

# UN5390: Scientific Computing I

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Week #03: 2016/09/13 and 2016/09/15; No Class

Cross-listed as BE5390, EE5390 and MA5390

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



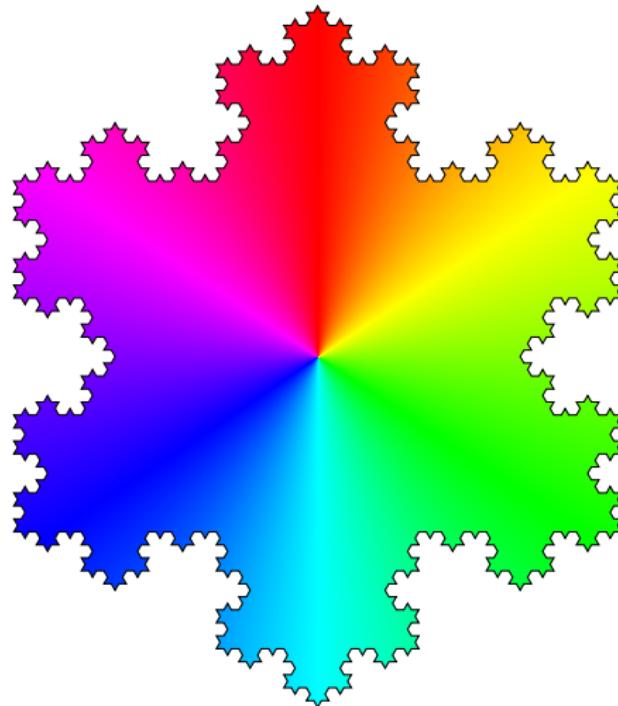
# No Class

Instructor in Alexandria, VA

Very limited internet access

## Before we meet again

- \* Review the syllabus, course material, grade through week #02, notations, active participation, free time exercises, tips, opportunities, mathematical results, videos, and training camps
- \* Complete assignment #01
- \* Catch up on life, research, and other courses



End of Tuesday lecture.

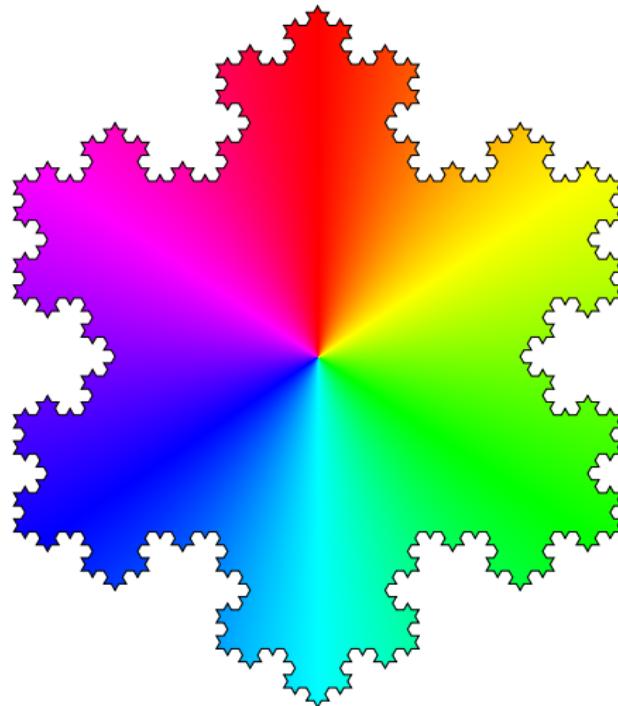
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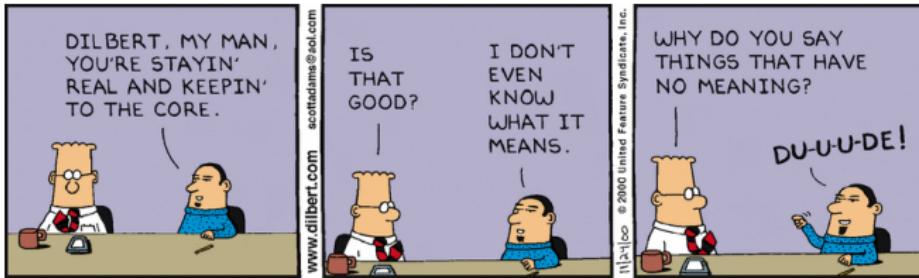
- \* Review the syllabus, course material, grade through week #02, notations, active participation, free time exercises, tips, opportunities, mathematical results, videos, and training camps
- \* Complete assignment #01
- \* Catch up on life, research, and other courses



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

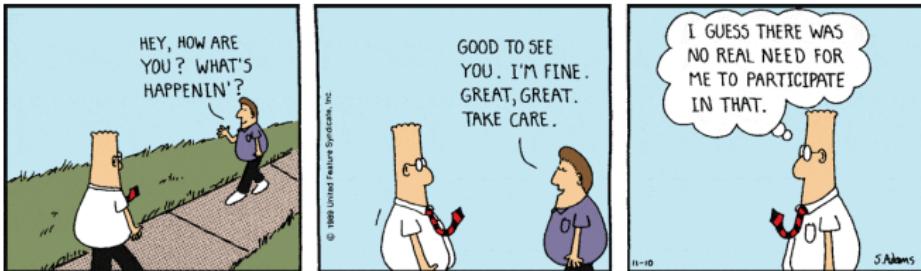
Potential pitfall ahead ... things can go lorem ipsumly wrong

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



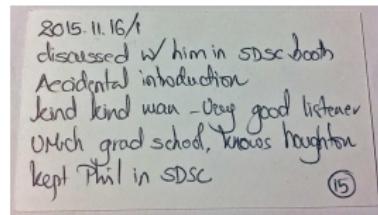
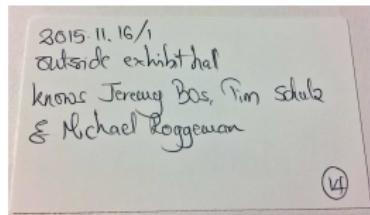
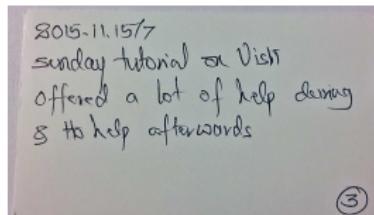
<http://dilbert.com/strip/2011-10-07/>

# Research Marketing II

## Professional business cards

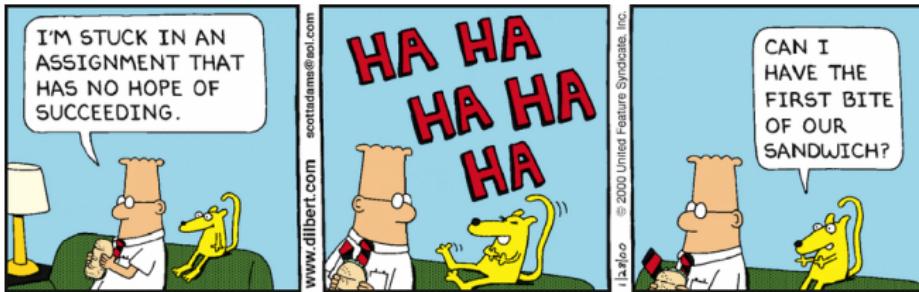
Visit Printing Services in the garden level of the Administration Building (a part of [University Marketing and Communications](#)) and get 100 professional business cards printed with the official Michigan Tech logo.

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
```

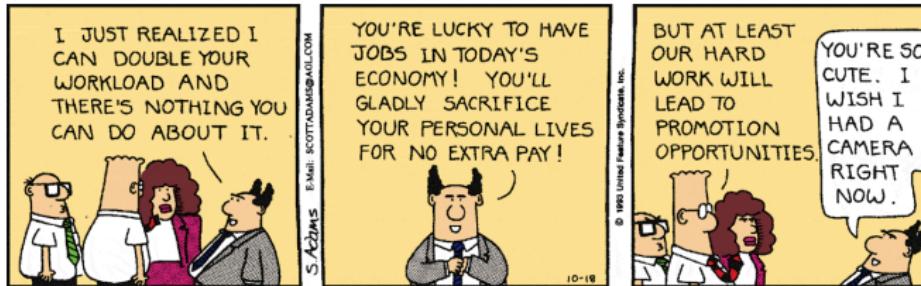


Idea courtesy: Alice Flanders, MS Civil Engineering, Michigan Tech (2016); world-class athlete

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

# 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  $\Delta t$  between lightning and thunder

[https://en.wikipedia.org/wiki/SI\\_base\\_unit](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.



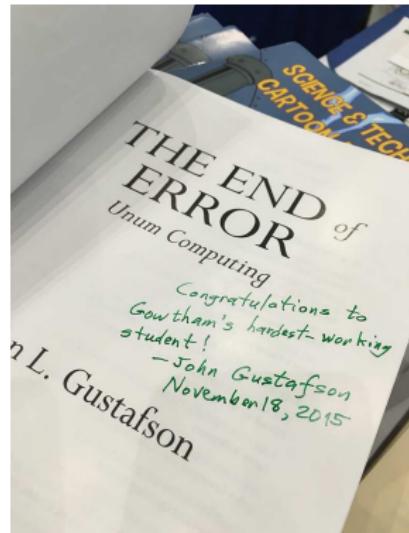
# Doing them all

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.



# 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 ( $\approx 1$  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.

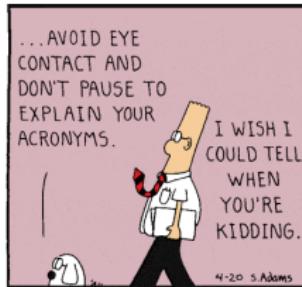
# Modify the subroutines

`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.

# 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<sup>A</sup>T<sub>E</sub>X 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<sup>A</sup>T<sub>E</sub>X workflow for assignments

Whenever you are working on the assignment

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

Replace 01 with the appropriate week number.



