on all participating processors and puts the result in one processor.

Collective communication

Barrier



Barrier function creates a barrier to synchronize all participating processors.

Serial and parallel examples

Instructor

Generation of Fibonacci sequence for $n > 2$ and $F(1) = F(2) = 1$

$$F(n) = F(n - 1) + F(n - 2)$$

Matrix multiplication of $A(n \times m)$ and $B(m \times p)$

$$C_{ij} = \sum_{k=1}^m A_{ik} B_{kj}$$

Discussion took place on Thursday of week #11 but included in **Message Passing Interface** section (Tuesday of week #11) for completeness purposes.

Serial and parallel examples

Adam Mitteer

Hunting with a gun/bow/rifle.

Fishing (trolling behind a boat they use many lines).



Serial and parallel examples

Akhil Kurup

Satellite launch: the rocket that carries the satellite has to disintegrate in stages in the predefined order and cannot just "burn out" all at once.

Image processing involves a lot of mathematical "convolution" operation where every element is shifted and multiplied with other elements. Since the image is available, the matrix manipulations can be done in parallel and the result combined in the end on a "master core" to produce the desired result.

Serial and parallel examples

Ashley Kern

When developing a model, one first takes ~75% of the data for model training and hold out ~25% for model validation. During the training step one can perform 10-fold cross validation where each fold can be used in parallel. After the model is trained, one applies the model to the hold out validation data which must be done in series following the model development.

Serial and parallel examples

Avinaash Kovvuri

Yet to complete

Serial and parallel examples

Cal Riutta

A surgery can be broken down into multiple threads handled by different "processors" or hospital staff. Anesthetics, distribution of tools and equipment, physical surgery, imaging, and so on – all part of the task of surgery, yet broken down into parallel tasks happening at the same time. Other specific tasks can only remain serial, however. Drug interactions could be an example: some drugs must be given carefully administered so as not to have an unwanted drug interaction. In some cases this may limit the drug administration to a certain sequential schedule.

Serial and parallel examples

Eisa Hedayati

Deep Packet Inspection (DPI), to be able to discover the type of connection in network. There is a rule of thumb that says we should have 4 serial transmitted packet to be able to DPI it and find the correct information, so here parallel processing won't work, since the inspection results are fully dependent to the previous transmitted packet.

DPI: For each connection we need to work on serial, but the total network has millions of connections, so by separating the connections, it is possible to make the job parallel, e.g., each 1000 connection can be assigned to one processor.

Serial and parallel examples

Hashim Al Mahmud

MD simulation of nanocomposite materials is generally parallel. However, sometimes serial tasks need to be performed in the workflow. For example, a complex curing reaction (cross link) for epoxy molecules cannot be done using LAMMPS alone. I need to start the first step in the reaction for each stoichiometric molecules in LAMMPS. Then, a Python script will complete the reaction process. In other words, each step depends on the preceding one. A sequential steps of using LAMMPS and Python can be controlled by a BASH script.

Serial and parallel examples

Ian Cummings

The core mathematics coursework from high school through university must be taken in sequence (roughly): Algebra, Geometry Trigonometry/Precalculus, Calculus, Linear Algebra, Differential Equations, Fourier/Laplace Transforms.

The education program as a whole can be parallelized; students take multiple subjects concurrently (science, mathematics, general education, and technical electives, etc).

Serial and parallel examples

Jeff Brookins

When reading a sentence, there is an agreed upon order of deciphering the text.

When a list of hashed passwords, for example, are pulled from a Windows machine; it is impossible to decrypt the hashes. However, brute force attacks, such as a dictionary attack, can be used to try every possible permutation of letters/numbers/symbols until the output matches the original hash.

Serial and parallel examples

Prithvi Kambhampati

Runge-Kutta method can be done serially only as the constants k_1 , k_2 , and so on depend on each other.

Visual encryption: Images can be encrypted using parallel processors. Each row of pixels can be assigned to a core.

Serial and parallel examples

Paul Roehm

Computations to determine next Genetic Algorithm runs to be performed (depends on previous).

Genetic Algorithm runs within a step.

Serial and parallel examples

Qing Guo

When applying electric field (EF) to the system, the outputs files of the system with smaller EF value are needed by system with bigger EF for quick convergence. So the progress should be using $I(n + 1) = O(n)$.

All systems with different density of defect numbers can be computed at the same time.

Serial and parallel examples

Zhiqiang Zhao

Addition in serial sequence

$$sum(n) = sum(n - 1) + 1$$

LU factorization algorithm

$$A = LU$$

Serial and parallel examples

Sandeep Lanka

Task scheduling and queuing, interrupt handling, etc.

Applying transformations to one or a group of pixels for any image processing purpose if the transformation doesn't depend on the neighbouring pixels.

Serial and parallel examples

Subin Thomas

Printing from printer.

Computing factorials.

Serial and parallel examples

Sameer Saraf

Yet to complete

Serial and parallel examples

Shuo Wang

The transfer function of a control system with feedback

$$\frac{Y(s)}{X(s)} = \frac{G(s)}{1 + G(s)H(s)}$$

Jacobi iteration

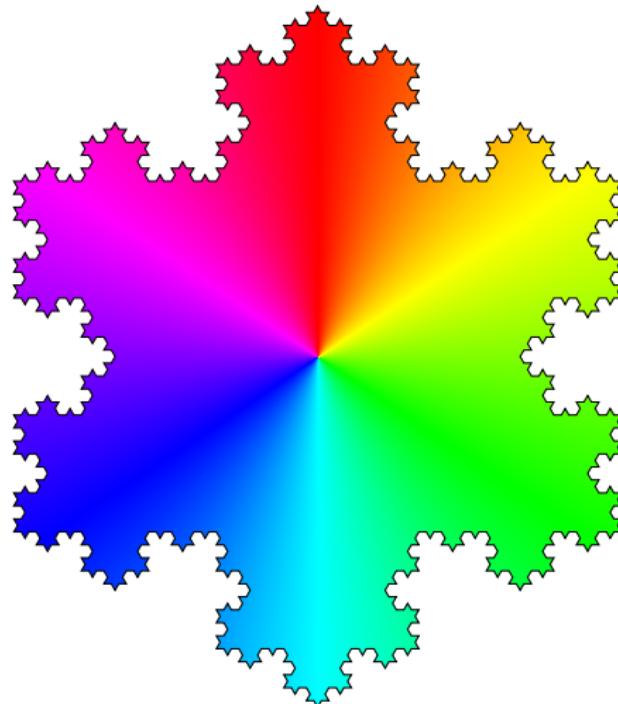
$$x^{(T+1)} = -D_A^{-1}(L_A + U_A)x^{(T)} + D_A^{-1}b$$

Additional references

- * [OpenMP](#)
- * [MPICH](#)
- * [Intel MPI Library](#)
- * [MATLAB](#)
 - [Parallel Computing Toolbox](#)
 - [Speeding Up Applications | Parallel Computing](#) (recorded webinars)
- * [Python: MPI4Python | Parallel Processing And Multi-Processing](#)
- * [R: R Bloggers | Glenn Lockwood](#)

Before we meet again

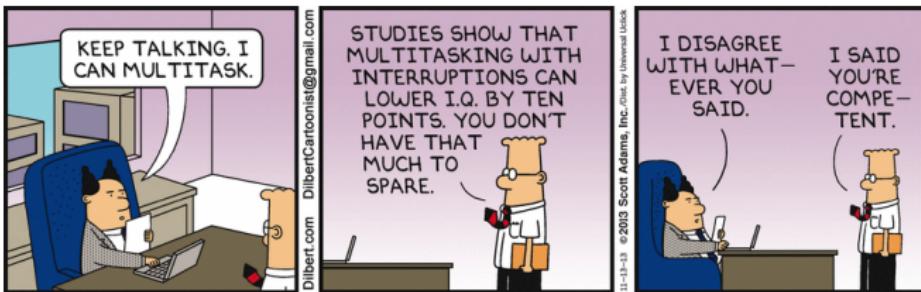
- * Review the syllabus, course material, grade through week #11, notations, active participation, free time exercises, tips, opportunities, mathematical results, and videos
- * Make progress in assignment #07
- * Make progress in the term project
- * Make progress towards Research Marketing III
- * Review program compilation using single source file
- * Review Fibonacci sequence and matrix multiplication



End of Tuesday lecture.

OpenMP

Parallel Programming/Message Passing Interface

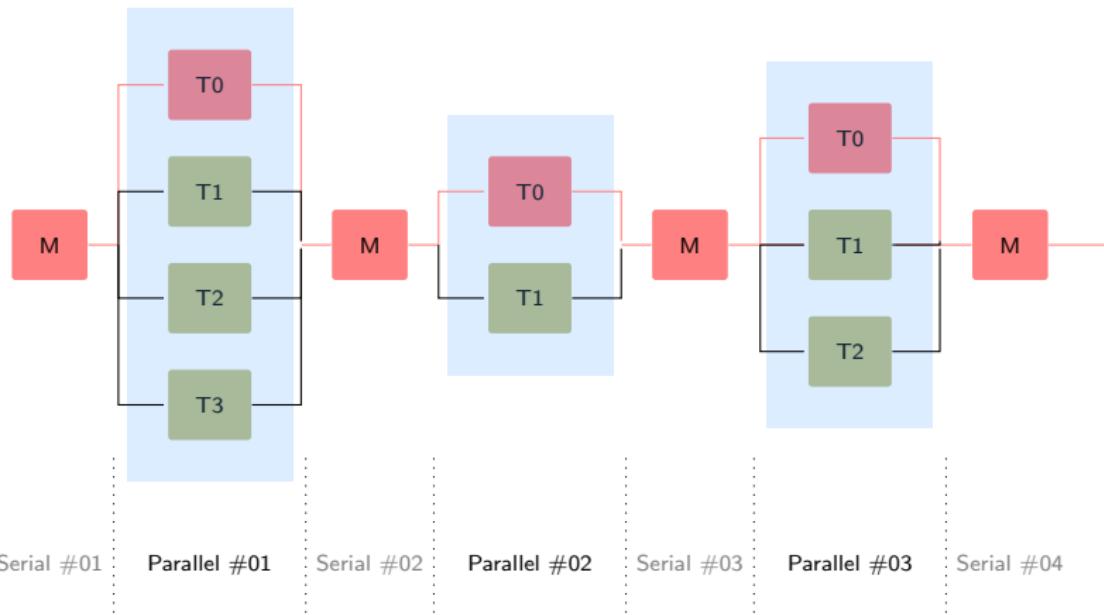


<http://dilbert.com/strip/2013-11-13/>

Features

- * An explicit and compiler directive based programming model
- * Limited by the number of processors/threads physically available
- * Accomplishes parallelism through the use of threads
- * Facilitates nested parallelism and dynamic threads
- * Employs fork-join model of parallel execution
 - * All programs begin as a single process, the master thread
 - * Master thread executes sequentially until a parallel region is encountered
 - * Master thread creates a team of parallel threads
 - * When the team of threads complete the statements in parallel region, they synchronize and terminate leaving only the master thread

Fork-join and dynamic threading



M denotes master thread (serial region).

T denotes task thread (parallel region); master thread, M, can be treated as the first task thread, T0, in parallel region.

Number of task threads can be different in different parallel regions.

Components

- * Compiler directives
 - * Appear as comments in source code
 - * Used for spawning a parallel region, dividing blocks of code among threads, synchronizing work among threads, etc.
 - * Have the following form

sentinel directive-name [clause]

C/C++

```
#pragma omp parallel shared(VAR1, VAR2) private(VAR3, VAR4)
```

It is programmer's responsibility to identify and decide the amount of each of these components.
Changes to **shared** variables are global and seen by other participating threads.
Changes to **private** variables are local and not seen by other participating threads.



