Methods and Practice of Scientific Computing (NERS/ENGR 570)

Prof. Brendan Kochunas



Outline

Overview of the course

Overview of Contemporary Scientific Computing

Introduction to Linux

Learning Objectives: By the end of Today's Lecture you should be able to

• (Knowledge) Understand objectives of course

• (*Knowledge*) Have a sense/expectation for the course format and logistics

• (Knowledge) be able to give a definition of scientific computing

• (Knowledge) Provide an educated response to the survey

Course Overview

Who are we?

Prof. Brendan Kochunas

- at University of Michigan
 - Assistant Professor (2019)
 - Adjunct Lecturer since (2016)
 - Assistant Research Scientist since (2015)
 - Post-doc (2014)
 - PhD student (2009-2013)
- Education
 - PhD in Nuclear Engineering from UM (2013)
 - M.S.E in Nuclear Engineering from UC Berkeley (2008)
 - B.S. in Nuclear Engineering from Purdue University (2006)
- Developed this course from scratch
 - 7th year teaching it

GSI and Guest Lecturers

- GSI Kyle Vaughn (kcvaughn@umich.edu)
 - PhD Candidate in NERS
- Guest Lectures TBD
 - I will have some travel

Course Objectives

- Enable students who complete the course to produce software in their research that can eventually grow into high quality software used in:
 - industry
 - national labs
 - the open-source community
- What this means is, you'll learn:
 - Best practices in software engineering
 - How to optimize code
 - How to use HPC resources
 - What are the tools available (and how to use them)
 - Overall become better and more productive programmers and computational scientists

Course Policies (1)

Lecture and Lab

- Lecture (10% of grade)
 - Simple assessment guizzes after some lectures
 - If in person, please silence cell phones
 - If remote, please stay on mute
 - Laptops & Tablets are encouraged
- Lab (40% of grade)
 - Typically 7-10 days to complete labs
 - This is to accommodate having multiple assignments at once.
- Non-In-Person Instruction Modality
 - Synchronous participation strongly encouraged!
 - All lectures and labs will be recorded and posted to Canvas

Homework and Project

- Homework (15% of grade)
 - Assignment deliverables should be your own work—unless it is a group activity
 - You are encouraged to work with others on assignments
 - It is ok to use the internet as a resource for completing exercises
 - But if you do, you should reference the sources for your solution and be able to explain it.
 - If we find you neglected to cite others' work you get a zero for that exercise.
- Project (35% of grade)
 - Teams of 2 to 4 (will try to divide evenly)
 - You will propose projects and iterate with us on topic, objectives, scope, etc.
 - So be thinking about them!
 - topics that are relevant to your research. We want you to choose

Course Policies (2)

Format of assignments

- The format of assignment deliverables will be specified on a case-by-case basis.
- Expected formats include:
 - Typed documents
 - Source code
 - LaTeX
 - Google Forms
 - Program output
 - Repository commits
 - Canvas Quizzes

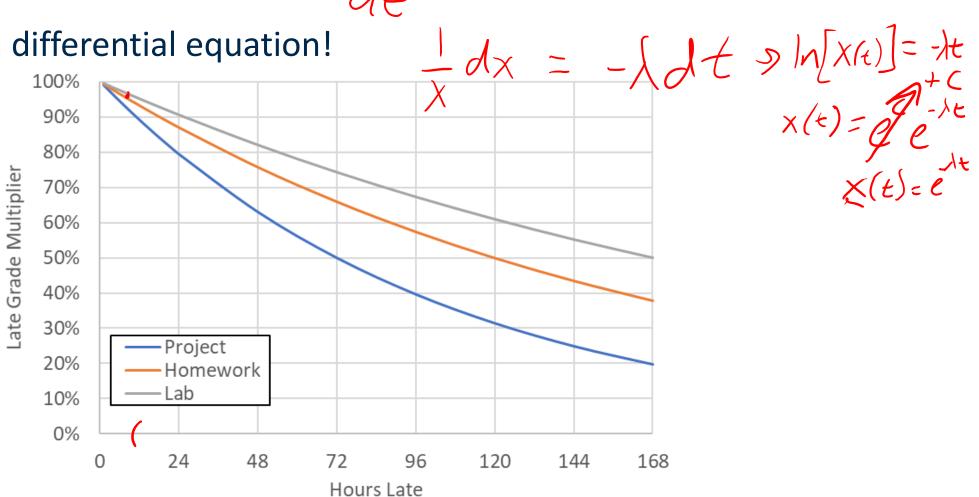
Late Assignments

- Late lab assignments will have a 7-day half-life.
 - e.g. If a lab assignment is completed
 1-week late its maximum possible
 value is 50%
- Late project deliverables have a 3-day half-life.
- Late homework assignments have a 5-day half-life.

