High Performance Computing

Autumn, 2018

Lecture 1

Imperial College
London

Instructor

Prasun Ray
Teaching Fellow
Department of Mathematics
p.ray@imperial.ac.uk
Huxley 6M20
Office hours Tuesdays 5-6pm, MLC
Thursdays 4-5pm, MLC
(First office hour on Tuesday, 9/10)

Weekly schedule

- **Lectures:**
  Tuesday, 2-3pm, Huxley 311
  Thursday, 9-10am, Huxley 340

- **Labs:**
  Tuesday, 4-5pm, MLC (Huxley 414)
  or
  Wednesday, 10-11am, MLC

- **Only need to attend *one* lab session**

CDT students: alternate lab sessions have been arranged

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

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

Assessment (tentative)

3 Programming assignments
HW1: Assigned 22/10, due 1/11 (**20%**)
HW2: Assigned 5/11, due 16/11 (**25%**)
HW3: Assigned 19/11, due 28/11 (**25%**)

1 Programming Project (30%)
Assigned 29/11, due 14/12

Submitting HW1 **commits you to the course**

CDT students: Will be contacted about assessment separately

Online material

- Main resource is course webpage:

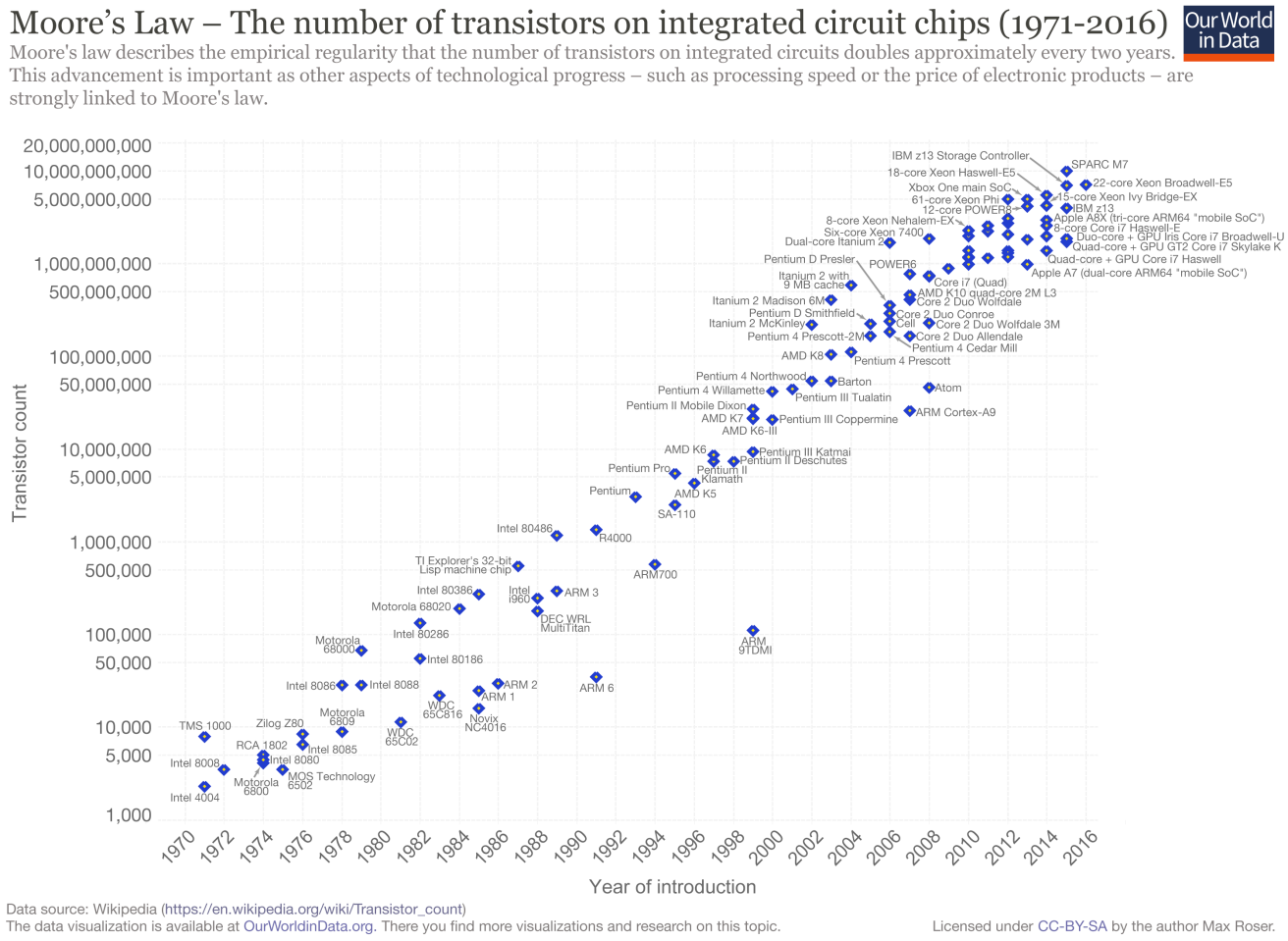
  http://imperialm3c.bitbucket.io/

- Slides will be available before every lecture

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

  https://bitbucket.org/imperialm3c/m3c2018

Moore’s law

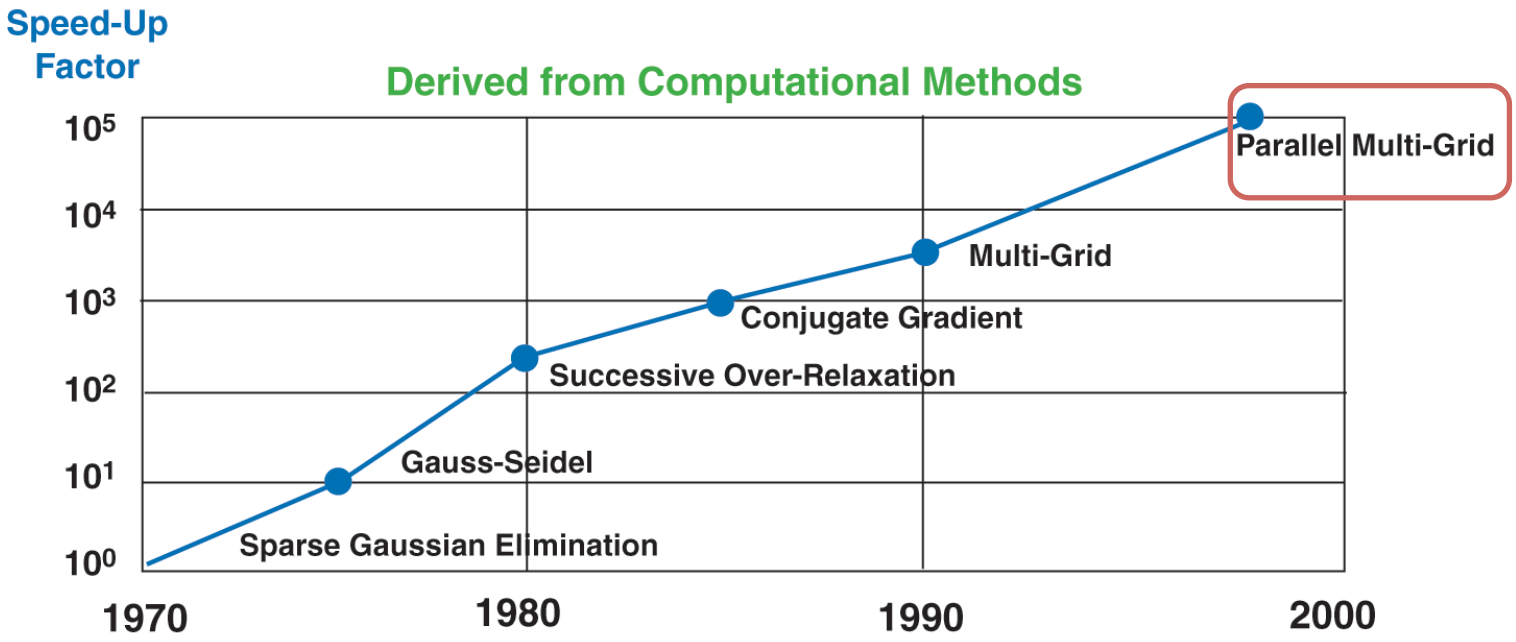


Data source: Wikipedia (https://en.wikipedia.org/wiki/Transistor_count)
The data visualization is available at OurWorldinData.org. There you find more visualizations and research on this topic.

Licensed under CC-BY-SA by the author Max Roser.

