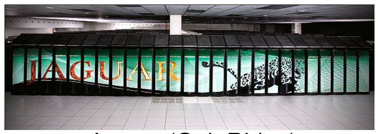
High-Performance Scientific Computing

Instructor: Randy LeVeque
TA: Grady Lemoine

Applied Mathematics 483/583, Spring 2011
http://www.amath.washington.edu/~rjl/am583

“World’s fastest computers”
http://top500.org

Roadrunner (Los Alamos)
122,400 cores



Jaguar (Oak Ridge)
224,162 cores

Notes:

Outline of today’s lecture

- Goals of this course, strategy for getting there
- Mechanics of homeworks
- Computer/software requirements
- Brief overview of computational science and challenges

Notes:

Overview

High Performance Computing (HPC) generally means heavy-duty computing on clusters or supercomputers with 100s to million(s) of cores.

Our focus is more modest, but we will cover much background material that is:

- Essential to know if you eventually want to do HPC
- Extremely useful for any scientific computing project, even on a laptop.

Focus on scientific computing as opposed to other computationally demanding domains, for which somewhat different tools might be best.

Notes:

Focus and Topics

Efficiently using single processor and multi-core computers

- Basic computer architecture, e.g. floating point arithmetic, cache hierarchies, pipelining
- Using Unix (or Linux, Mac OS X)
- Language issues, e.g. compiled vs. interpreted, object oriented, etc.
- Specific languages: Python, Fortran 90/95
- Parallel computing with OpenMP, MPI, IPython

Efficient programming as well as minimizing run time

- Version control: Mercurial (hg),
- Makefiles, Python scripting,
- Debuggers

Notes:

Strategy

So much material, so little time....

- Concentrate on basics, simple motivating examples.
- Get enough hands-on experience to be comfortable experimenting further and learning much more on your own.
- Learn what's out there to help select what's best for your needs.
- Teach many things "by example" as we go along.

Notes:

Lecture notes

- html and pdf versions at (green = link in pdf file) **http://www.amath.washington.edu/~rjl/am583**
- Written using Sphinx: Python-based system for writing documentation. Learn by example!!
- Source for each file can be seen by clicking on "Show Source" on right-hand menu.
- Source files are in class hg repository. You can clone the repository and run Sphinx yourself to make a local version.

```
$ hg clone http://bitbucket.org/.../uwamath583s11
$ cd uwamath583s11/sphinx
$ make html
$ firefox _build/html/index.html
```


Notes:

Lecture slides

Slides from lectures will be linked from the Slides section of the class notes.

Generally in 3 forms, including one with space for taking notes.

With luck they will be posted at least 2 hours before class if you want to print and bring along.

Note: Slides will contain things not in the notes, lectures will also include hands-on demos not on the slides.

Notes:

Prerequisites

Some programming experience in some language,
e.g., Matlab, C, Java.

You should be comfortable:

- editing a file containing a program and executing it,
- using basic structures like loops, if-then-else, input-output,
- writing subroutines or functions in some language

You are not expected to know Python or Fortran.

Some basic knowledge of linear algebra, e.g.:

- what vectors and matrices are and how to multiply them
- How to go about solving a linear system of equations

Some comfort level for learning new sofware and willingness to dive in to lots of new things.

Notes:

Homeworks

There will be 6 homeworks, plus a take-home final “exam”.

Electronic submission: via Mercurial (in order to get experience using Mercurial!)

Homework assignments will be in the notes.

Main goal: introduce many topics and get some hands-on experience with each.

Notes:

Homework #1

Homework #1 is in the notes.

Tasks:

- Make sure you have a computer that you can use with
  - Unix (e.g. Linux of Mac OSX),
  - Python 2.5 or higer,
  - Mercurial

  See next slide.
- Use Mercurial (hg) to clone the class repository and set up your own repository.
- Copy a Python script from one to the other and run it, putting the output in a second file.
- Commit these files and push them to your repository for us to see.

Notes:

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Computer/Software requirements

You will need access to a computer with a number of things on it, see the section of the notes on Downloading and Installing Software.

Note: Unix is often required for scientific computing.

Windows: Many tools we'll use can be used with Windows, but learning Unix is part of this class.

Options:

- Install everything you'll need on your own computer,
- Install VirtualBox and use the Virtual Machine (VM) created for this class.
- Use a Linux machine in the Applied Mathematics department (via ssh).

R.J. LeVeque, University of Washington AMath 483/583, Lecture 1, March 28, 2011

Notes:

R.J. LeVeque, University of Washington AMath 483/583, Lecture 1, March 28, 2011

TA and Office Hours

TA: Grady Lemoine

See the Class Catalyst Page for contact info, updated hours.

Office hours in Guggenheim 406

Monday, Tuesday, Friday 1:30 – 2:30

There is also a Discussion Board on the Class Catalyst Page, feel free to post **(and answer!)** questions about getting things to work.

R.J. LeVeque, University of Washington AMath 483/583, Lecture 1, March 28, 2011

Notes:

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Survey

Please take the survey found on the Class Catalyst Page to let us know about your background and computing plans.

As soon as possible.

Notes:

Computational Science (and Engineering)

Often called the third pillar of science, complementing the traditional pillars of theory and experiment.

Direct numerical simulation of complex physics / biology / chemistry is possible.

Typically requires solving very large systems of mathematical equations.