λ Half-Life Example



Let's solve a differential equation!



Course Policies (3)

Announcements & Materials

- Announcements
 - Email announcements will be made on Canvas
 - Announcements may also be given verbally in class
 - These will be posted on Canvas
- Materials
 - Electronic material presented during lectures will be posted before the lecture.

Resources

- CAEN Lab
 - Redhat Linux environment
- HPC Machines (DO NOT ABUSE)
 - Great Lakes (University of Michigan)
- Git & Continuous Integration
 Servers
 - For some assignments

Engineering Honor Code

- Engineers must possess personal integrity both as students and as professionals. They must be honorable people to ensure safety, health, fairness, and the proper use of available resources in their undertakings.
- Students in the College of Engineering community are honorable and trustworthy persons.
- The students, faculty members, and administrators of the College of Engineering trust each other to uphold the principles of the Honor Code. They are jointly responsible for precautions against violations of its policies.
- It is dishonorable for students to receive credit for work that is not the result of their own efforts.

Office Hours & Contact info

- Prof. Kochunas
 - Email: bkochuna@umich.edu
 - Office: Cooley 2958B
 - Phone: 734-763-3867
- Office Hours (Tentative)
 - Prof. Kochunas: Monday 3:30 pm to 4:30 pm
 - Friday after lab also works, but I can't promise my availability here will be regular.
 - GSI's: Tuesday and Thursday
 - Location: PML 3017.

Go to Syllabus

Class Selected Modules

Topic			Description	
	Lecture 1		Heterogeneous Architectures	
GPU Parallelism	Lecture 2		Programming models for GPUs	
		Lab	Hardware Abstraction with Kokkos	
Testing, Testing,	Lecture 1		Testing, Verification, and Validation	
	Lecture 2		How to write a Unit Test	
Testing		Lab	Automated Testing Infrastructure	
Data and Mesh	Lecture 1		Data Format Libraries: HDF5, NetCDF, SILO	
Libraries	Lecture 2		Mesh Libraries: Libmesh, Exodus, others	
Libialies		Lab	Working with Data Libraries	
Package	Lecture 1		Package and Dependency Management with Spack	
Management &	Lecture 2		Containers: Docker and Singularity	
Containers		Lab	Spack and Singularity on Great Lakes	
	Lecture 1		Using Jupyter Notebooks with HPC	
Python for HPC	Lecture 2		Packages for Scientific Computing	
		Lab	TBD	
Debugging and	Lecture 1		Debugging Tools: DDT, GDB, and Valgrind	
Profiling Tools	Lecture 2		Performance Tools: MAP, HPCToolKit, TAU	
Profilling roots		Lab	Make it work; Make it fast Debug and Optimize	
	Lecture 1		QA, deployment, copyrights, and licensing	
Misc. Topics	Lecture 2		Visualization Tools and Best Practices	
		Lab	Working with Paraview	

Disclaimers

- Live programming is hard and computers are temperamental... please bear with us.
- Be prepared to learn (our expectations)
 - ...how to figure things out for yourself.
 - This is an invaluable skill as a researcher and computational scientist.
 - ...how to program in different languages.
 - You'll have assignments in C/C++ and Fortran.
 - None of your grade will be directly based on code written in MATLAB (Python is discouraged).
 - ...a lot about a lot of things
 - Several of the topics deserve their own semester long course, and its our job to condense this into a lecture (or 2) and give you an overview, but some depth as well.
 - By the end you will each be a "Jill" or "Jack" of "all trades", but a "master of none"
- There is no silver bullet. This is not magic. You will learn through failure, frustration, and hard work.