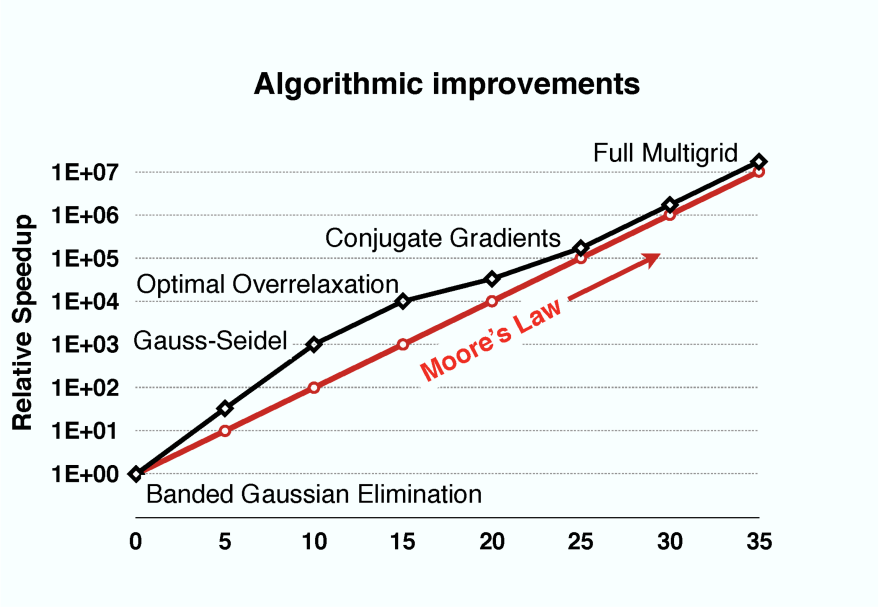
- **Number of transistors on chip doubles every 2 years**
- **From ~2005, multicore processors (why?)**
- **2 core, then 4, 6, 8, 16**
- **Intel Xeon Phi: 60+ cores!**

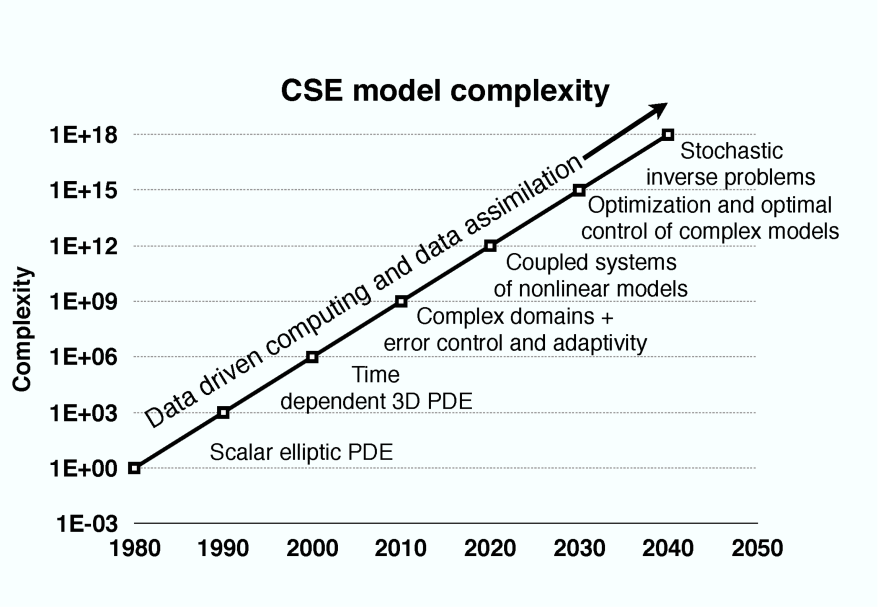
Algorithms and hardware



SIAM Rev (2001)

Algorithms and hardware





SIAM Rev (2001)