# L<sup>A</sup>T<sub>E</sub>X workflow for assignments

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

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

Replace 01 with the appropriate week number.

For more information, visit [https://github.com/MichiganTech/LaTeX\\_GettingStarted](https://github.com/MichiganTech/LaTeX_GettingStarted)



# $\text{\LaTeX}$ 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](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,  $\text{\LaTeX}$ , and Doxygen

It supports multiple output formats including  $\text{\LaTeX}$  (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.



# 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

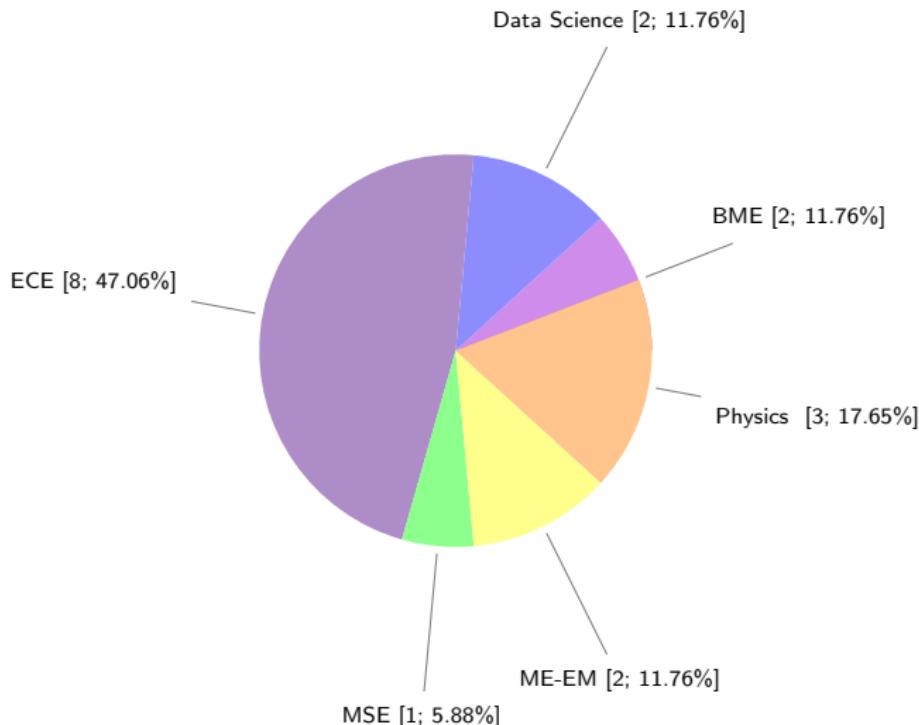
#	Name	Email	Advisor
09	Cal Riutta *	cdriutta	Jinfeng Jiang

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  $\text{\LaTeX}$  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 ( $\text{\LaTeX}$ )



- \* 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 ( $\text{\LaTeX}$ )



# 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.



# Mathematical Results

Standing the test of time

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

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