The Method and the Madness

Lectures and Labs

- Each lecture has 2-4 Learning Objectives
 - Assessment of learning objectives are the basis of assignments
- General Lecture format is 50 min of lecture and 30 min of hands on.
- Labs vary, but usually follow along and then work on your own for a bit.

Learning Models: Bloom's Taxonomy

EVALUATION SYNTHESIS **ANALYSIS** APPLICATION COMPREHENSION KNOWLEDGE

Bloom's Taxonomy



Produce new or original work

Design, assemble, construct, conjecture, develop, formulate, author, investigate

evaluate

Justify a stand or decision

appraise, argue, defend, judge, select, support, value, critique, weigh

analyze

Draw connections among ideas

differentiate, organize, relate, compare, contrast, distinguish, examine, experiment, question, test

apply

Use information in new situations

execute, implement, solve, use, demonstrate, interpret, operate, schedule, sketch

understand

Explain ideas or concepts

classify, describe, discuss, explain, identify, locate, recognize, report, select, translate

remember

Recall facts and basic concepts define, duplicate, list, memorize, repeat, state

What is Scientific Computing?

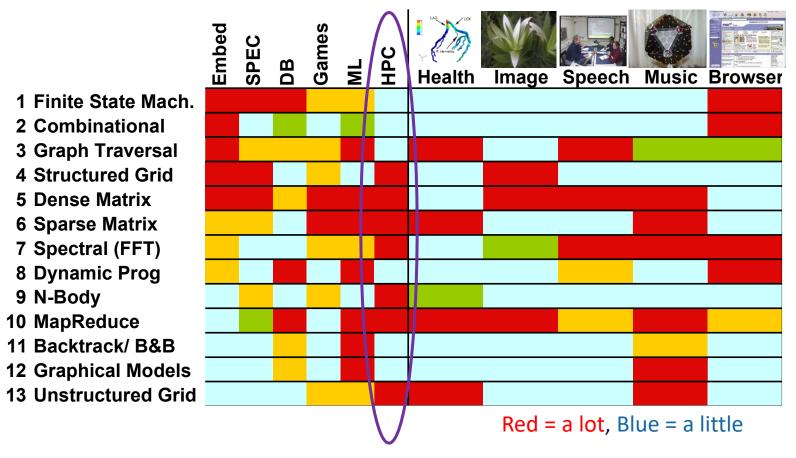
Scientific Computing as the Third Pillar of Science

- Why so much effort on computing?
- Traditional scientific and engineering method:
 - 1. Do theory or paper design
 - 2. Perform experiments, build prototypes, etc.
- Limitations
 - Too difficult—build a large wind tunnel
 - Too expensive—build a passenger jet and throw it away
 - Too dangerous—nuclear weapons
 - Too slow—climate change or astral evolution
- Computational science and engineering paradigm
 - 3. Use computers to simulate and analyze phenomenon

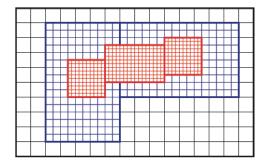


What are people doing with HPC?

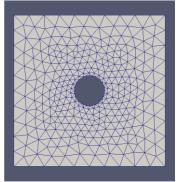
- "Landscape view of Parallel Computing Research"
 - https://www2.eecs.berkeley.edu/P ubs/TechRpts/2006/EECS-2006-183.pdf
 - https://pdfs.semanticscholar.org/p resentation/515f/88754f5d8d1d22 edaf94130cb1e6b4b0519c.pdf
- 13 Motifs (still dwarfs) in parallel computing
 - Previously 7 dwarfs



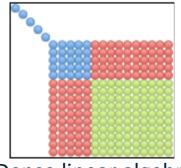
Motifs in HPC



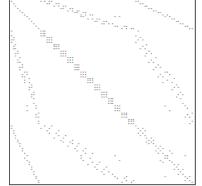
Structured Grid



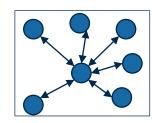
Unstructured Grid



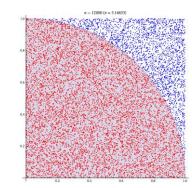
Dense linear algebra



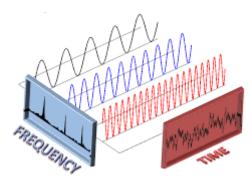
Sparse linear algebra



N-body (Fast Multipole Method)