Components

- * Run-time library routines

- * Used for setting and querying the number of threads (`num_threads`), querying a thread's unique identifier (`thread_id`), setting and querying the dynamic threads feature, querying if in a parallel region (and at what level), querying wall clock time, etc.

Commonly used routines, and the necessary header file

```
#include <omp.h>

omp_get_num_procs()      # Total number of available processors
omp_get_max_threads()    # Maximum number of usable threads
omp_get_num_threads()    # Number of threads in the current team
omp_get_thread_num()     # Unique ID of each participating thread
omp_get_wtime()          # Wall time
```

C/C++ routines are case sensitive; FORTRAN routines are not.

It is programmer's responsibility to identify and decide the amount of each of these components.



Components

- * Environment variables

- * Help control the execution of parallel code at run-time
- * Used for setting number of threads, binding threads to processors, enabling/disabling nested parallelism and dynamic threads, etc.

BASH

```
export OMP_NUM_THREADS=4
```

Setting OMP_NUM_THREADS

If more than one OpenMP program (or more than one instance of the same program) is running concurrently, set this variable on a per program basis using a parent shell script to prevent resource contention/over-subscription.

It is programmer's responsibility to identify and decide the amount of each of these components.

Value of this variable can be changed during run-time at the command line OR within the parent shell script. **If this variable is not explicitly set, then PROGRAM.x uses all available processors/cores for its execution.**



Conventions

- * Processor/Thread count begins at 0, and ends at N-1. The program will not use more processors/threads than physically available
- * Dynamic threading and nested parallelism will be ignored
- * Master thread (i.e., `thread_id = 0`) will perform write operations. Worker threads (i.e., `thread_id = 1:N-1`) will perform read/write operations, and communicate with master and/or other workers iff there is a need

Using more processors/threads than physically available

can lead to reduced performance and potentially damage the hardware.
Instructor's carefully crafted examples will demonstrate the sluggish performance.

Compilation and execution

Compilation

```
gcc -Wall -g -pg -lm -fopenmp PROGRAM.c -o PROGRAM.x  
g++ -Wall -g -pg -lm -fopenmp PROGRAM.cpp -o PROGRAM.x
```

Execution

```
OMP_NUM_THREADS=2      # CHANGE TO 1, 2, 4, 8, ETC.  
./PROGRAM.x
```

clock() vs omp_get_wtime()

A serial C program that employs `clock()` provided by `time.h` will estimate the CPU time (t_{CPU}). Prefixing the program execution with `time` command as described in **Tip #3** can provide an estimate of the wall time (t_{Wall}). `omp.h` provides `omp_get_wtime()` for estimating t_{Wall} in OpenMP C parallel programs.



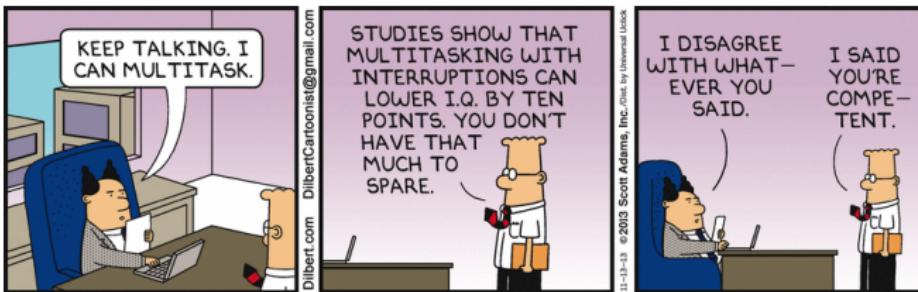
Additional references

- * [OpenMP \(The Official Website\)](#)
- * [Quick Reference – Compiler Directives, Run-time Library Routines And Environment Variables](#)
- * Twitter
[@OpenMP](#)

PDF in [AdditionalMaterial](#) folder.

MATLAB

Parallel Programming/Parallel Computing Toolbox



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

Features

- * Parallel Computing Toolbox (PCT) is one of ~60 toolboxes included in Michigan Tech's unlimited use campus license
 - Parallelization approach is similar to OpenMP in that it is limited by the number of processors physically available in a machine
- * Distributed Computing Server (DCS; per research group acquisition)
 - Parallelization can use processors from different physical machines connected by a network

MATLAB and Parallel Computing Toolbox (GUI)

```
# Open MATLAB  
ver  
# CHECK IF Parallel Computing Toolbox IS LISTED
```

Conventions

- * Processor count begins at 0, and ends at N-1. The program will not use more processors than physically available
- * No support for nested parallelism
- * Master processor (i.e., `proc_id = 0`) will perform write operations. Worker processor (i.e., `proc_id = 1:N-1`) will perform read/write operations, and communicate with master and/or other workers iff there is a need

Code parallelization

Using Parallel Computing Toolbox

```
# OPEN THE SCRIPT m FILE
# ADD THIS LINE AT THE TOP (NPROC = # OF PROCESSORS)
parpool('local', NPROC)
# REPLACE EVERY for LOOP WITH parfor LOOP
# SAVE AND CLOSE THE SCRIPT m FILE
```

Nested parallelism

is NOT supported in Parallel Computing Toolbox. MATLAB's built-in debugger/profiler will detect nested `parfor` statements and provide suitable warnings/solutions (observe the color in the sidebar of MATLAB Editor pane).

Execution

Serial programs (command line)

```
# HelloWorld_s.m IS THE MATLAB SCRIPT m FILE
matlab -nodisplay -nosplash -singleCompThread \
-r HelloWorld_s -logfile HelloWorld_s.log
```

Parallel programs (command line)

```
# HelloWorld_p.m IS THE MATLAB SCRIPT m FILE
matlab -nodisplay -nosplash \
-r HelloWorld_p -logfile HelloWorld_p.log
```

What happens to figures/plots in command line?

Modify the MATLAB script `m` file so that figures and plots are written to the disk as files. Most HPC infrastructures do not have a GUI, and simulations with unmodified MATLAB `m` files could fail to complete.

Additional references

- * MathWorks
 - * Parallel Computing Toolbox
 - * Distributed Computing Server
 - * Twitter
- @MATLAB

PDF in AdditionalMaterial folder.

Parallel Computing Examples

MATLAB and OpenMP (C) programs



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

Embarrassingly/Perfectly parallel scenario

- * No explicit communication between processors/threads
- * Every processor/thread performs its share of the work
- * Applicable to languages that do not support parallelism
- * Common examples

Hello, World!

Array population

Dart board algorithm for π



MATLAB and OpenMP 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: MATLAB and OpenMP samples #11"  
git push origin master
```

Hello, World!

MATLAB; In-class activity

To be performed in `colossus.it`

```
cd ${UN5390}/CourseWork/Week_11/${USER}_11
cd Parallel/Embarrassing
BASENAME="HelloWorld"

# SERIAL
cat ${BASENAME}_s.m | more
matlab -nodisplay -nosplash -singleCompThread \
-r ${BASENAME}_s -logfile ${BASENAME}_s.log

# PARALLEL
cat ${BASENAME}_p.m | more
matlab -nodisplay -nosplash \
-r ${BASENAME}_p -logfile ${BASENAME}_p.log
```



Hello, World!

OpenMP; In-class activity

To be performed in `colossus.it` (1/3)

```
cd ${UN5390}/CourseWork/Week_11/${USER}_11
cd Parallel/Embarrassing
ln -sf ../functions.h functions.h
BASENAME="HelloWorld"

# SERIAL
cat ${BASENAME}_s.c | more
gcc -Wall -g -pg -lm ${BASENAME}_s.c -o ${BASENAME}_s.x
./${BASENAME}_s.x
```

Hello, World!

OpenMP; In-class activity

To be performed in `colossus.it` (2/3)

```
# PARALLEL VERSION #01
# EACH PARTICIPATING THREAD PRINTS
#   Hello, World! from thread M out of N
cat ${BASENAME}_p_01.c | more
gcc -Wall -g -pg -lm -fopenmp ${BASENAME}_p_01.c \
-o ${BASENAME}_p_01.x

OMP_NUM_THREADS=2    # CHANGE TO 1, 2, 4, 8
./${BASENAME}_p_01.x
```

Hello, World!

OpenMP; In-class activity

To be performed in `colossus.it` (3/3)

```
# PARALLEL VERSION #02
# VERSION #01 FEATURES +
# MASTER THREAD PRINTS ADDITIONAL INFORMATION
# EMPLOYS omp_get_wtime() TO PRINT WALL TIME
cat ${BASENAME}_p_02.c | more
gcc -Wall -g -pg -lm -fopenmp ${BASENAME}_p_02.c \
-o ${BASENAME}_p_02.x

OMP_NUM_THREADS=2      # CHANGE TO 1, 2, 4, 8, ETC.
./${BASENAME}_p_02.x

rm -f *.h *.out *.x
```



Before we meet again

- * Review the syllabus, course material, grade through week #11, notations, active participation, free time exercises, tips, opportunities, mathematical results, videos, and training camps
- * Complete assignment #07
- * Make progress in the term project
- * Turn in the project status by Friday 4:59 pm (weeks #11 & #12)
- * Make progress towards Research Marketing III
- * Estimate amount of work necessary to earn desired/possible grade (details to follow)

Before we meet again

- * No class during week #12

- Turn in the project status by Friday 4:59 pm

- Get some rest, catch up on life and other courses

- Get started on and make progress in assignment #12

- * 'Attend' SC16, if interested

- @SuperComputing | #HPCMatters | #SuperComputing | #SC16

- * Have a happy and safe Thanksgiving!



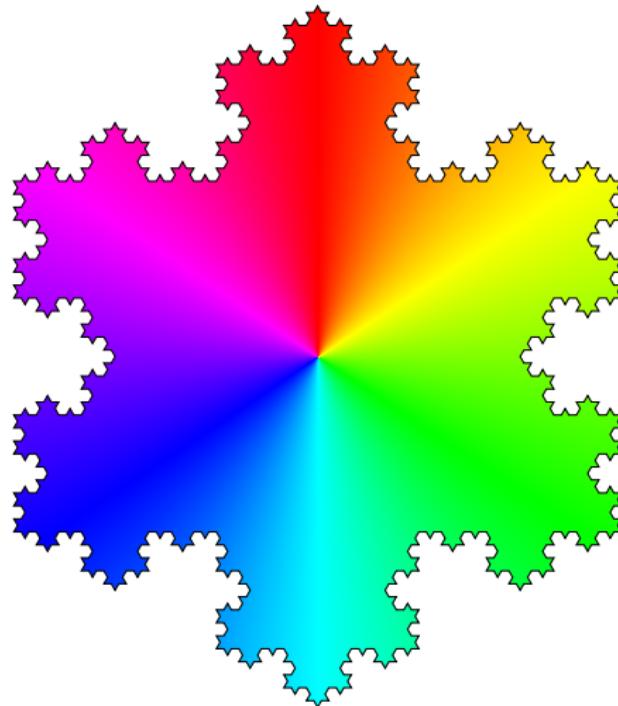
Before we meet again

Grade and workload estimator

| | Max % | My % | Cumulative % | Grade |
|-------------------------|--------------|------|--------------|-------|
| Attendance 01-11 | 05.00 | | | |
| Assignment #01 | 05.00 | | | |
| Assignment #04 | 10.00 | | | |
| Research Marketing I | 02.00 | | | |
| Research Marketing II | 02.00 | | | |
| PB&J Sandwich Recipe | 02.00 | | | |
| Project Report #10 | 01.00 | | | |
| You And The Board | 02.00 | | | |
| Do A Little More (DALM) | 09.00 | | | |
| Attendance 13, 14 | 01.00 | | | |
| Assignment #07 | 15.00 | | | |
| Assignment #12 | 20.00 | | | |
| Research Marketing III | 02.00 | | | |
| Project Report #11-14 | 04.00 | | | |
| Project Work | 20.00 | | | |
| Do A Little More | 09.00 - DALM | | | |

A: 93% and above; AB: 88% - 92.99%; B: 82% - 87.99%; BC: 76% - 81.99%; C: 70% - 75.99%; CD: 65% - 69.99%

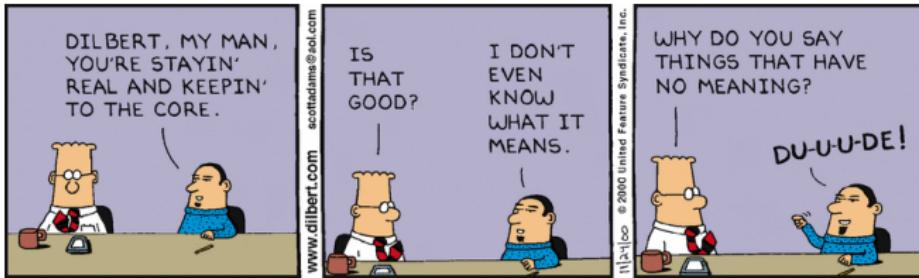
D: 60% - 64.99%; F: 59.99% and below



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 | @UseVim | @VimLinks | @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



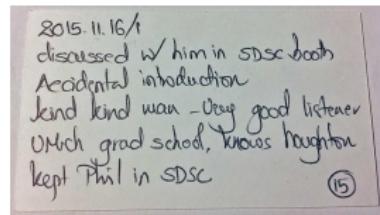
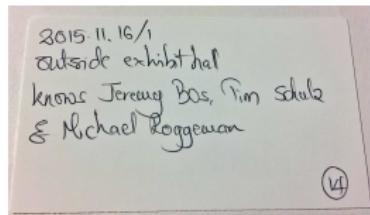
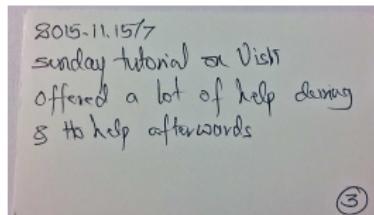
<http://dilbert.com/strip/2011-10-07/>

Research Marketing II

Professional business cards

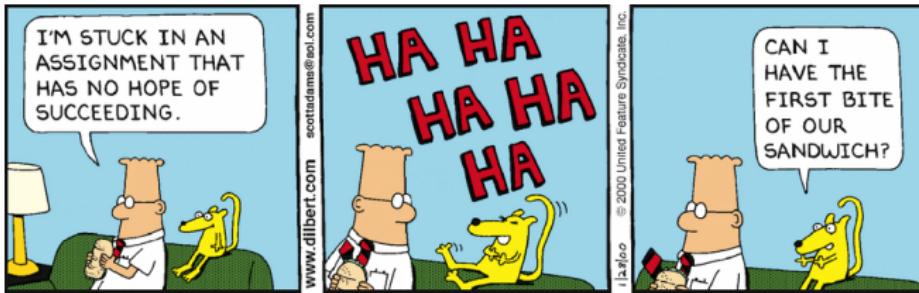
Visit Printing Services in the garden level of the Administration Building (a part of [University Marketing and Communications](#)) and get 100 professional business cards printed with the official Michigan Tech logo.

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
```

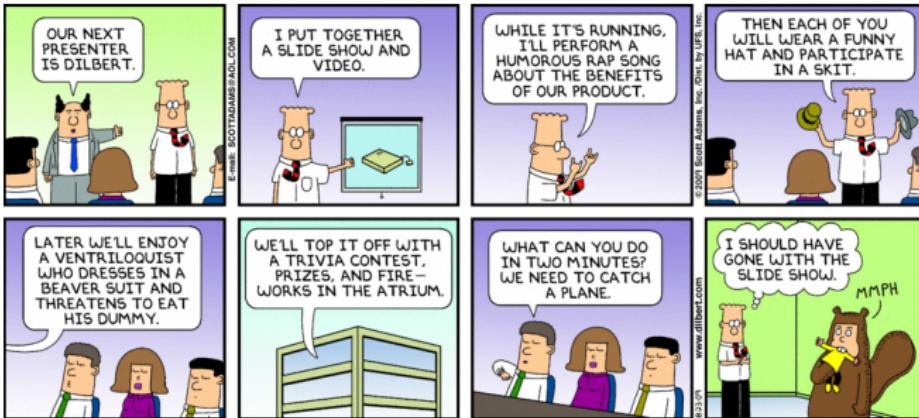


Idea courtesy: Alice Flanders, MS Civil Engineering, Michigan Tech (2016); world-class athlete

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?

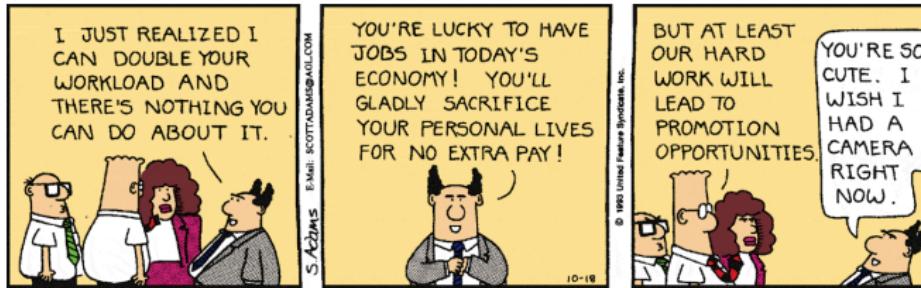
How to craft a winning elevator pitch

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.



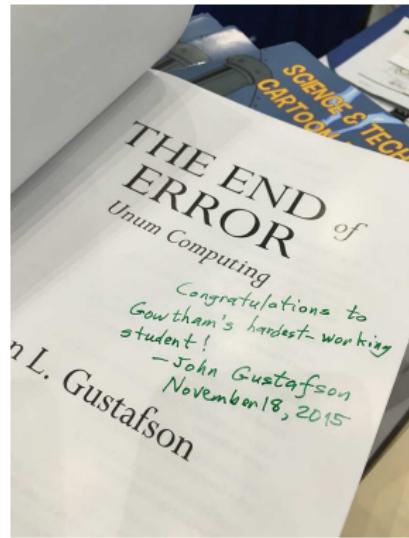
Doing them all

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 folder.



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 (≈ 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](#)



Identify the workflow

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.

Modify the subroutines

`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 `AdditionalMaterials/Profile` folder.

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.

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

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

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

Bugs in the roots of quadratic expression

Bugs in the roots of a quadratic expression

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 $1 < \alpha < 2$.

Error analysis

Integration



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



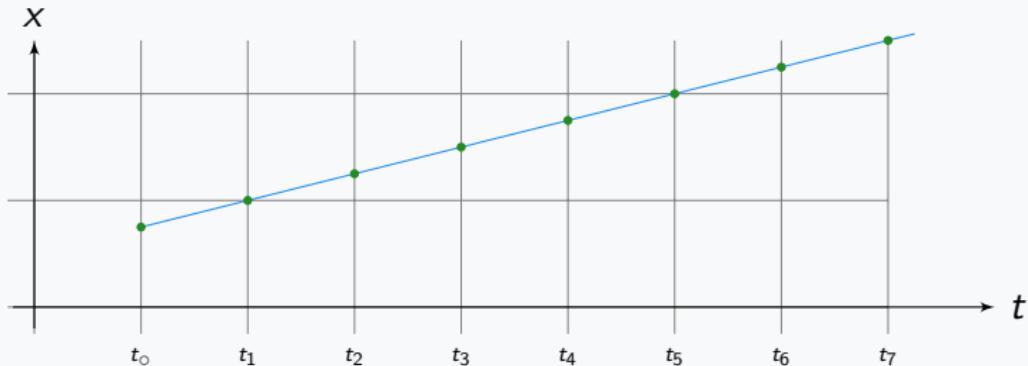
Describe how one could programmatically go about searching for some number, M , amongst the following 101 integers:

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

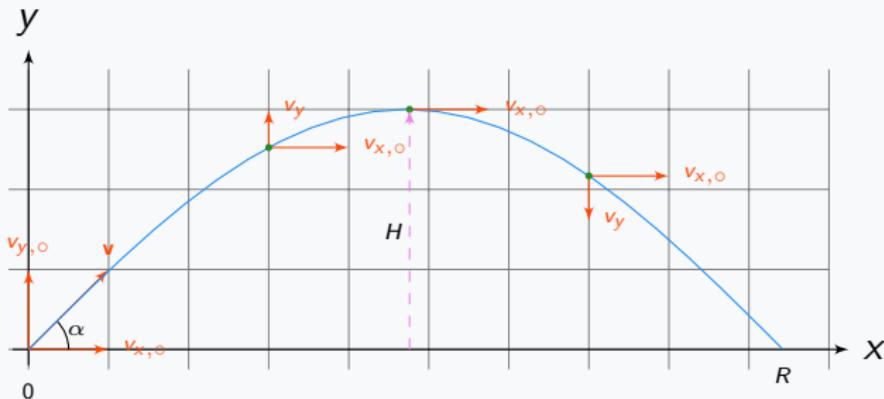
$$f(x_0, t_0) = \left. \frac{dx}{dt} \right|_{t=0} = v_0 ; x(t=0) = x_0$$

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 Gustfason'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.

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.



\LaTeX workflow for assignments

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

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

Replace 01 with the appropriate week number.