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

# Fundamental Theorem of Algebra

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

## Alternate statement #1 (proved using successive polynomial division)

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

## Alternate statement #2

The field of complex numbers is algebraically closed.

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



# Fundamental Theorem of Calculus

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

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

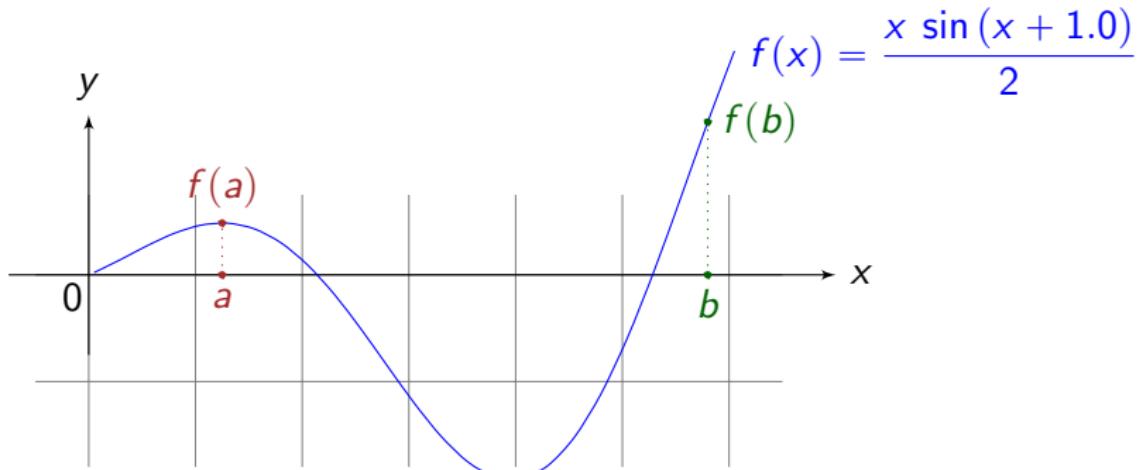
Changing the notations while retaining the underlying essence,

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

Re-arranging the terms,

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

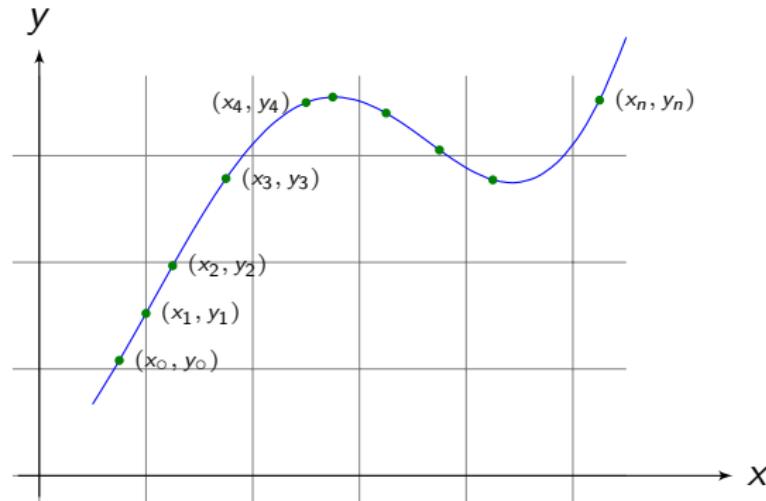
# Intermediate Value Theorem (IVT)



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

# Lagrange Polynomial Interpolation

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



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

# Lagrange Polynomial Interpolation

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

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

Lagrange basis polynomials are given by

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

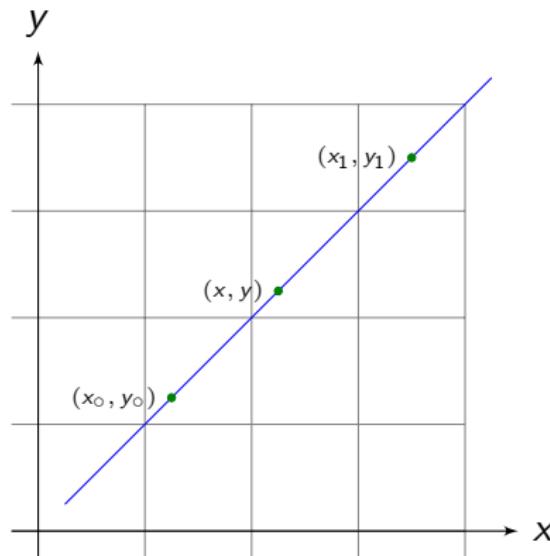
and are built to have the *Kronecker delta* property

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

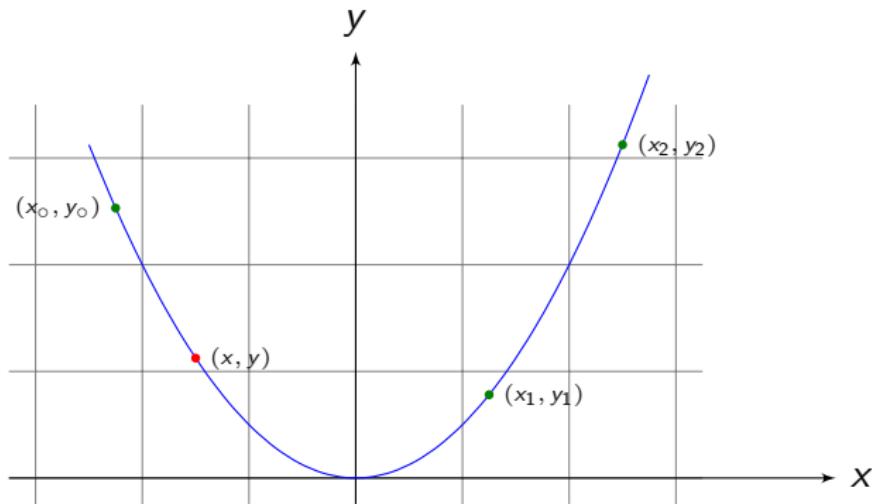
# Lagrange Polynomial Interpolation

Linear

Suppose that  $(x_0, y_0)$  and  $(x_1, y_1)$  are two known points. The linear interpolant is then a straight line between these two points.



# Lagrange Polynomial Interpolation Quadratic



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

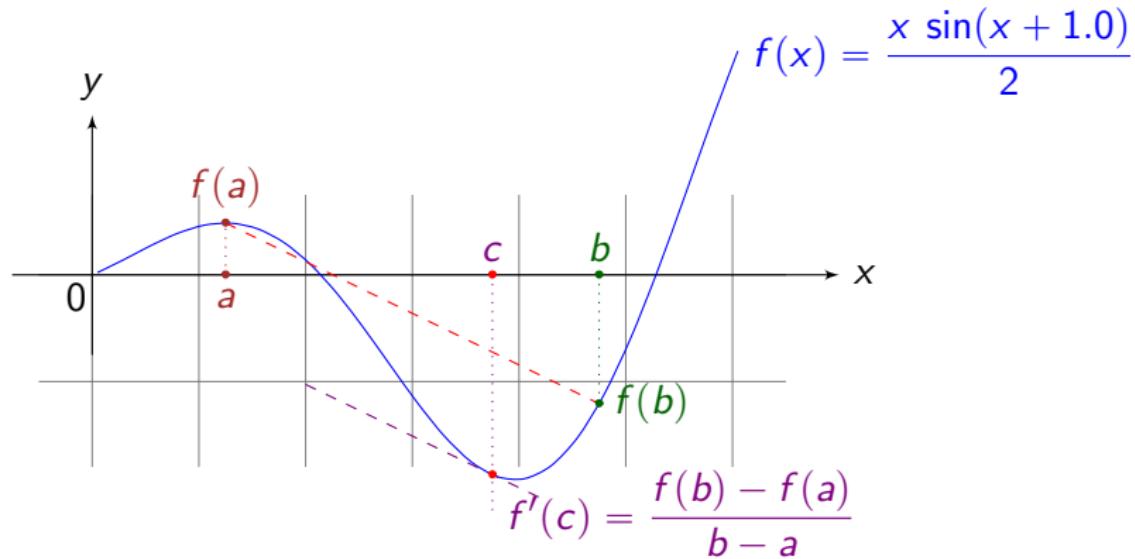
# Lagrange Polynomial Interpolation

Error analysis

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

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

# Mean Value Theorem



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



## Weighted Mean Value Theorem for Integrals

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

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

# Newton-Cotes Formula

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

Consider the integral



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