MapReduce (Monte Carlo)



Spectral (FFT)

Hardware /

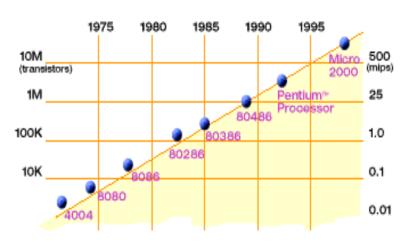
Overview of Contemporary Tools for Scientific Computing

e.g. what's been going on since you've been born $\neq 20$ $\vee eacs$

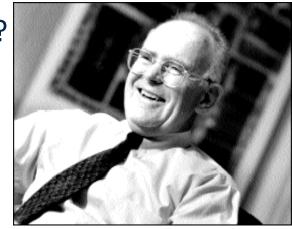


Moore's Law

- The number of transistors on a microprocessor will double every 18 months.
 - Largely been realized.
 - What does this mean for "performance"?

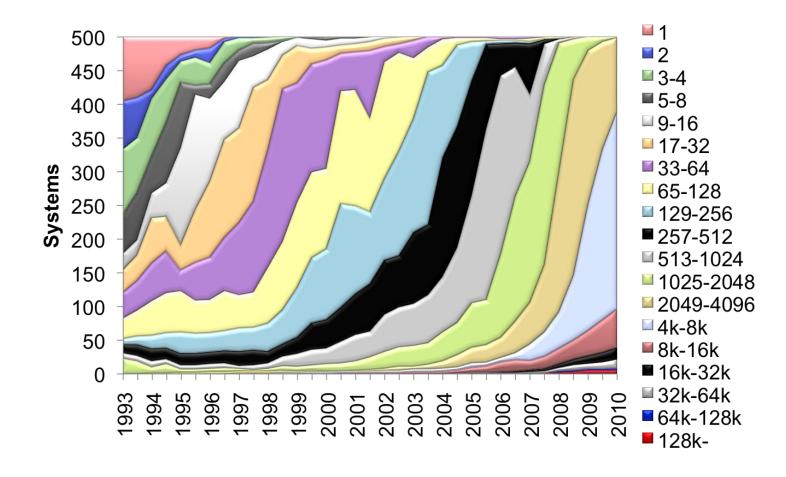


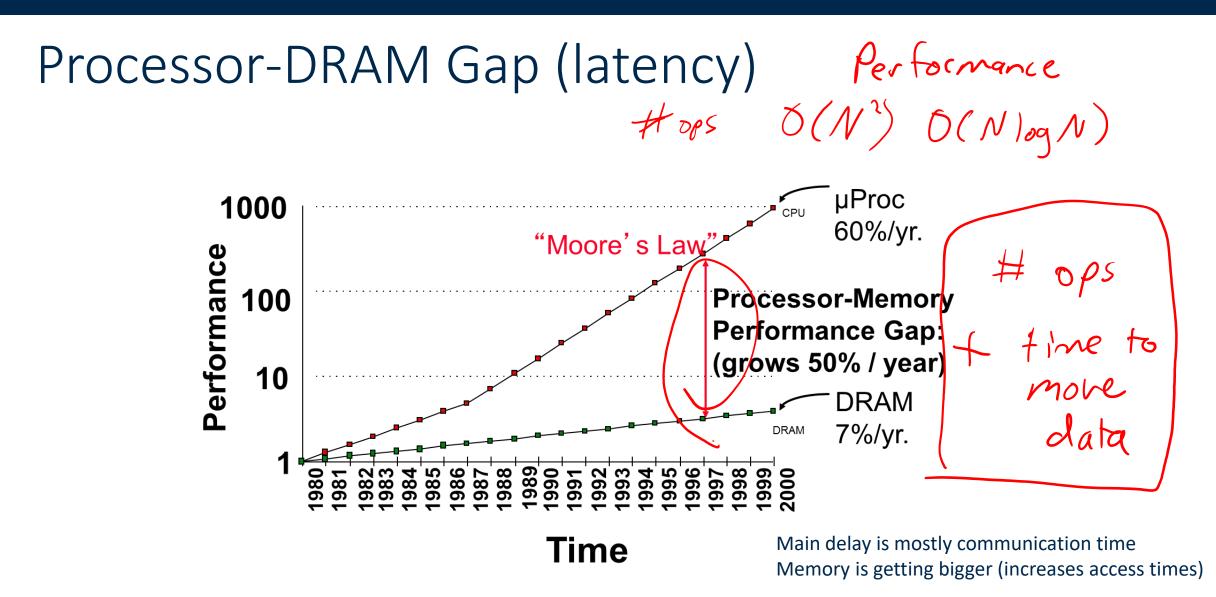
Microprocessors have become smaller, denser, and more powerful.