For more information, visit https://github.com/MichiganTech/LaTeX_GettingStarted



\LaTeX workflow for assignments

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

```
# 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 human readable format, 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 all 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 Eassa Hedayati



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_p_01.c"
        echo
    else
        local cbase=`echo "$1" | awk -F "." '{ print $1 }'`
        gcc -Wall -g -pg -fopenmp -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 `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.



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
```

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

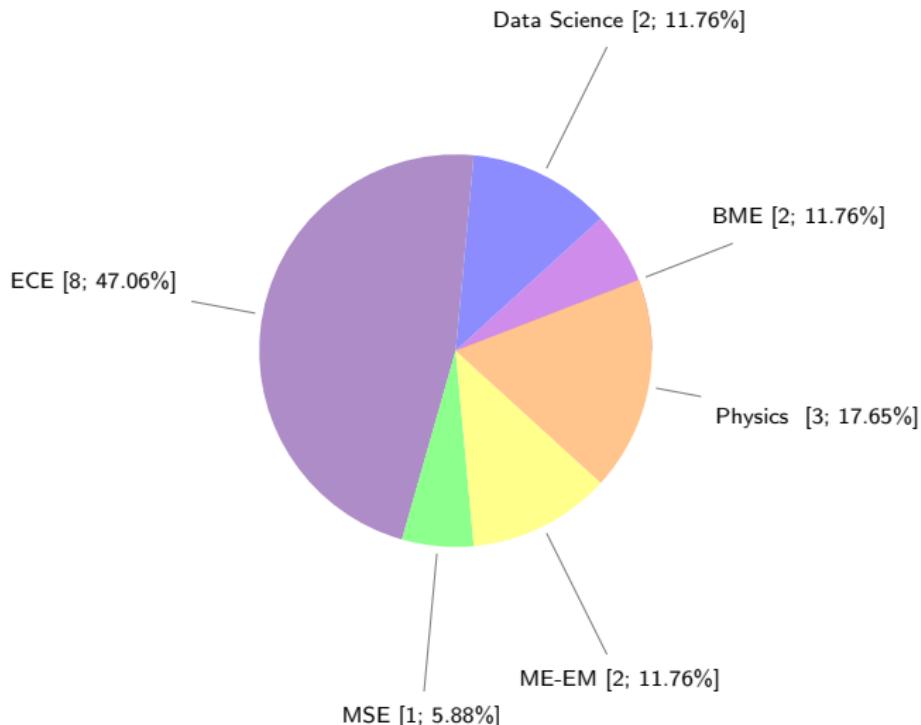
| # | Name | Email | Advisor |
|----|--------------|--|---------------|
| 09 | Cal Riutta * | cdriutta | Jinfeng Jiang |

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/>

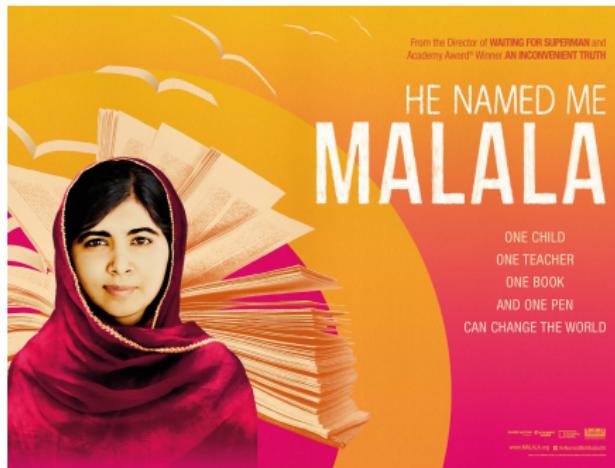


Before The Flood



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>

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

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

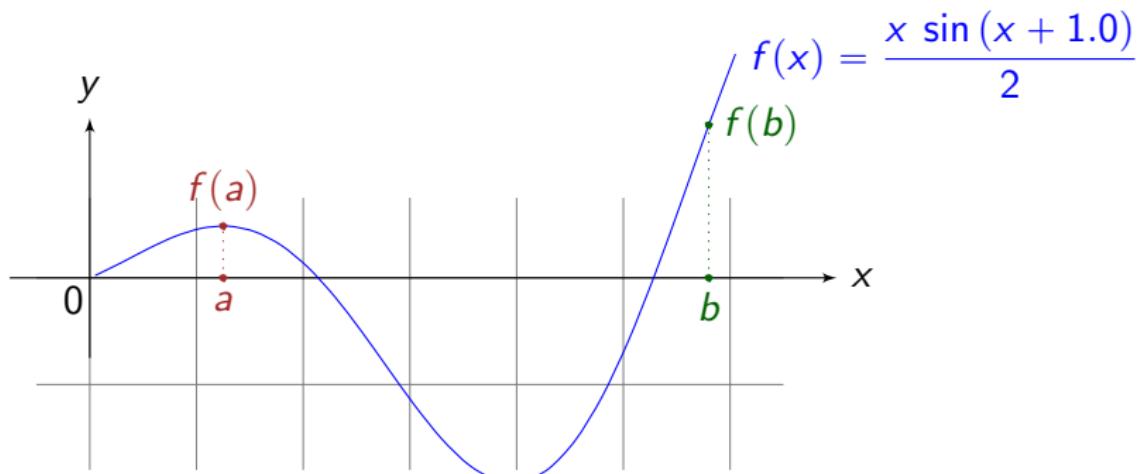
Changing the notations while retaining the underlying essence,

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

Re-arranging the terms,

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

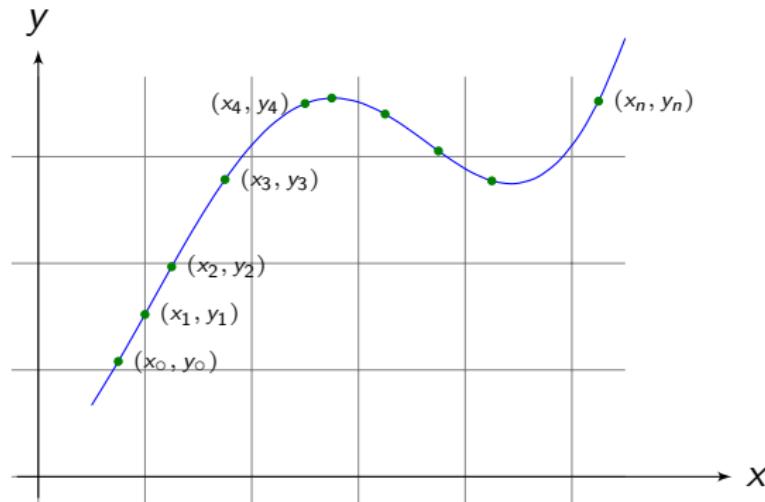
Intermediate value theorem (IVT)



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

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

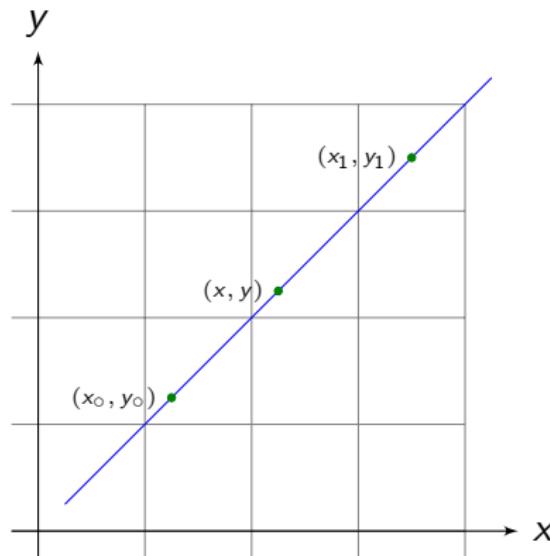
and are built to have the *Kronecker delta* property

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

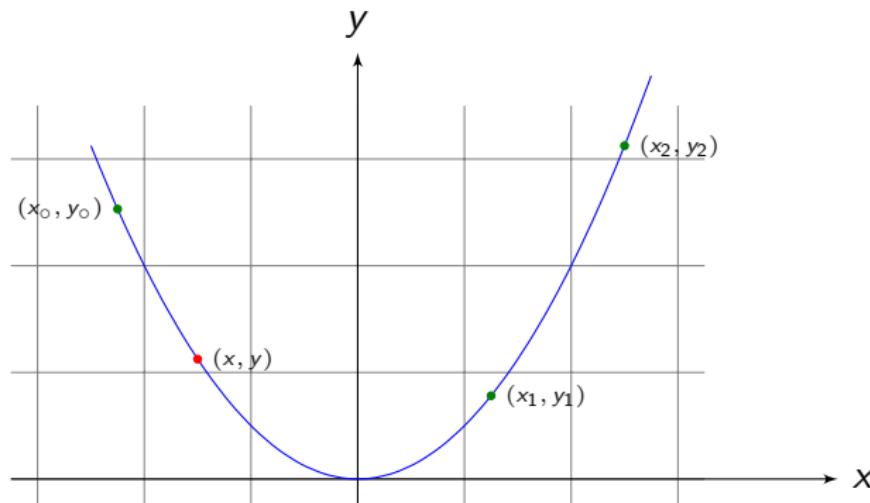
Lagrange polynomial interpolation

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



$$L_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} y_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} y_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} y_2$$

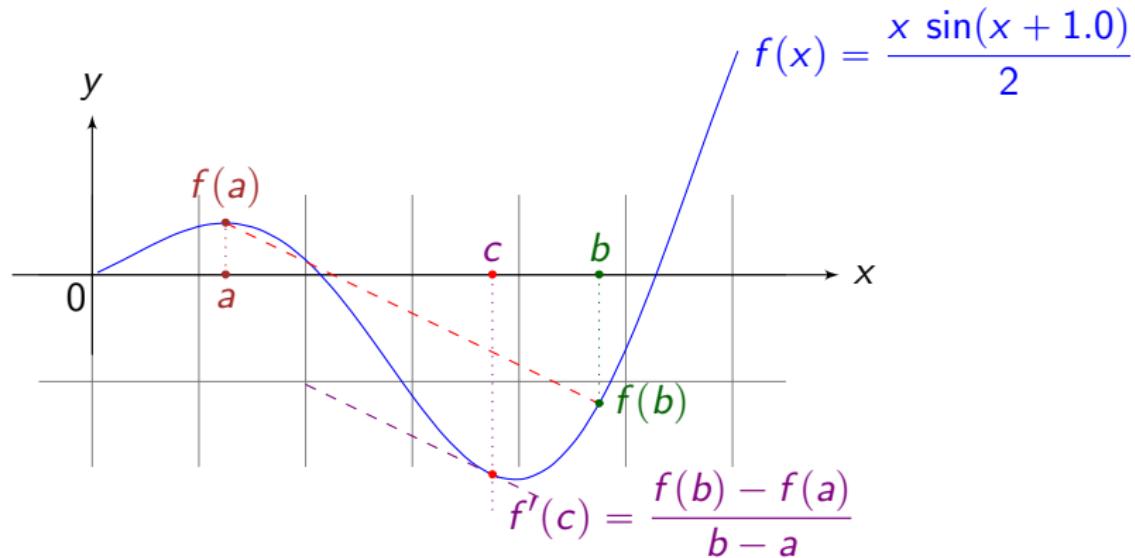
Lagrange polynomial interpolation

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

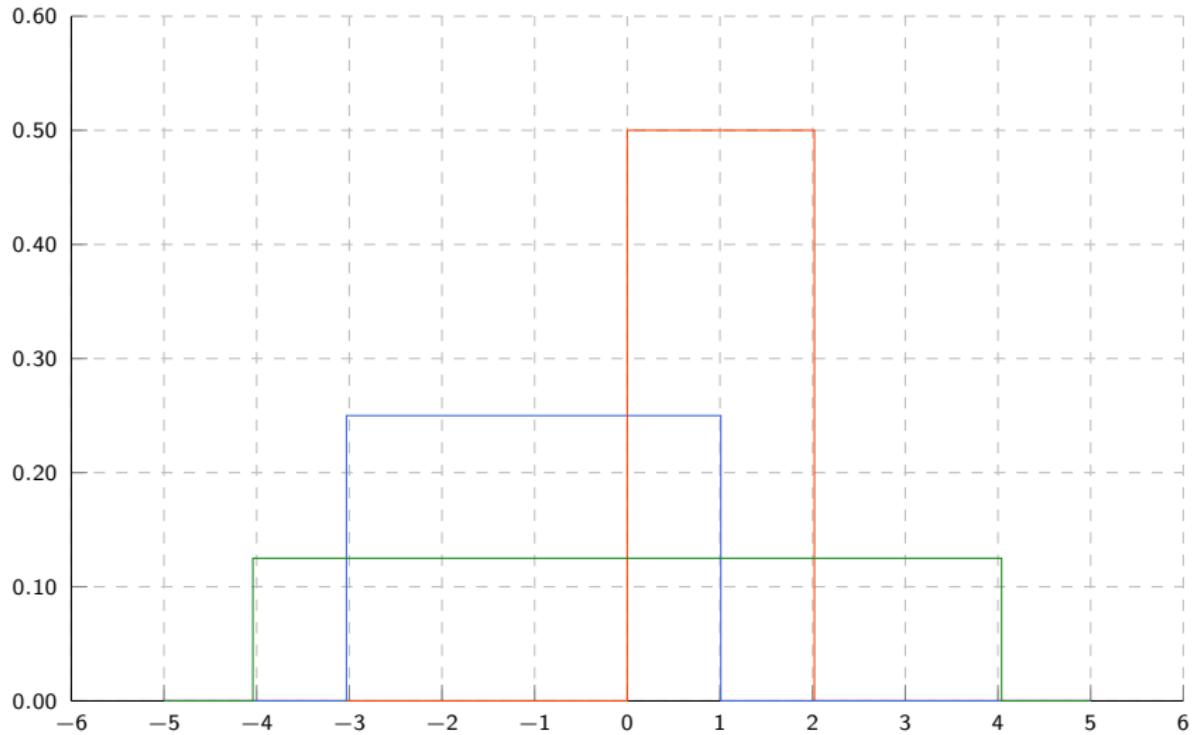
a finite number of values are equally likely to be observed. The probability density function on the interval $[a, b]$ is

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

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



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

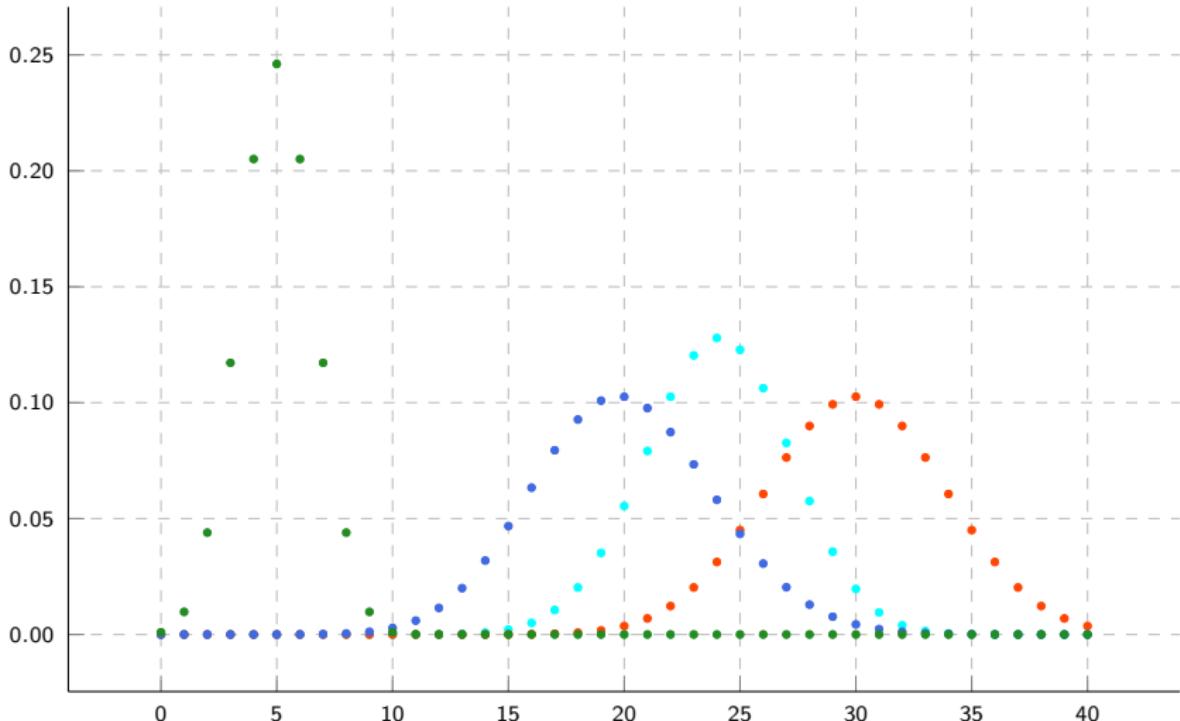
Discrete

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

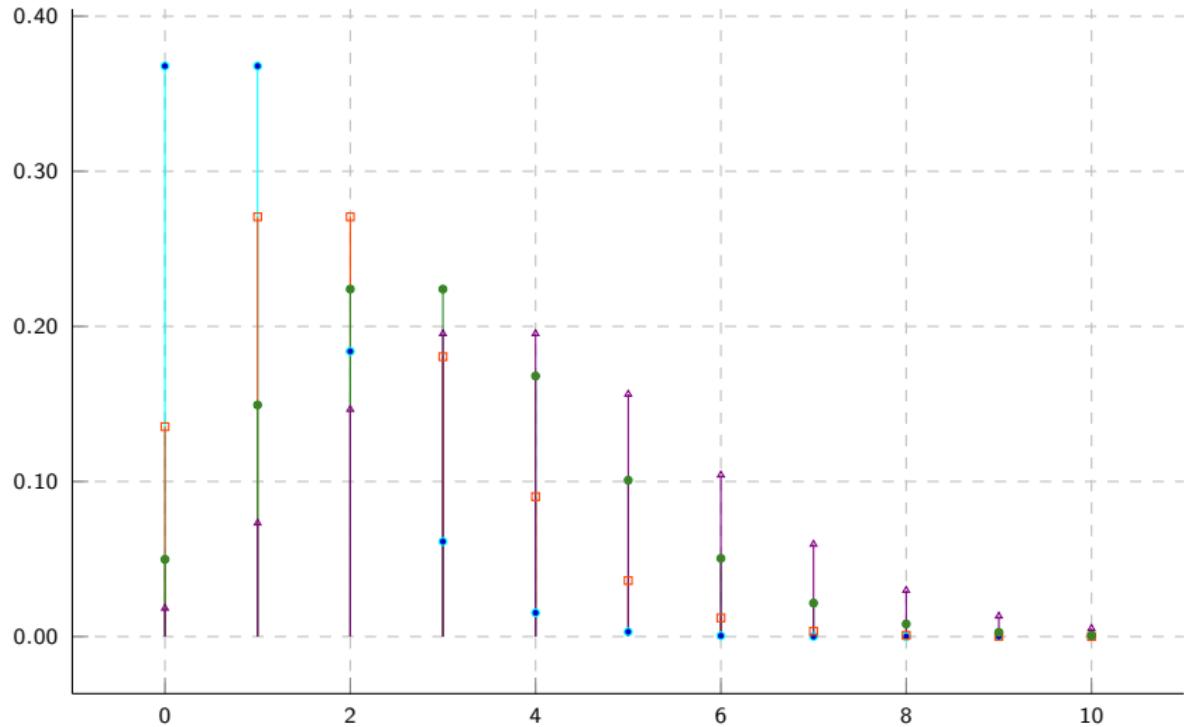
Discrete

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



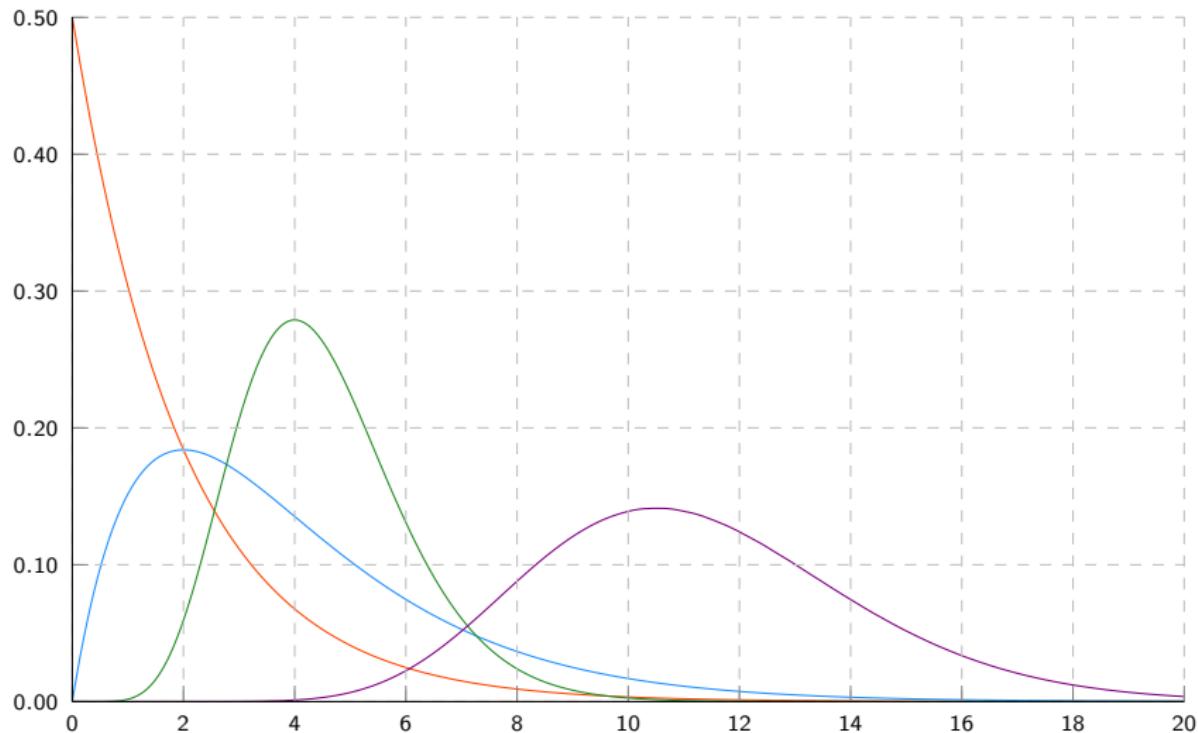
Gamma distribution

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

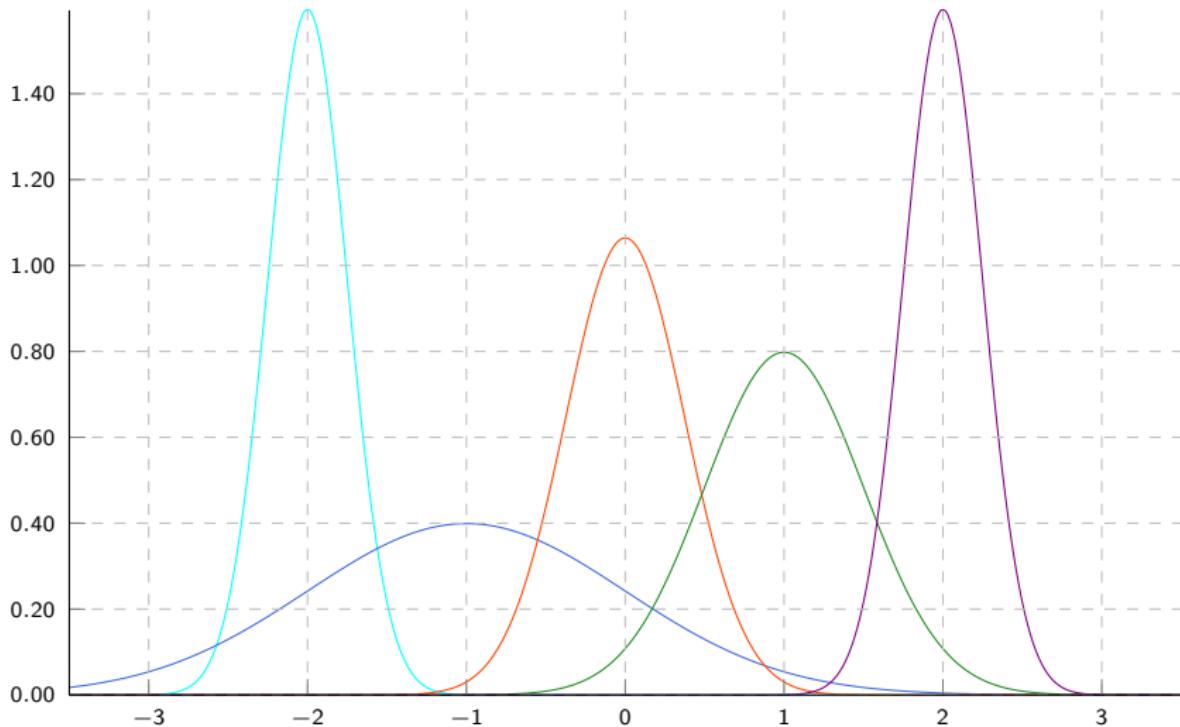
a limiting form of binomial distribution (De Moivre, 1733) and as a plausible distribution for measurement errors (Gauss, 1809). The probability density with mean μ and standard deviation σ is

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

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

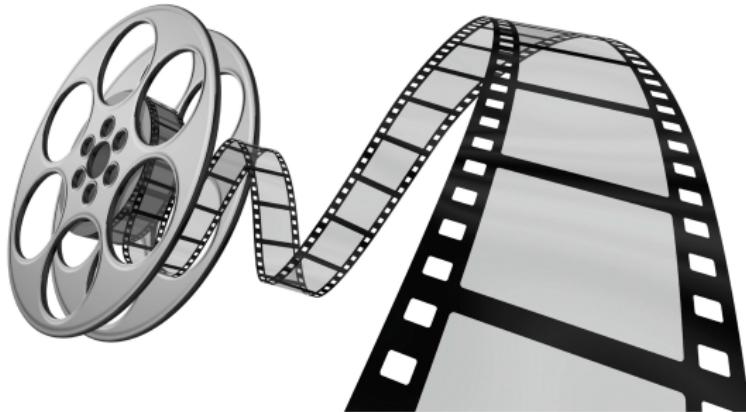
$$y_{n+1} = y_n + \frac{h}{6} k_1 + \frac{h}{3} k_2 + \frac{h}{3} k_3 + \frac{h}{6} k_4$$

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 ...



Computer History Museum



1401 N. Shoreline Blvd., Mountain View, CA 94043
(650) 810-1010

The Fairchild Notes



The Art of Writing Software



Supercomputing

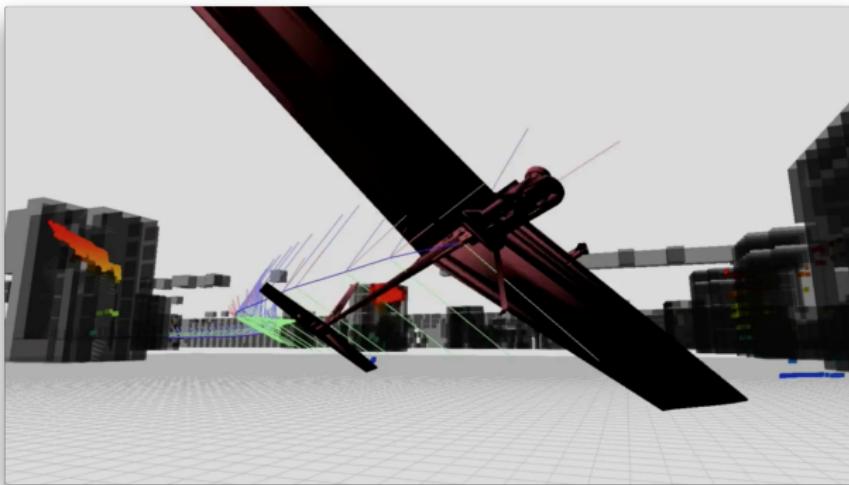


The International Conference for High Performance Computing,
Networking, Storage and Analysis

What is HPC?



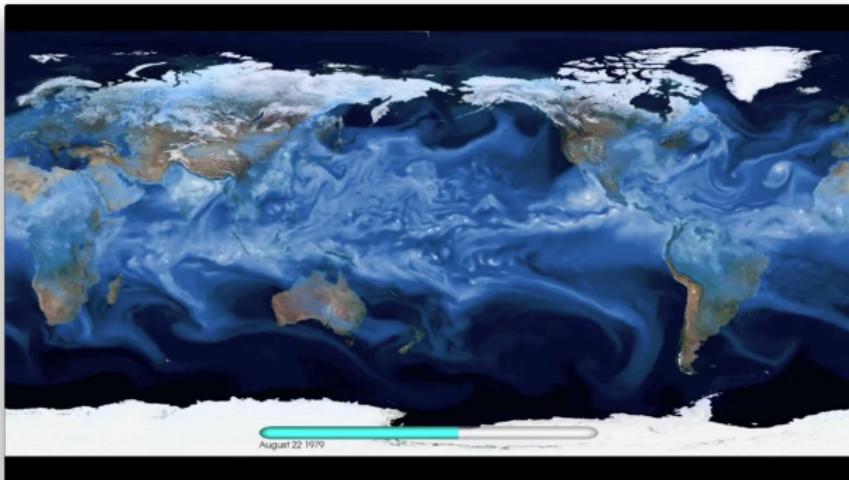
Aerospace



Batteries



Climate modeling



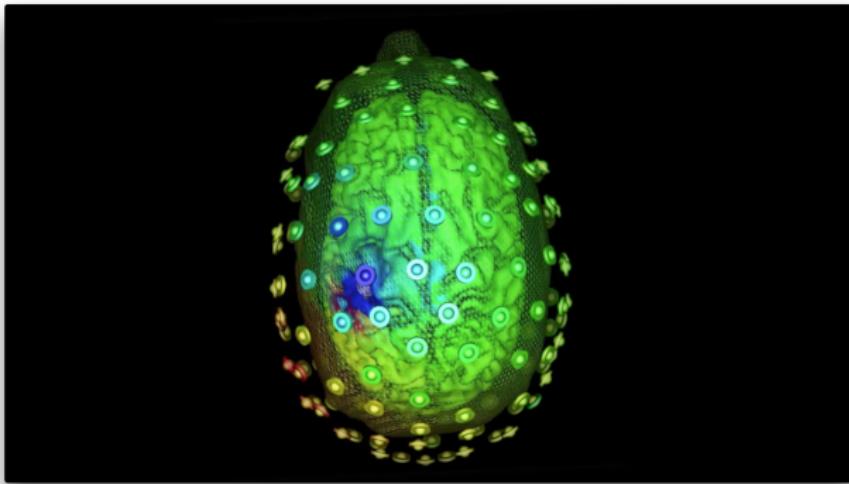
Diapers, detergents, shampoo



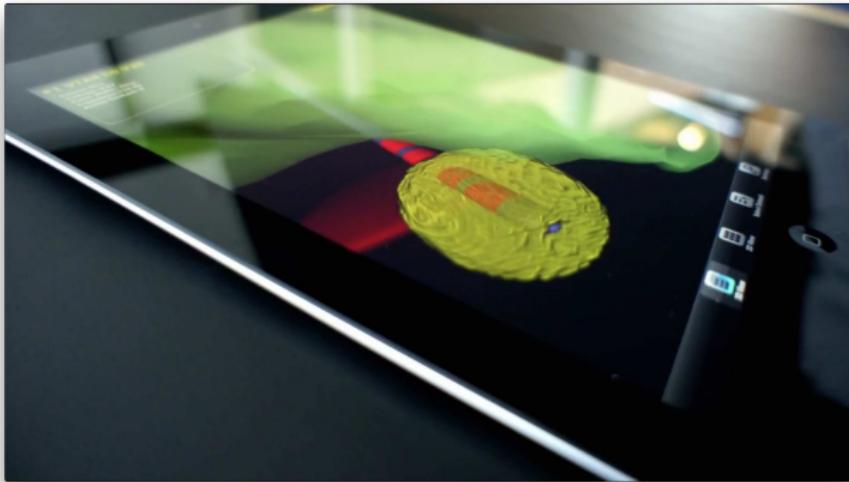
Entertainment



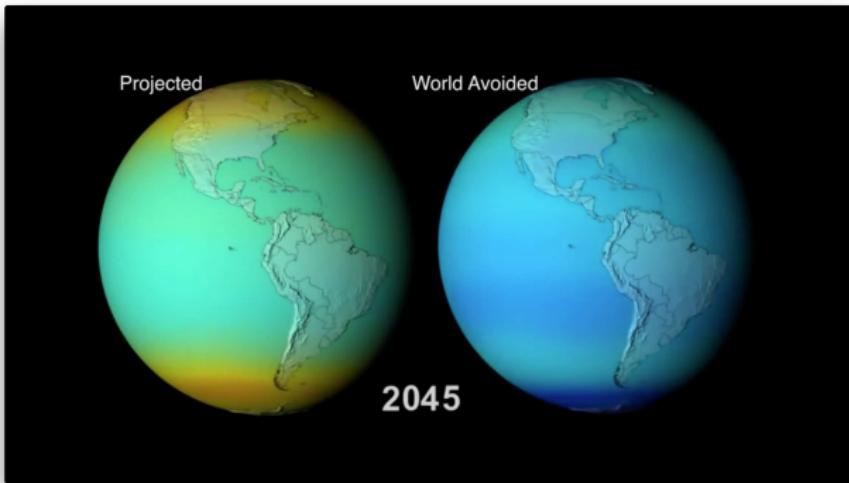
Epilepsy treatments



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 one hour after take-off on a flight from Kuala Lumpur to Beijing. The Boeing 777-200ER carried twelve crew members and 227 passengers. The airline has since announced that "it is believed that the aircraft crashed 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, although as this is, not all emergency survival equipment would have been deployed, there are contradictions in the available evidence.

The National Transportation Safety Board (NTSB) investigation found that Captain Sullenberger and his crew successfully ditched US Airways Flight 1549, an Airbus A320, into the Hudson River in New York City after a bird strike on take-off from LaGuardia Airport. This was on January 15, 2009.

Figure 12 and the video animation referenced on the second page of this article show what "typical" nose-diving of a commercial airplane looks like.

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Cong Gu is currently a member of the mathematics department of TAMU. His email address is conggu@math.tamu.edu.

Philip J. Morris is a Boeing 737 Walkin Professor of Aerospace Engineering at the University of Southern California. His email address is pjm@usc.edu.

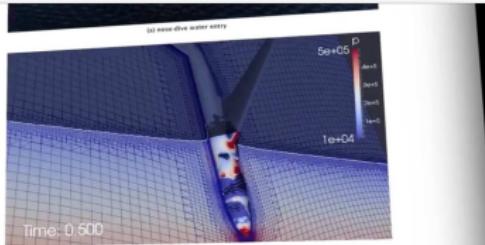


Figure 12. Pitch angle = -90° , angle of approach = 93° . This corresponds to Case 4. A video animation can be viewed at <https://www.dropbox.com/s/vaf0qenjw0lk5yz/comb-90.mp4>.

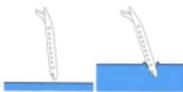
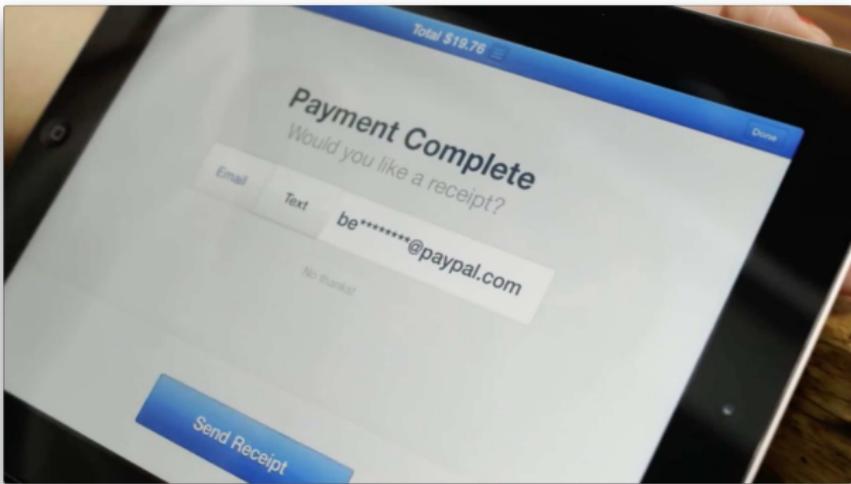


Figure 13. Schematics for nose-diving. The ocean current pushes the aircraft to the right, causing it possibly to finish belly-up on the ocean floor.
This corresponds to Case 4.

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 [WRR87]. These findings were published nearly three decades ago but remain valid today.

PayPal



Storm prediction

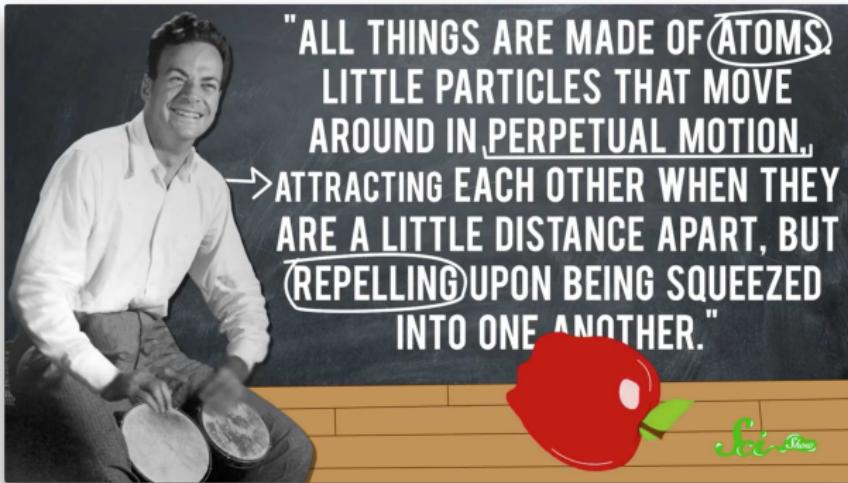


People and Personalities



and their stories

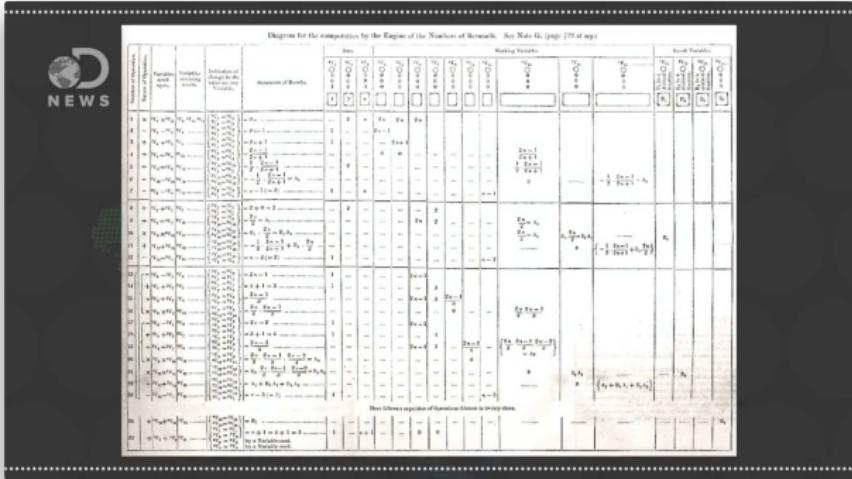
Richard Phillips Feynman 1918 – 1988



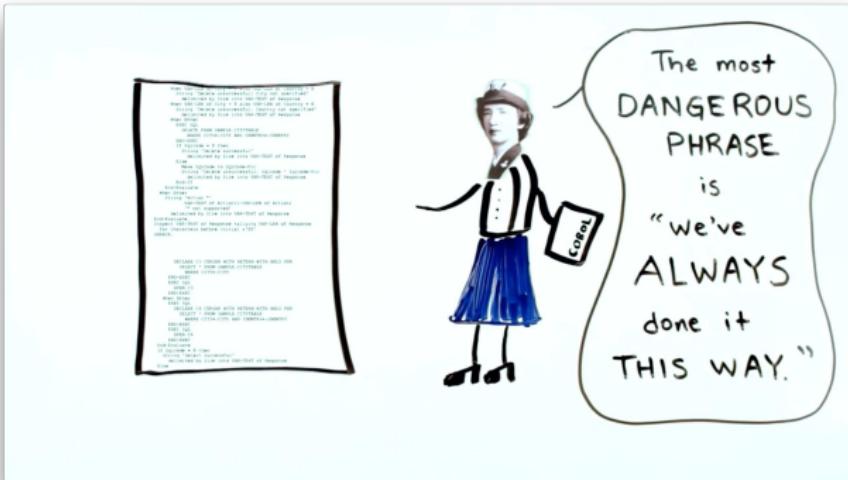
Alan Mathison Turing 1912 – 1954



Ada Lovelace 1815 – 1852



Grace Brewster Murray Hopper 1906 – 1992

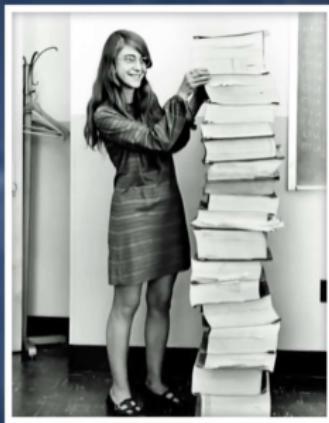


Margaret Heafield Hamilton

1936 – present

SHE BECAME
THE HEAD OF THE
APOLLO FLIGHT
SOFTWARE
DEVELOPMENT
TEAM

Credit: NASA

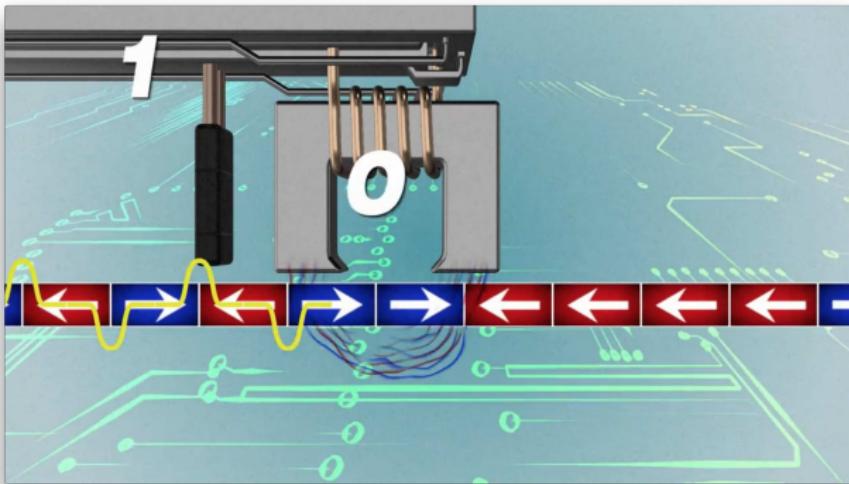


Sci

TED Ed

LESSONS WORTH SHARING

Hard Drives



Algorithm

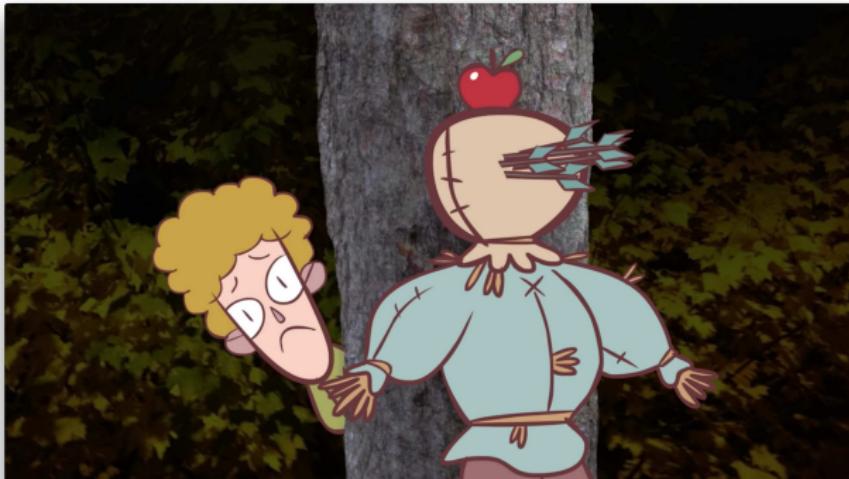
Pseudocode

let **N** = 0

For each person in room

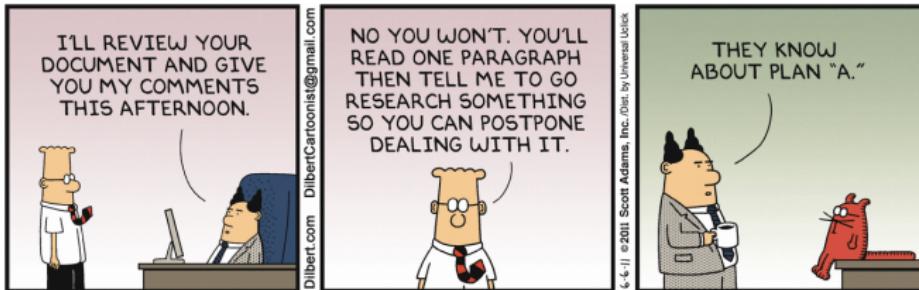
Set **N** = **N** + 1

Accuracy vs Precision



Review of Performance

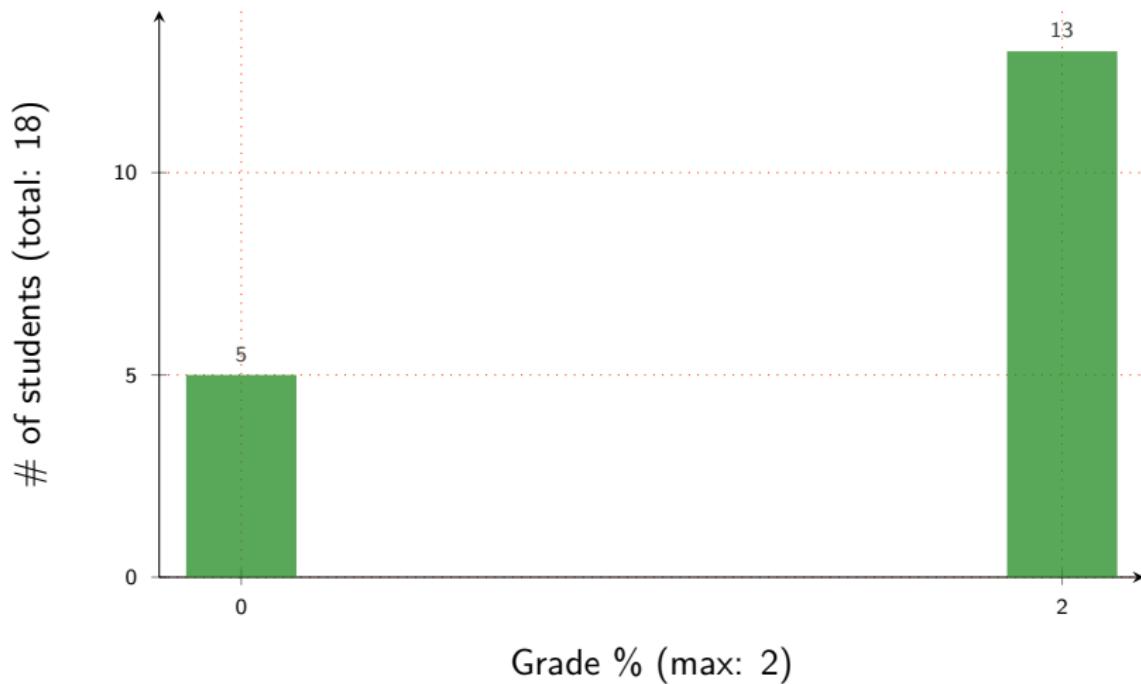
How well have we been performing?