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

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

then the integral,  $I$ , takes the form

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

Isaac Newton (1642 – 1727): English physicist and mathematician

Roger Cotes (1682 – 1716): English mathematician (no photo)

# Taylor Series Expansion

If  $f(x)$  is infinitely differentiable at  $x_0$ , then

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



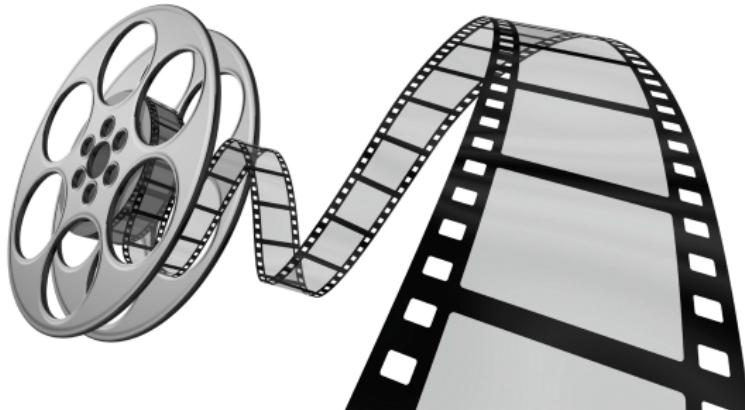
A more general form that clearly identifies the error term is given by the  $p^{th}$  order Taylor series expansion of  $f(x)$  with  $\tilde{x} \in [x, x + \Delta x]$

$$f(x + \Delta x) = \sum_{n=0}^p \frac{(\Delta x)^n}{n!} \left. \frac{d^n}{dx^n} f(x) \right|_{x=x} + \frac{(\Delta x)^{p+1}}{(p+1)!} \left. \frac{d^{p+1}}{dx^{p+1}} f(\tilde{x}) \right|_{\tilde{x} \in [x, x + \Delta x]}$$

Brook Taylor (1685 – 1731): English mathematician

# Videos

If a picture is worth a thousand words ...

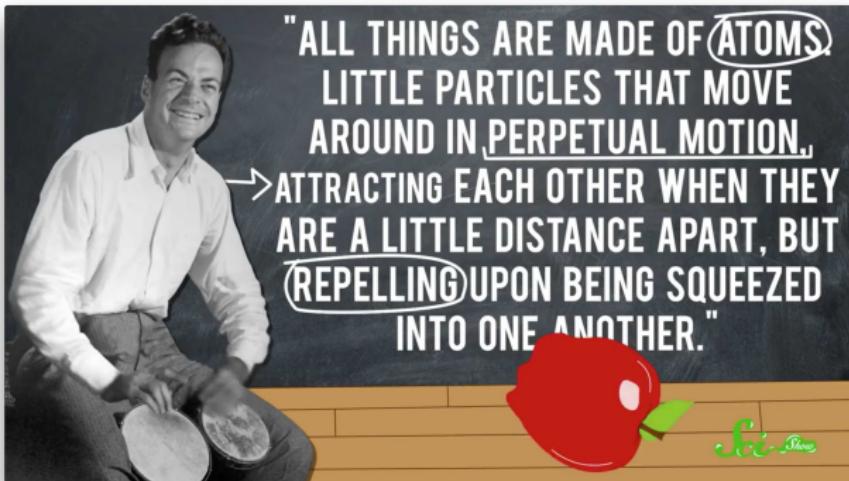


# People and Personalities

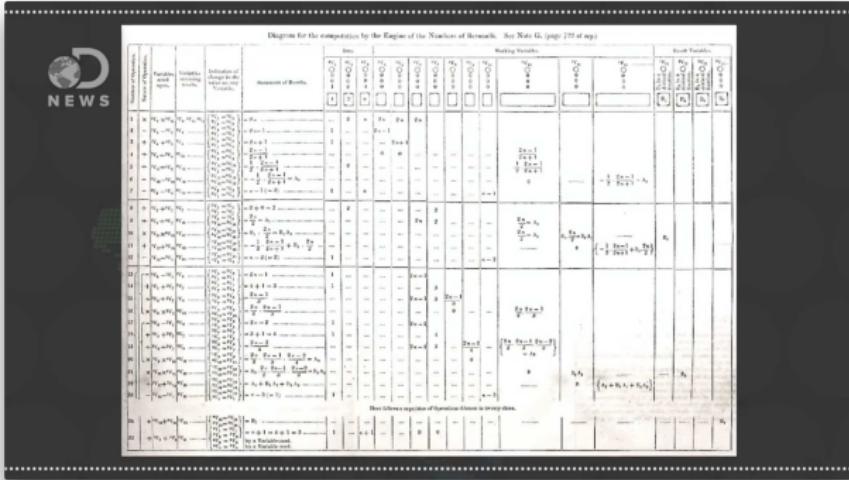


and their stories