High-end HPC

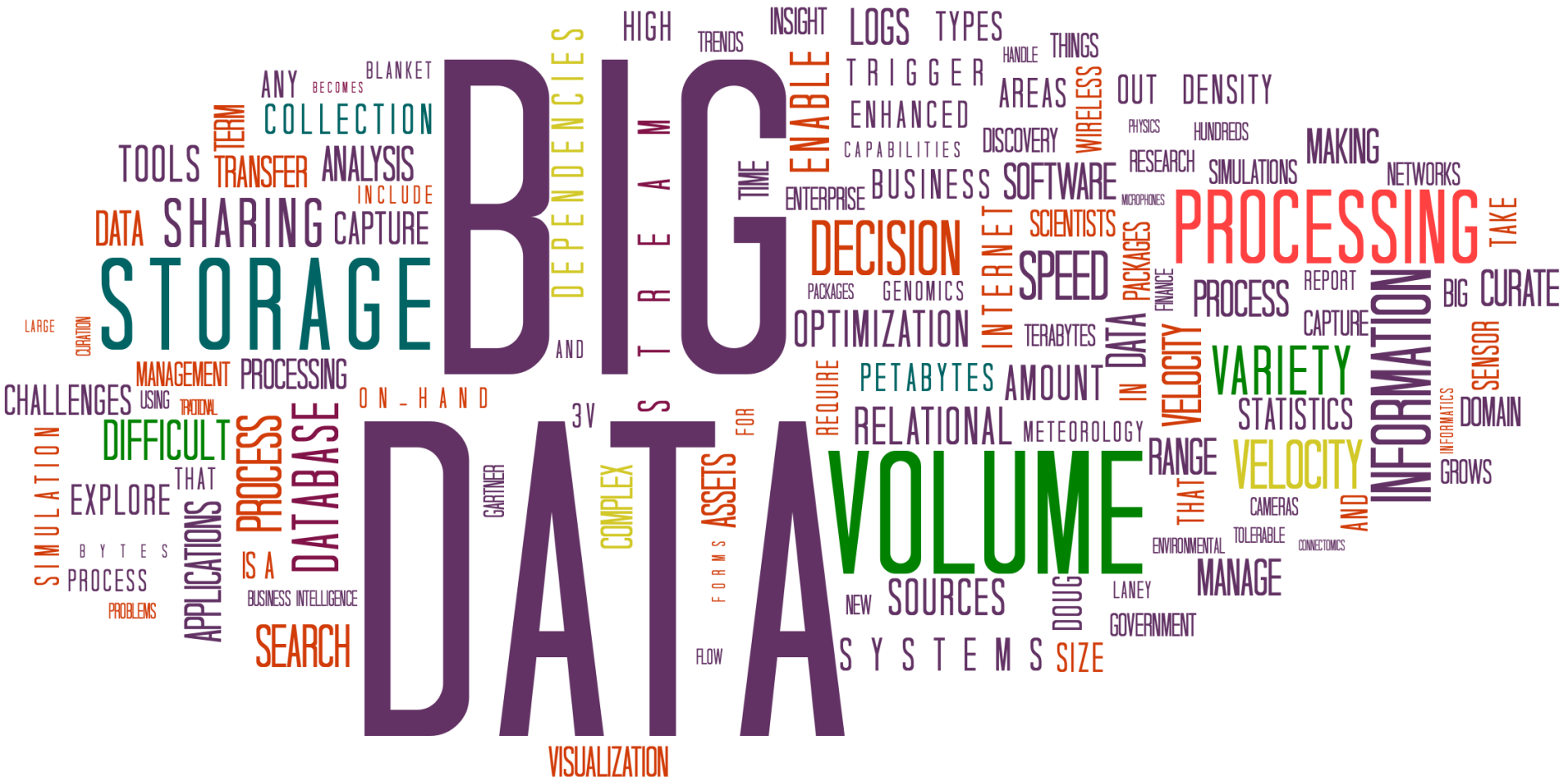
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,282,544	122,300.0	187,659.3	8,806
2	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
3	**Sierra** - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/NNSA/LLNL United States	1,572,480	71,610.0	119,193.6	
4	**Tianhe-2A** - 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	61,444.5	100,678.7	18,482
5	**AI Bridging Cloud Infrastructure (ABCI)** - PRIMERGY CX2550 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR , Fujitsu National Institute of Advanced Industrial Science and Technology (AIST) Japan	391,680	19,880.0	32,576.6	1,649
6	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 , Cray Inc. Swiss National Supercomputing Centre (CSCS) Switzerland	361,760	19,590.0	25,326.3	2,272
7	**Titan** - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x , Cray Inc. DOE/SC/Oak Ridge National Laboratory United States	560,640	17,590.0	27,112.5	8,209

Historically: cluster computing limited to national labs, research universities

But now…

Cluster computing is mainstream

Big data means big computers!