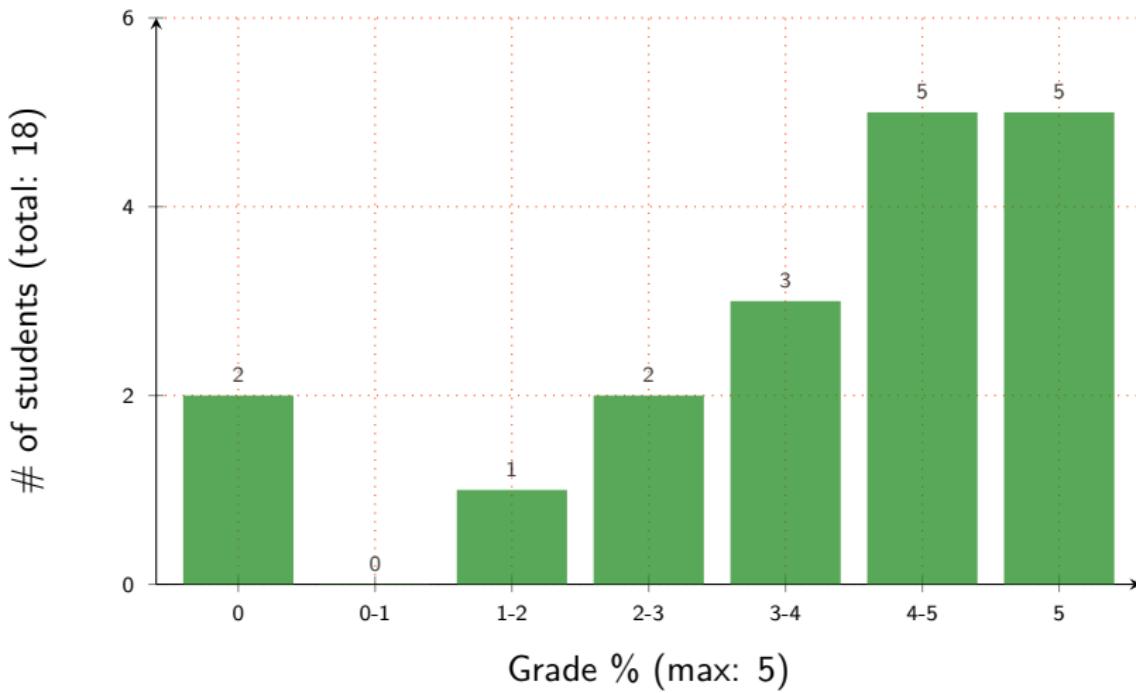
<http://dilbert.com/strip/2011-06-06/>

Active Participation #01

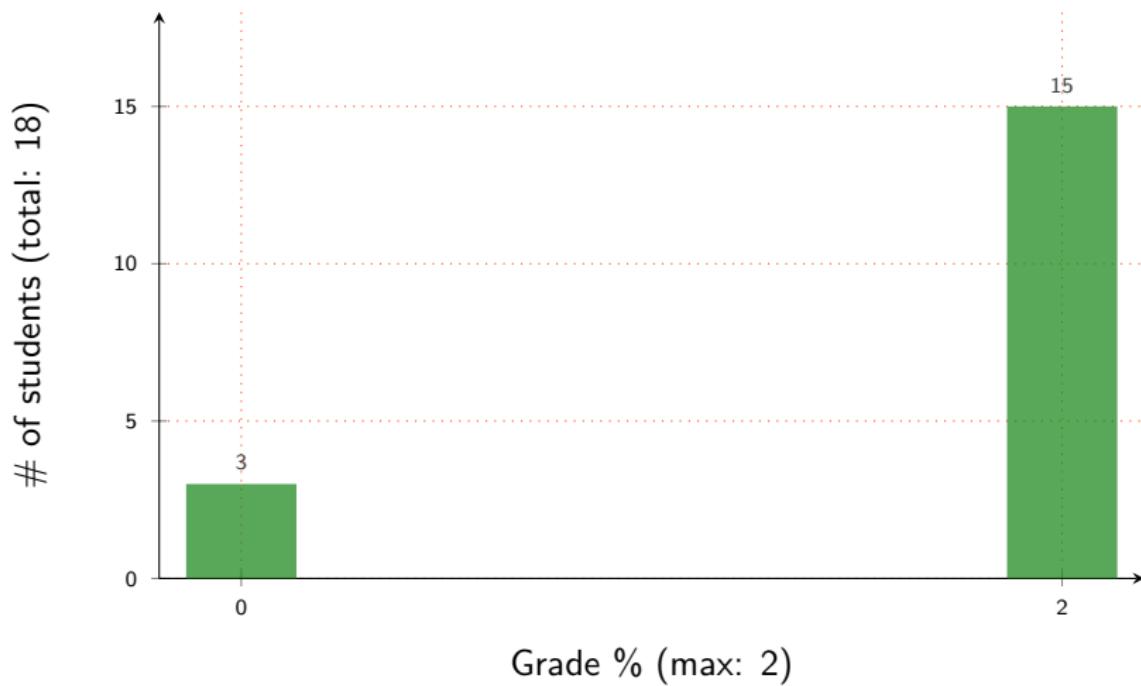
Research Marketing I: Twitter



Assignment #01

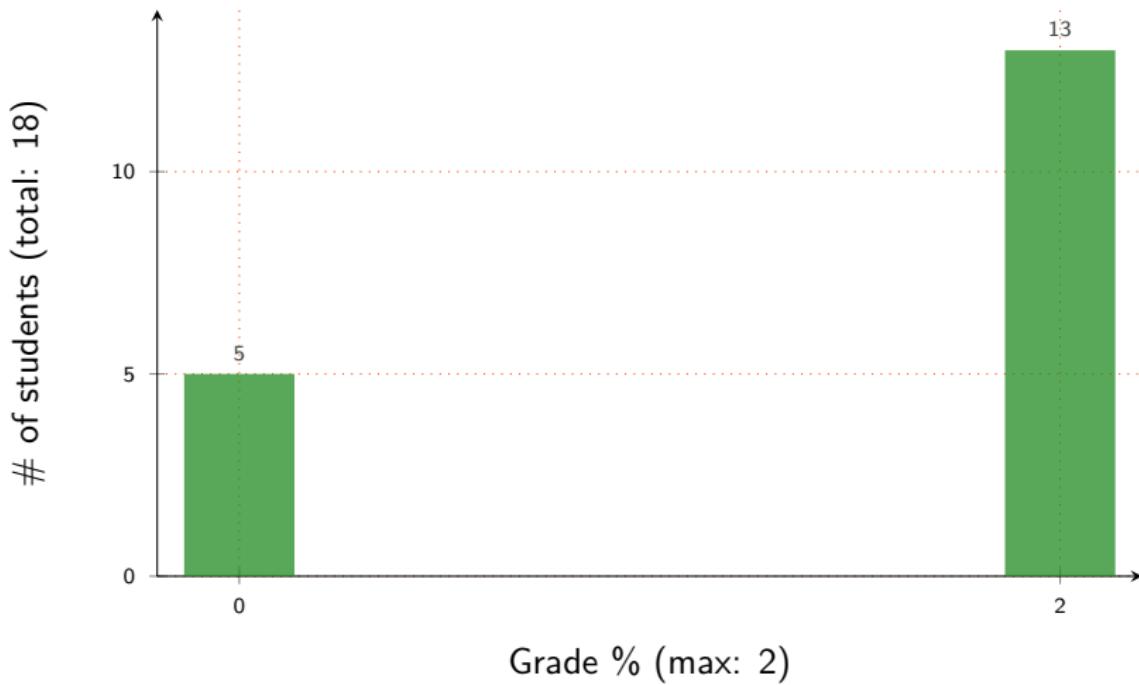


Active Participation #02 PB&J Sandwich Recipe

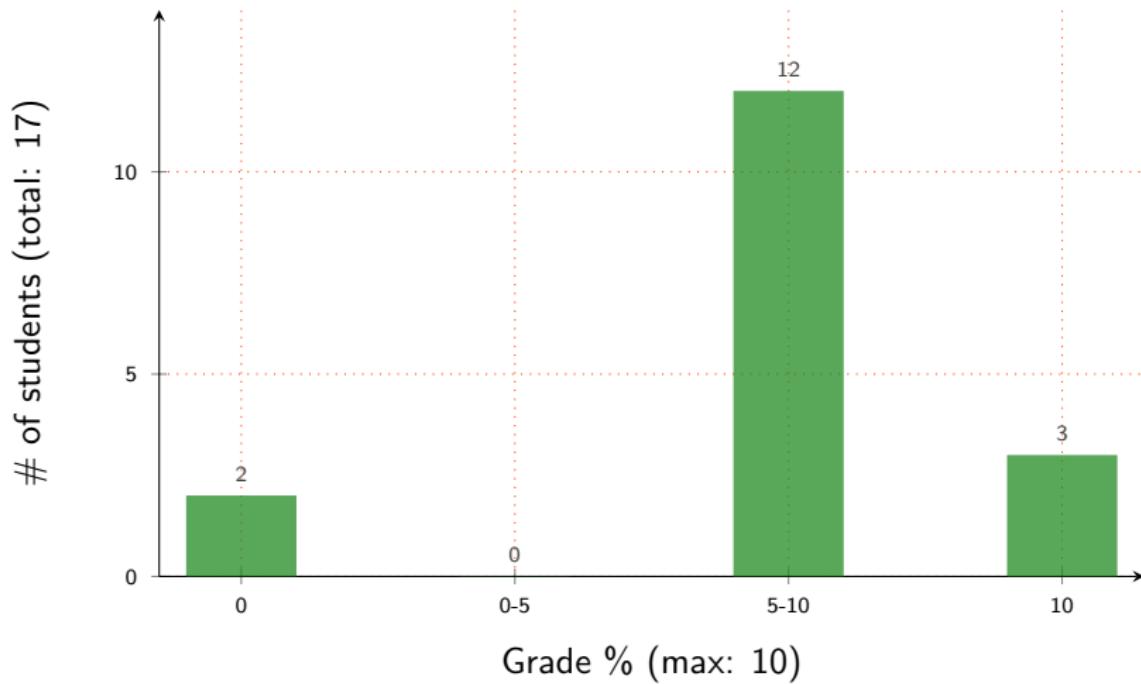


Active Participation #03

Research Marketing II: Professional/University Business Cards



Assignment #04



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

EERC B39 · (906) 487-4096 · g@mtu.edu · [@sgowtham](https://twitter.com/@sgowtham)

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