Gordon Moore (co-founder of Intel) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 18 months.

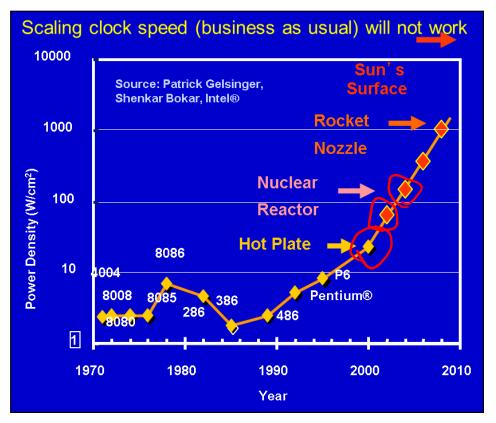
Core Counts





Present (2000-2020)

- A somewhat stable period of growth.
 - No significant changes to architecture x86 and x86_64)
- Power density begins to limit serial performance
 - clock-speeds stop increasing
- However, Moore's law continues (in an altered form)
 - Multi-core processors are de-facto standard now.
 - Parallelism (albeit modest) becomes commercial
- Heterogeneous architectures begin to appear
 - NVIDIA GPUs
 - Intel MICs
- Multiparais more energy efficient
 - Lower clock speeds
 - Less waste of power: e.g. speculation, dynamic dependence checking

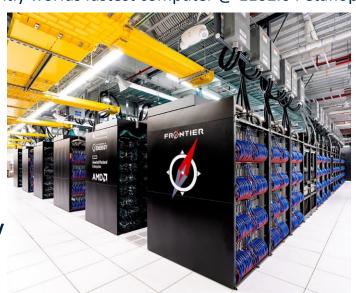


Power Density on microprocessors (The "Power Wall")

TOP500

- List the 500 most powerful computers in the world.
- Yardstick Rmax of LINPACK
 - Solve Ax=b, dense problem, matrix is random
 - Problem is dominated by dense matrix-matrix multiply
- List is updated twice a year
 - International Super Computing (ISC) conference in June in Germany
 - Super Computing conference in November in U.S.
- All information available from the TOP500 website: www.top500.org
 - Additional lists: www.green500.org (for most energy efficient supercomputers)



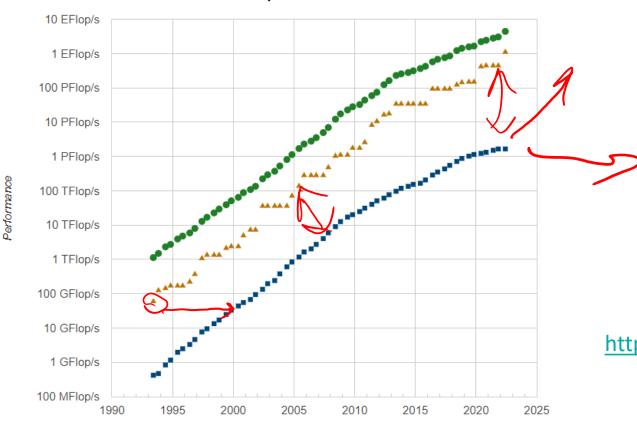


Top 10 on the Top 500

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	<u>Frontier</u> - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot- 11, HPE <u>DOE/SC/Oak Ridge National Laboratory</u> United States	8,730,112	1,102.00	1,685.65	21,100
2	<u>Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science</u> Japan	7,630,848	442.01	537.21	29,899
3	<u>LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC</u> Finland	1,110,144	151.90	214.35	2,942
4	<u>Summit</u> - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096
5	Sierra - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94.64	125.71	7,438
6	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93.01	125.44	15,371
7	Perlmutter - HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE DOE/SC/LBNL/NERSC United States	761,856	70.87	93.75	2,589
8	Selene - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	555,520	63.46	79.22	2,646
9	<u>Tianhe-2A</u> - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000, NUDT National Super Computer Center in Guangzhou China	4,981,760	61.44	100.68	18,482
10	Adastra - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot- 11, HPE Grand Equipment National de Calcul Intensif - Centre Informatique National de l'Enseignement Suprieur (GENCI-CINES) France	319,072	46.10	61.61	921

Trends in HPC Platforms (Top 500)

Performance Development



- ▲ #1 Computer
- #500 Computer
- Sum of Top500

https://www.top500.org/statistics/perfdevel/

HPC in the next 5 years (Transition to Exascale)

• Gigahertz-Kilocore-Meganode = Exascale

- We have GHzprocessprs:
 - 2.x GHz
- We have Kilocore nodes:
 - Actually 10-kilocore (4x14,080 processors)
- What about Meganode clusters:
 - Not quite there... but that's ok (9,408)







Scaling to Exascale							
	Tianhe-2 (2013)	Exa (2020)	Ratio to go				
Number of nodes	16,000 (each 2 Ivy + 3 Phi)	1,000,000	~60				
Node concurrency	24 Ivy + 171 Phi = 195 cores	1,000	~5				
Node memory (GB)	88 Ivy + 8 Phi = 96	64	(1)				
Node peak perf (GF/s)	422 Ivy + 3,009 Phi = 3,431	1,000	(1)				
Total concurrency	3,120,000	1 B	~320				
Total memory (PB)	1.536	64	~40				
Total peak perf (PF/s)	54.9	1,000	~20				
Power (MW)	17.8 (+ 24 MW cooling !)	20	(1)				

Scaling to Evascale

Big challenges to Exascale on the hardware side

- How do you control power?
- How do you cool it?
- How do you handle concurrency?
- Next generation of leadership computers recently deployed
 - OLCF Frontier (AIMID)
 - ALCF Polaris (AMD & Nvidia)
 - NERSC Perlmutter (AMD & Nvidia)

Energy to operate Supercomputer

- Today's (...well yesterdays) power costs
 - DP Double Precision
 - FMADD –Fused Multiply Add

Operation	approximate energy cost		
DP FMADD flop	100 pJ		
DP DRAM read-to-register	4800 pJ		
DP word transmit-to-neighbor	7500 pJ		
DP word transmit-across-system	9000 pJ		

- Remember that a pico (10⁻¹²) of something done exa (10¹⁸) times per second is a mega (10⁶) somethings per second
 - 100 pJ at 1 Eflop/s is 100 MW!!!!!!!!!!
 - For the flop/s!!!!!
- In the USA, the average home uses ~1.25 kW continuously (on average)
 - Commercial nuclear power plant produces 1000 MW.

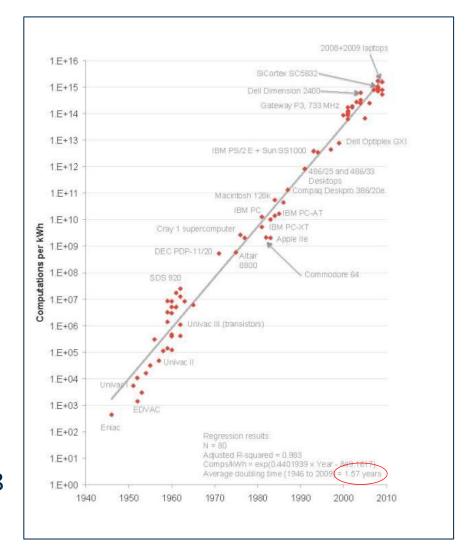
Koomey's Law

- Relates computation to energy
 - Observed exponential behavior
- "at a fixed computing load, the amount of battery you need will fall by a factor of two every year and a half."



