Introduction to High Performance Scientific Computing

Autumn, 2017

Lecture 1

Instructor

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Office hours: Mondays 5-6pm, MLC
Thursdays 4-5pm, MLC
(First office hour on Monday, 9/10)

Weekly schedule

- Lectures:
  Monday, 11-12, Huxley 340
  Thursday, 11-12, Huxley 340
- Labs:
  Tuesday, 5-6pm, MLC (Huxley 414)
  or
  Wednesday, 10-11am, Huxley 340
- Only need to attend *one* lab session

  CDT-only lab: 11am-12pm, RSM 3.38
- Wednesday 10am lab requires laptop with necessary software installed (more on this later)

Syllabus

Lectures 1-2: Unix basics, version control with git/bitbucket

Lectures 3-6: Programming and scientific computing with Python

Lectures 7-10: Modular programming with Fortran, libraries, makefiles, coupling Fortran+Python

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Syllabus

Lectures 11-14: Introduction to parallel computing and OpenMP

Lectures 15-16: Distributed memory computing with MPI, parallel libraries

Lectures 17-20: Basic computer architecture, cloud computing, cluster computing with Python and Spark

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Assessment

3 Programming assignments
HW1: Assigned 23/10, due 2/11 (**20%**)
HW2: Assigned 6/11, due 16/11 (**20%**)
HW3: Assigned 20/11, due 29/11 (**15%**)

1 Programming Project (45%)
Assigned 30/11, due 15/12

Submitting HW1 **commits you to the course**

CDT students: Will be contacted about assessment separately

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Online material

- Main resource is course webpage:

  http://imperialhpsc.bitbucket.io/

- Slides will be available before every lecture

  All course material will be available on course bitbucket page (more on this later):

  https://bitbucket.org/ImperialHPSC/m3c2017

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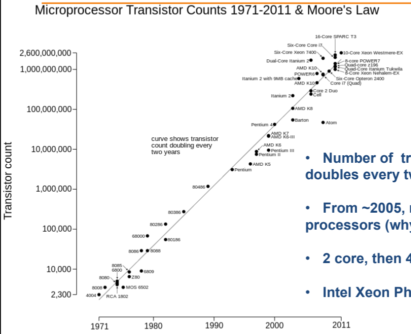
Moore's law



- Number of transistors on chip doubles every two years
- From ~2005, multicore processors (why?)
- 2 core, then 4, 6, 8, 16
- Intel Xeon Phi: 60+ cores!

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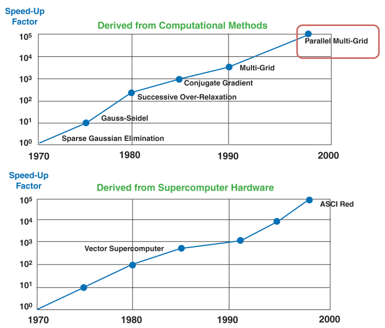
"Transistor Count and Moore's Law - 2011" by Wgsimon - Own work. Licensed under CC BY-SA 3.0 via Wikimedia Commons - http://commons.wikimedia.org/wiki/File:Transistor_Count_and_Moore%27s_Law_-_2011.svg#/media/File:Transistor_Count_and_Moore%27s_Law_-_2011.svg

Algorithms and hardware



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SIAM Rev (2001)

High-end HPC

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660

Historically: cluster computing limited to national labs, research universities

But now…

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Cluster computing is mainstream

Big data means big computers!

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Cluster computing is mainstream

amazon web services™

Google Cloud Platform

Microsoft | Cloud Services
We're all in.

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Course objective

- Cluster computing is not free!
- Important to:
  - choose right tools
  - use them effectively

This course provides foundation for "intelligent, informed" computing.

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Software tools

Useful to classify tools as *scientific* or *general purpose*

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Software tools

Useful to classify tools as *scientific* or *general purpose*

Examples:

Scientific	General purpose
Matlab	Python
Fortran	C++
R	Java

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Software tools

Languages are *compiled* or *interpreted*

Software tools

Languages are *compiled* or *interpreted*

Compiled	Interpreted
Fortran	Python
C++	Matlab
Java	R

Software tools

This course:

Python: interpreted, general purpose

Fortran: compiled, scientific

Operating systems

Most HPC and scientific computing requires Unix (or Unix-like terminals)

Linux and Mac OS are built on Unix (and have terminal apps)
- Fairly straightforward to install course software

Windows:
- Not well-suited for HPC
- Can get Unix terminal with cygwin
- For this course: Should install Linux virtual machine (VM) and install software within the VM
- MLC computers have Linux VMs installed (go try them out!)