# Richard Phillips Feynman 1918 – 1988



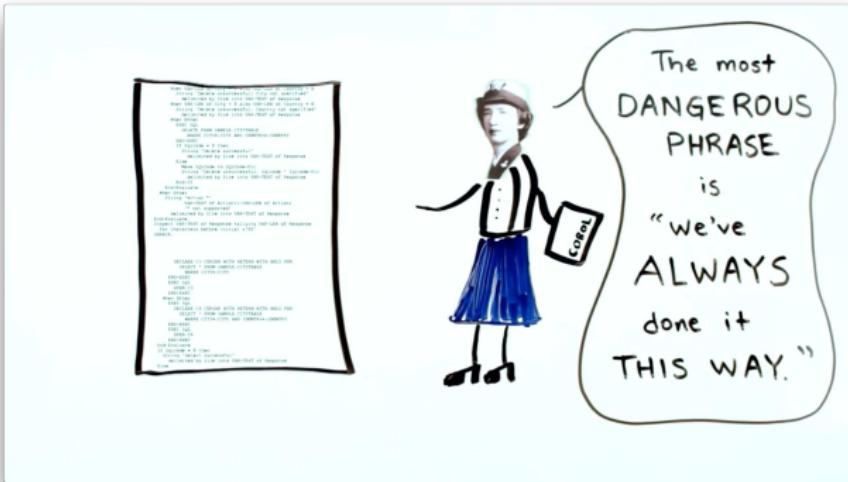
Ada August King, Countess of Lovelace 1815 – 1852



# Alan Mathison Turing 1912 – 1954



# Grace Brewster Murray Hopper 1906 – 1992



# Computer History Museum



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

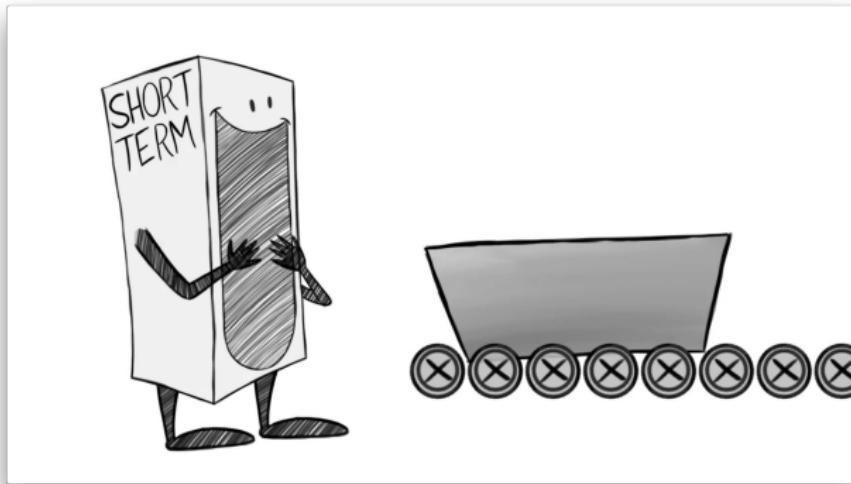
# The Fairchild Notes



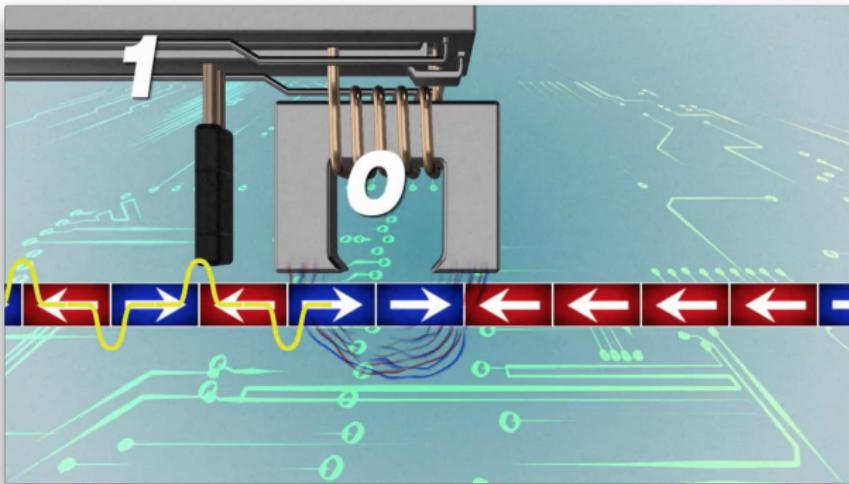
# **TED** Ed

**LESSONS WORTH SHARING**

# Computer Memory



# Hard Drives



# Turing Test



# Algorithm

## Pseudocode

let **N** = 0

For each person in room

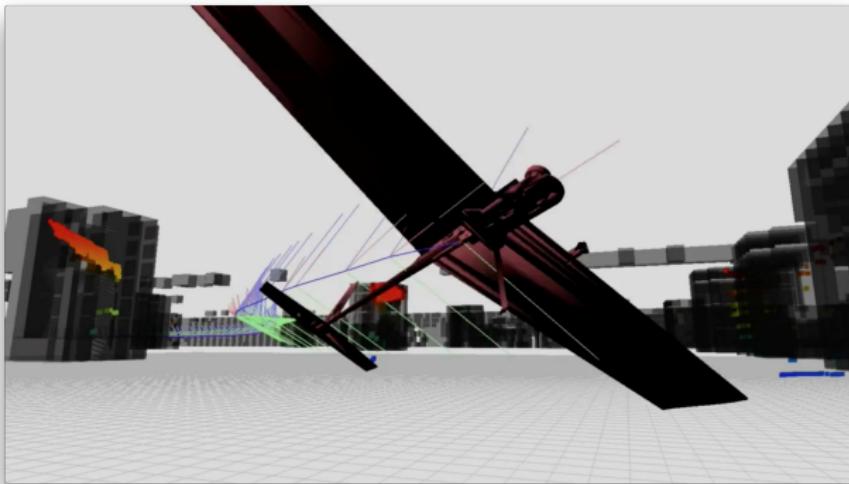
Set **N** = **N** + 1



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

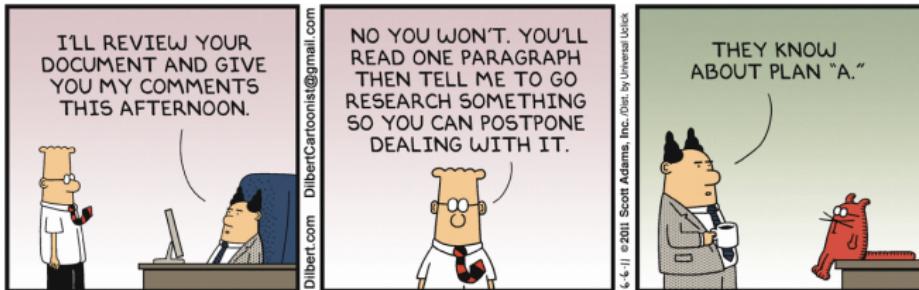
What is HPC?

# Aerospace



# Review of Performance

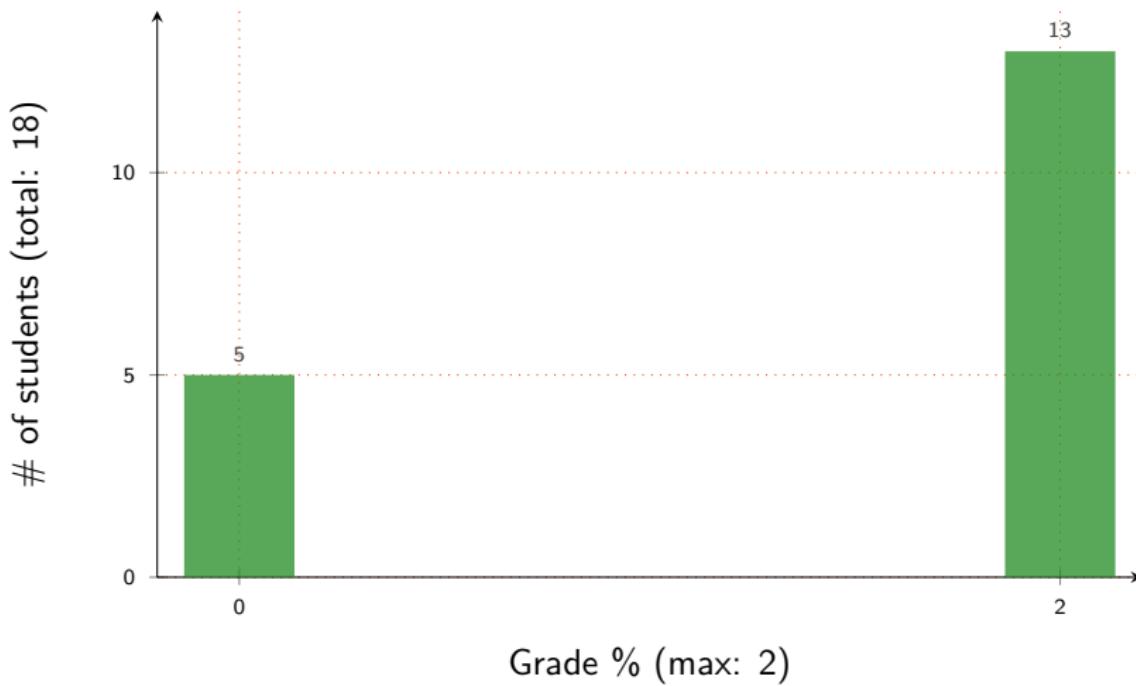
How well have we been performing?



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

# Active Participation #01

Research Marketing I: Twitter



## 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,

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

# Got questions?

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

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