Jonathan Koomey

- Computation is becoming more energy efficient
 - Cannot continue indefinitely. Projected to deviate ~2048





Introduction to Linux

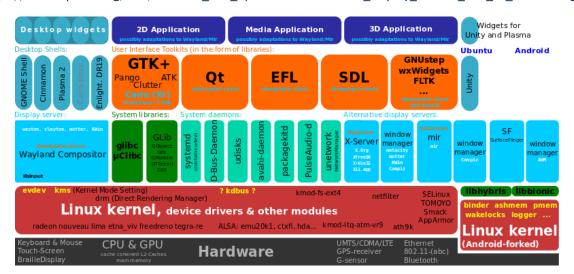
Lab on Friday: http://linuxcommand.org/tlcl.php

Background

- Linux is the open-source operating system.
 - Originally developed for the x86 architecture.
 - First released in 1991.
 - Available in many distributions both free and commercial
- Dominates the HPC world as the de-facto operating system.
 - Free or low-cost
 - Customizable
 - "Lighweight" (does not necessarily require a lot of system resources).
 - There is a Windows OS (Windows HPC Pack 2012)
- Generally preferred by programmers & developers
 - Consequently, some of its features are tailored towards these activities.
- MacOS and Android are built on Linux
- Microsoft recently deployed the Windows Subsystem for Linux

Basic Linux Software Stack

https://en.wikipedia.org/wiki/File:Free and open-source-software display servers and UI toolkits.svg



The Shell

- The linux shell is the environment (and set of rules) for the human/machine interface.
 - Command line interface
- The Shell is generally:
 - An interactive command language or scripting programming language
- Numerous types of shells
 - Bourne Shell (sh)
 - Written by Jason Bourne Stephen Bourne at Bell Labs
 - Bourne-Again Shell (bash)
 - Written as part of GNU project by Brian Fox. Default on most Linux and Mac systems.
 - · Korn Shell (ksh).
 - Written by hard rock group Korn David Korne at Bell Labs, combined sh with csh
 - C Shell (csh)
 - Written by Bill Joy (as a graduate student at Berkeley), modeled on C
 - TENEX C shell (tcsh)
 - Fancier C shell. Written by Ken Greer for TENEX operating system.
 - Z Shell (zsh)
 - Extension of sh with some useful features from bash, tcsh, and ksh
- In this course we will focus on bash.

The Command Line Interface

NO GRAPHICS: JUST TEXT

- Three standard "units"
 - Standard input (stdin) the keyboard
 - Standard output (stdout) the screen (may be buffered)
 - Standard error (stderr) also the screen, but appears immediately.

Special Characters (bash)

- Special characters can be used to "redirect" the standard units when running a command
 - Output can be "piped", (e.g. forwarded) to another command with the "|" character
 - e.g. redirect standard output to standard input of following command
 - Output can be redirected to a file with the ">" character
 - Other input can be redirected to a program with the "<" character instead of using standard input
- Commands can be sent to the background with "&"
- Old commands can be executed with "!" character
- Commands can also be chained together with ";",
 "&&", and "||"
- Evaluate commands inline with "`" or "\$ ()"

The Environment

- Environment is defined by environment variables
- Some common environment variables
 - \$PATH the default location(s) where the shell looks for executable files
 - \$LD LIBRARY PATH where to find shared libraries
 - \$HOME the home directory
 - \$USER you
 - \$HOSTNAME the machine you are on
- You can define your own environment variables
 - Useful for scripting. May be used by certain programs.
- Example
 - export PATH=/usr/bin/
 - echo \$PATH /usr/bin/

Useful commands: How to RTFM

- Several commands to show more information about a program or command
 - info
 - man
 - help
 - Command options -h, --help
- Google is your best friend
 - Before asking the GSIs or me, try Google!
- All kinds of complicated commands can be found on Stack Overflow or other forums
 - 99.9% chance that someone else has already asked your question

Useful commands: Working with files

Directories

- cd "change directory"
 - ".." is parent directory, "." is current directory, "-" is previous directory
- ls "List Segments" (list files/directories)
- pwd "Present Working Directory" (current location)
- mkdir "Make Directory"
- rmdir "Remove Directory" (must be empty)
 - rm -r "Remove (recursively)" can delete nonempty directories