Instructions for installing course software available online: http://imperialhpsc.bitbucket.io/

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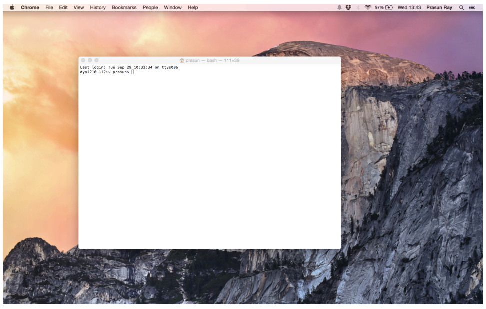
Unix terminal

Terminal on a mac:



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12 Unix commands

Navigation:

pwd: print working directory (where am I?)
ls: list of directory contents (what is here?)
cd: change directory (let's go somewhere else)

```
$ pwd
/Users/prasun/Documents/repos/m3c2017
$
$ ls
Readme.md lectures
$
$ cd lectures
$
$ ls
lecture1
```

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12 Unix commands

Manipulate files and directories:

cp: Make copy of a file
mv: Move or rename a file
rm: Remove a file
rm –r : Remove directory and all of its contents (dangerous!)

```
$ ls
Readme.md lectures
$
$ cp Readme.md Readme.md_copy
$
$ ls
Readme.md Readme.md_copy
    lectures
$
$ mv Readme.md_copy
Readme.md_copy2
$
$ ls
Readme.md Readme.md_copy2
    lectures
$
$ rm Readme.md_copy2
$
$ ls
Readme.md lectures
```

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12 Unix commands

Info about contents of file:

cat: List contents of file
head -n: List first n lines
tail -n: list last n lines
grep: search within file for a string

```
$ cat example.txt
This is an example text file.
This is line 2.
This is line 3.
This is the last line.
$
$ head -1 example.txt
This is an example text file.
$
$ tail -2 example.txt
This is line 3.
This is the last line.
$
$ grep last example.txt
This is the last line.
```

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12 Unix commands

Getting help:
man: manual page for a command

Try *man ls*. What does *ls -l* do? *ls -a*?

What if you don't know name of command?

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

or google.

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12 Unix commands

The 12 commands:

1. pwd
2. ls
3. cd
4. cp
5. mv
6. rm
7. rm –r
8. cat
9. head –n
10. tail –n
11. grep
12. man

This is "basic" Unix. Can do much more!

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A little more Unix

Instead of outputting to screen, can output to file using ">"

```
$ ls
example.txt  lecture1

$ grep last example.txt > output.txt

$ ls
example.txt  lecture1  output.txt

$ cat output.txt
This is the last line.
```

Lines in example.txt containing "last" are written to output.txt

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A little more Unix

Command can be executed sequentially (they can be "piped") using "|"

```
$ head -2 example.txt | grep line > output.txt
$
$ cat output.txt
This is line 2.
```

First two lines in example.txt are searched for the string "line" with results being written to output.txt

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An example

You run optimization software that gives output that looks like:

```
INPUT:endgeom
INPUT:azimuthal 9 0.1
INPUT:polar 5
INPUT:begin

 k-cactus is   1.402458

TIMING: Module: cpu        10.03 wall        10.04 Overall: cpu        29.00 wall        29.29
==================================================================================
==================
INPUT:EDIT 4

CALLING EDIT(INTERFACE_NO=  4)

INPUT:begin
**************************************************************************************************************
INTERFACE    4  EIGENVALUE  1.402458  OVERALL MWd/t   0.0000E+00 BURNUP TIME   0.0000E+00
DAYS

==================================================================================
=======================================
RUN SET    1
```

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An example

We only care about the "k-cactus" values which appear several times. How do we extract them?

```
INPUT:endgeom
INPUT:azimuthal 9 0.1
INPUT:polar 5
INPUT:begin

 k-cactus is   1.402458

TIMING: Module: cpu        10.03 wall        10.04 Overall: cpu        29.00 wall        29.29
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DAYS

==================================================================================
=======================================
RUN SET    1
```

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An example

Using grep:

```
$ grep cactus datafile.out
 k-cactus is   1.402458
 k-cactus is   1.386050
 k-cactus is   1.377296
 k-cactus is   1.352324
 k-cactus is   1.328779
```

But what if we only want the numbers?

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An example

Using grep:

```
$ grep cactus datafile.out
 k-cactus is   1.402458
 k-cactus is   1.386050
 k-cactus is   1.377296
 k-cactus is   1.352324
 k-cactus is   1.328779
```

But what if we only want the numbers?

Use "cut":

```
$ grep cactus datafile.out | cut -d s -f 3
   1.402458
   1.386050
   1.377296
   1.352324
   1.328779
```

Questions: How do we store these numbers in a file? How do we find out what the flags after "cut" are doing?

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What next?

- **If you have your own laptop/desktop: start installing course software – see webpage for instructions**
- **If you don't, try out the virtual machines and these Unix commands on the MLC computers -- look for the "oel" icon on the desktop**
- **Start working through introductory Python videos and exercises**
  - **1st video should be online Friday morning**

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