Cluster computing is mainstream

Google Cloud Platform

Course objective

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

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

Software tools

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

Software tools

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

Examples:

Scientific	General purpose
Matlab	Python
Fortran	C++
R	Java

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

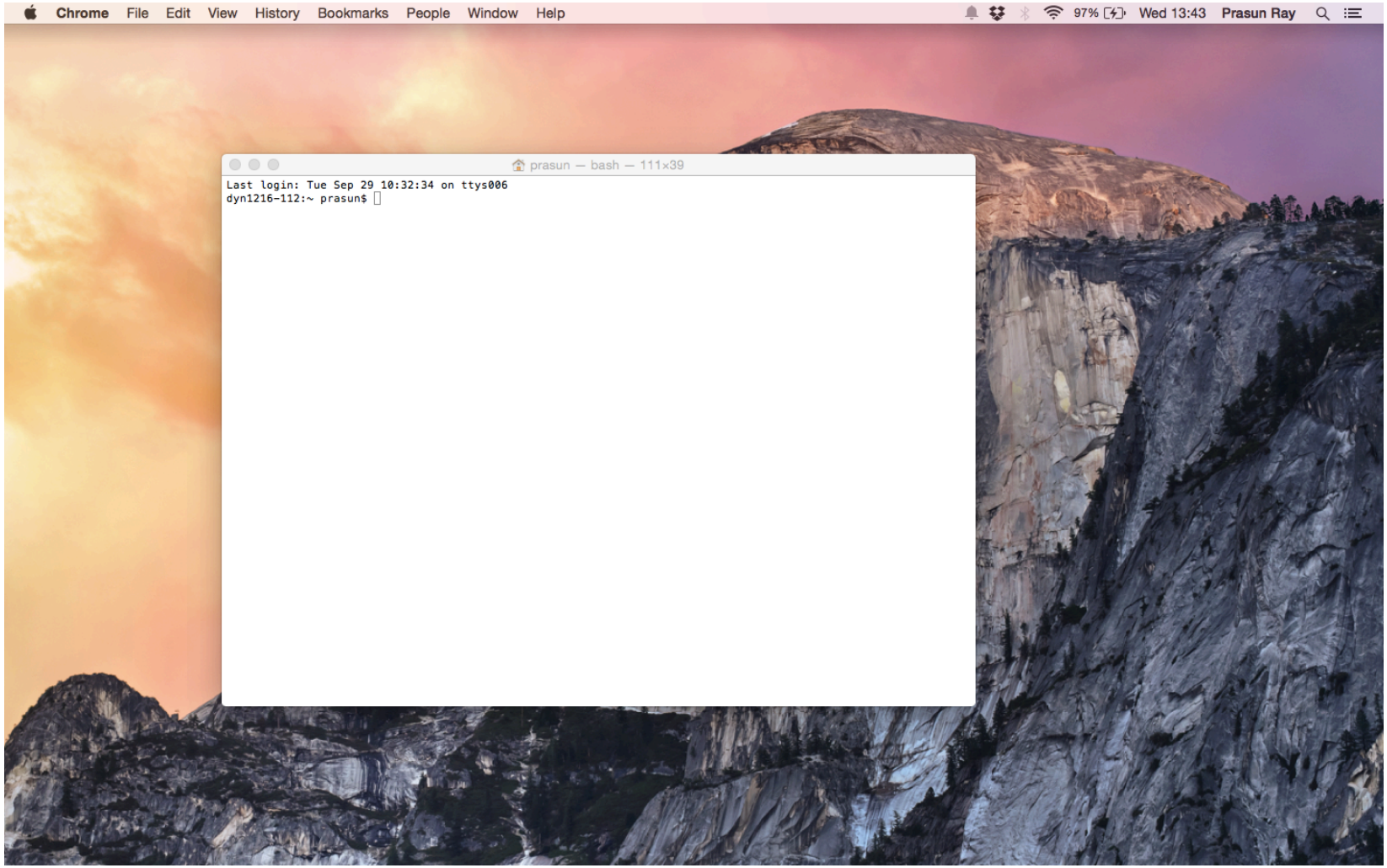
Windows:

- 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://imperialm3c.bitbucket.io/

Unix terminal

Terminal on a mac:



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
```

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
```

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.
```

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.

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!

A little more Unix

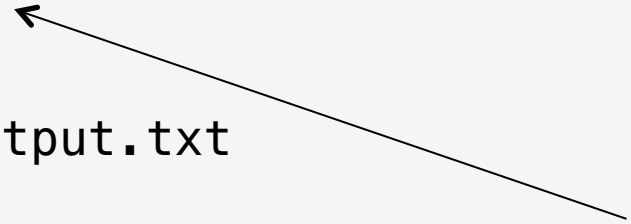
Instead of outputting to screen, can output to file using “>”

```
$ 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

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

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
```

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
================================================================================
==================
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
```

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?

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?

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 – go to software hub and search for "Linux – Maths" (and let me know if you have problems)
- Start working through introductory Python videos and exercises