Files

- cp "Copy"
- mv "Move"
- rm "Remove"
- ln link (e.g. create a shortcut)
- chmod modify file permissions
- chgrp "Change Group" ownership
- chown "Change owner"
- tar "Tape Archive." Stores/Extracts files from tape/disk archives
- gzip/gunzip-File compression/decompression

Useful commands: Probing

Specifically

- top (or htop) "Table of Processes". List of all processes running on machine
- who list all users logged in
- ps list all processes running (brief version of top)
- kill stop running a process
- lscpu show machine specs
 - cat /proc/cpuinfo
- hostname the name of the machine you're on
- du "disk usage" see how big a directory is
- df "disk free space" see how much space is left
- which shows you full path to command

Generally

- Depending on the machine, there may be several other commands used to probe different
- For HPC platforms it is useful to be able to view who is running jobs, how long they have left, how many CPU
 - We will cover all of this later.

Users

- finger list information about user
- groups list groups that a user is a member of
- date the current time

Useful commands: Navigating Servers

- ssh Secure Shell. Basis for remote connections in Linux (e.g. login to a remote server)
- scp Secure Copy. copy files to/from a remote server
- sftp Secure File Transfer Protocol. more interactive version of scp
- rsync remote synchronization, a little better than scp
- wget Web get. Download stuff from webpages.

Useful commands: Searching

- grep "Globally search Regular Expression Print"
 - Finds and prints all lines matching a given string/regex in files within a specified scope
- find Finds all files matching a certain criterion
- find -name "blah*"
 - Find all files whose names begin with "blah"
- <tab> auto-complete command, directory name, filename
 - Press it twice to list available matches

Useful commands: Parsing

- sed
 - Can print specific lines from a file
 - sed -n '50,100 p' blah.txt
 - Print lines 50 through 100 from blah.txt
 - Find & replace strings in a file
 - sed -i 's/foo/bar/g' blah.txt
 - Replace all instances of 'foo' with 'bar' in blah.txt
- awk (gawk) Text file parsing language
- cat concatenate two files
- diff (sdiff) show differences between two files

Useful Commands: History

- ctrl+r searches command history for a command
- !<exp> rerun the last command starting with <exp>
- history shows your command line history
 - history -cw clear your history (what are you hiding?! admin passwords?!)
 - Don't forget the .bash history file.

Useful commands: Misc

- ctrl+c kills a process
- ctrl+z pauses a process
- bg resume paused process in background
- fg either sends background process to foreground, or resumes paused process in foreground
- pushd, popd, dirs useful for storing and returning to a specific directory path
- head, tail, more, less quickly view (pieces of) files without entering a text editor
- touch change the time-stamp of a file
- mail send emails from the command line.

Regular Expressions (regex)

Regular Expressions

- A sequence of characters that define a search pattern
- Many special characters to facilitate advanced commands
 - . wildcard (any character is a match)
 - ? matches preceding element 0 or 1 times
 - * matches preceding element 0 to many times
 - + matches preceding element 1 to many times
 - [abc] = a OR b OR c
 - [^abc] = NOT (a OR b OR c)

Other Special Characters

- ^ = beginning of line
- \$ = end of a line
- \d matches a digit (equivalent to [0-9])
- \D matches a non-digit (equivalent to [^0-9])
- | separates multiple expressions
- {M,N} gives a range of minimum M to maximum N matches
 - {M} matches exactly M times
 - {M,} matches at least M times
 - {0,N} matches at most N times

Examples:

- egrep '^foo|bar\$' blah.txt match any line in blah.txt that starts with foo or ends with bar
- egrep (0-9) + (0-9)' blah.txt match any line with a digit, one or more spaces, and a letter
- egrep '^[aeiou]' blah.txt match any line that starts with a vowel

Bonus Useful commands: Basic Sysadmin

- sudo "Super User DO" execute command with administrator privileges
 - Will ask for admin password
 - Usually won't be available on a large shared machine, but be careful if you actually have privileges
- useradd create a new user
- usermod modify an existing user
- passwd change password
- yum (rpm) Yellowdog Updater, Modified (Redhat/CentOS).
 Manage installed software.
 - apt Advanced Packaging Tool (Ubuntu). Manage installed software.
 - apt-get, apt-cache
- cron (crontab) schedule a recurring task