Notes:

Computational Science (and Engineering)

Unknowns represent values of some physical quantities, e.g.,

- (x, y, z) locations and velocities of individual atoms in a molecular dynamics simulation,
- (x, y, z) locations and velocities of individual stars in a cosmology simulation, e.g. galaxy formation.
- Density, pressure, velocities of a fluid at billions of points in a fluid dynamics simulation,
- Stress, strain, velocity of a solid at billions of points in a solid mechanics simulation.

Note: $1000 \times 1000 \times 1000$ grid has 1 billion grid points.

Need 8 gigabytes to store one variable at all grid points.

Notes:

Computational Science and Engineering

A few examples of large scale problems for motivation.

Currently, that often means Tera-scale or Peta-scale.

Next comes Exa-scale.

Notes:

How fast are computers?

Kilo = thousand (10^3)
Mega = million (10^6)
Giga = billion (10^9)
Tera = trillion (10^{12})
Peta = 10^{15}
Exa = 10^{18}

Processor speeds usually measured in Gigahertz these days.

Hertz means "machine cycles per second".

One operation may take a few cycles.

So a 1 GHz processor can do
$> 100,000,000$ operations per second.

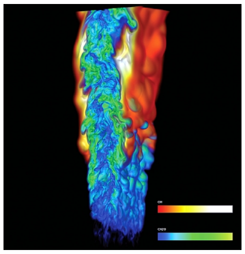
Exascale is a billion times more than Gigascale.
(More speed and/or data.)

Notes:

Combustion

Goal: Developing more fuel efficient and cleaner combustion processes for petroleum and alternative fuels.

Sample computation at Oak Ridge National Laboratory:



Ethylene combustion (simple!)

More than 1 billion grid points,
$\Delta x = \Delta y = \Delta z =$15 microns

4.5 million processor hours on Jaguar's 31,000 cores

Generated > 120 terabytes of data

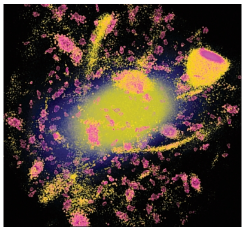
http://www.scidacreview.org/0902/html/news1.html

Notes:

Milky Way's dark matter halo

Goal: Understand nature of the universe.

Sample computation at Oak Ridge National Laboratory:



1.1 billion particles of dark matter,

simulated for 13.7 billion years

> 1 million processor hours on Jaguar (3000 cores)

http://www.scidacreview.org/0901/html/bt.html

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Notes:

How long does it take to solve a linear system?

Solving an $n \times n$ linear system $Ax = b$ requires $\approx \frac{1}{3}n^3$ flops.
(Using Gauss elimination for a dense matrix.)

On a 100 MFlops system:

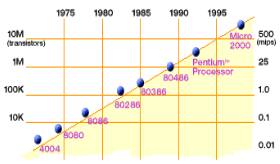
n	flops	time
10	3.3×10^2	0.0000033 seconds
100	3.3×10^5	0.0033 seconds
1000	3.3×10^8	3.33 seconds
10000	3.3×10^{11}	333 seconds $=$ 5.5 minutes
100000	3.3×10^{14}	333333 seconds $=$ 92.5 hours
1000000	3.3×10^{17}	92500 hours $=$ 105 years

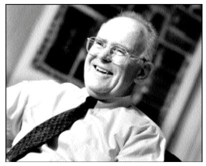
Assuming data transfer is not a problem!
It is a problem: It's often the bottleneck, not compute speed!
$10^6 \times 10^6$ matrix has 10^{12} elements $\implies$ 8 terabytes.

Notes:

Moore’s Law

Technology Trends: Microprocessor Capacity





2X transistors/Chip Every 1.5 years
Called “Moore’s Law”

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.

Slide source: Jack Dongarra

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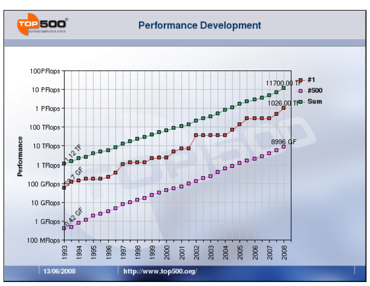
Notes:

Increasing speed

Moore’s Law: Processor speed doubles every 18 months.
$\Longrightarrow$ factor of 1024 in 15 years.

Going forward: Number of cores doubles every 18 months.



Top: Total computing power of top 500 computers

Middle: #1 computer

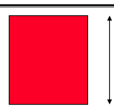
Bottom: #500 computer

`http://www.top500.org`

Notes:

More Limits: How fast can a serial computer be?

1 Tflop/s, 1 Tbyte sequential machine



r = 0.3 mm

- Consider the 1 Tflop/s sequential machine:
  - Data must travel some distance, r, to get from memory to CPU.
  - To get 1 data element per cycle, this means 10^{12} times per second at the speed of light, $c = 3 \times 10^8$ m/s. Thus $r < c/10^{12} = 0.3$ mm.
- Now put 1 Tbyte of storage in a 0.3 mm x 0.3 mm area:
  - Each bit occupies about 1 square Angstrom, or the size of a small atom.
- No choice but parallelism

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Slide Source: Kathy Yellick

Notes:

Take away messages

- Massively parallel machines are needed for Petascale or Exascale (millions or billions of cores).
- But also, all machines going to be multicore soon, with lots of cores.
- If you want to continue seeing benefiting from hardware improvements, you need to know something about parallel computing.

Notes: