Outline:

• Binary storage, floating point numbers
• Version control — main ideas
• Client-server version control, e.g., CVS, Subversion
• Distributed version control, e.g., git, Mercurial

Reading:

• class notes: Storing information in binary
• class notes: version control section
• class notes: git section
• Bitbucket 101

Homework #1

Homework #1 is in the notes.

Tasks:

• Make sure you have a computer that you can use with
  • Unix (e.g. Linux or Mac OSX),
  • Python 2.5 or higher, matplotlib
  • gfortran
  • git

• Use git to clone the class repository and set up your own repository on bitbucket.

• Copy some files from one to the other, run codes and store output.

• Commit these files and push them to your repository for us to see.

Class Virtual Machine

Available online from class webpage

This file is large! About 765 MB compressed.

After unzipping, about 2.2 GB.

Also available from TAs on thumb drive during office hours,
Or during class on Wednesday or Friday.
TAs and office hours

Two TAs are available to all UW students:
Scott Moe and Susie Sargsyan (AMath PhD students)

Office hours: posted on Canvas course web page
https://canvas.uw.edu/courses/812916

Tentative:
M 1:30-2:30 in Lewis 208,
T 10:30-11:30 in Lewis 212 (*)
W 1:30-2:30 in Lewis 208 (*)
F 12:00-1:00 in Lewis 212

(*) GoToMeeting also available for 583B students

My office hours: M & W in CSE Atrium, 9:30 – 10:45.

Notes:

Outline of quarter

Some topics we'll cover (nonlinearly):
• Unix
• Version control (git)
• Python
• Compiled vs. interpreted languages
• Fortran 90
• Makefiles
• Parallel computing
• OpenMP
• MPI (message passing interface)
• Graphics / visualization

Notes:

Unix (and Linux, Mac OS X, etc.)

See the class notes Unix page for a brief intro and many links.

Unix commands will be introduced as needed and mostly discussed in the context of other things.

Some important ones...
• cd, pwd, ls, mkdir
• mv, cp

Commands are typed into a terminal window shell, see class notes shells page.

We will use bash. Prompt will be denoted $, e.g.

$ cd ..
Other references and sources

- Links in notes and bibliography
- Wikipedia often has good intros and summaries.
- Software Carpentry, particularly these videos
- Other courses at universities or supercomputer centers. See the bibliography.
- Textbooks. See the bibliography.

Steady state heat conduction

Discretize on an $N \times N$ grid with $N^2$ unknowns:

Assume temperature is fixed (and known) at each point on boundary.
At interior points, the steady state value is (approximately) the average of the 4 neighboring values.

Storing a big matrix

Recall: Approximating the heat equation on a $100 \times 100$ grid gives a linear system with 10,000 equations, $Au = b$ where the matrix $A$ is $10,000 \times 10,000$.

Question: How much disk space is required to store a $10,000 \times 10,000$ matrix of real numbers?

It depends on how many bytes are used for each real number. 1 byte = 8 bits, bit = “binary digit”

Assuming 8 bytes (64 bits) per value:
A 10,000 $\times$ 10,000 matrix has $10^8$ elements, so this requires $8 \times 10^8$ bytes = 800 MB.
And less than 50,000 values are nonzero, so 99.95% are 0.
Measuring size and speed

Kilo = thousand \((10^3)\)

Mega = million \((10^6)\)

Giga = billion \((10^9)\)

Tera = trillion \((10^{12})\)

Peta = 10^{15}

Exa = 10^{18}

Computer memory

Memory is subdivided into bytes, consisting of 8 bits each.

One byte can hold \(2^8 = 256\) distinct numbers:

\[
\begin{align*}
00000000 & = 0 \\
00000001 & = 1 \\
00000010 & = 2 \\
\vdots & \\
11111111 & = 255
\end{align*}
\]

Might represent integers, characters, colors, etc.

Usually programs involve integers and real numbers that require more than 1 byte to store.

Often 4 bytes (32 bits) or 8 bytes (64 bits) used for each.

Integers

To store integers, need one bit for the sign (+ or −)

In one byte this would leave 7 bits for binary digits.

Two-complements representation used:

\[
\begin{align*}
10000000 & = -128 \\
10000001 & = -127 \\
10000010 & = -126 \\
\vdots & \\
11111110 & = -2 \\
11111111 & = -1 \\
00000000 & = 0 \\
00000001 & = 1 \\
00000010 & = 2 \\
\vdots & \\
01111111 & = 127
\end{align*}
\]

Advantage: Binary addition works directly.
Integers

Integers are typically stored in 4 bytes (32 bits). Values between roughly \(-2^{31}\) and \(2^{31}\) can be stored.

In Python, larger integers can be stored and will automatically be stored using more bytes.

Note: special software for arithmetic, may be slower!

```
$ python
>>> 2**30
1073741824
>>> 2**100
1267650600228229401496703205376L
```

Note L on end!

R.J. LeVeque, University of Washington
AMath 483/583, Lecture 2

Fixed point notation

Use, e.g. 64 bits for a real number but always assume \(N\) bits in integer part and \(M\) bits in fractional part.

Analog in decimal arithmetic, e.g.:
- 5 digits for integer part and
- 6 digits in fractional part

Could represent, e.g.:
- 00003.141592 (\(\pi\))
- 00000.000314 (\(\pi / 10000\))
- 31415.926535 (\(\pi \times 10000\))

Disadvantages:
- Precision depends on size of number
- Often many wasted bits (leading 0's)
- Limited range; often scientific problems involve very large or small numbers.

R.J. LeVeque, University of Washington
AMath 483/583, Lecture 2

Floating point real numbers

**Base 10** scientific notation:

\[0.2345 \times 10^{-18} = 0.2345 \times 10^{-18} = 0.00000000000000002345\]

**Mantissa**: 0.2345, **Exponent**: −18

**Binary** floating point numbers:

**Example**: **Mantissa**: 0.101101, **Exponent**: −11011 means:

\[0.101101 = 1(2^{-1}) + 0(2^{-2}) + 1(2^{-3}) + 1(2^{-4}) + 0(2^{-5}) + 1(2^{-6})\]

\[= 0.703125\] (base 10)

\[-11011 = -1(2^{4}) + 1(2^{3}) + 0(2^{2}) + 1(2^{1}) + 1(2^{0}) = -27\] (base 10)

So the number is

\[0.703125 \times 2^{-27} \approx 5.2386894822120667 \times 10^{-9}\]
Floating point real numbers

Python float is 8 bytes with IEEE standard representation. 53 bits for mantissa and 11 bits for exponent (64 bits = 8 bytes). We can store 52 binary bits of precision. 

\[ 2^{-52} \approx 2.2 \times 10^{-16} \implies \text{roughly 15 digits of precision.} \]

Notes:

Floating point real numbers

Since \( 2^{-52} \approx 2.2 \times 10^{-16} \) this corresponds to roughly 15 digits of precision.

For example:

```python
>>> from numpy import pi
>>> pi
3.1415926535897931
>>> 1000 * pi
3141.5926535897929
>>> pi/1000
0.0031415926535897933
```

Note: storage and arithmetic is done in base 2 Converted to base 10 only when printed!

Version control systems

Originally developed for large software projects with many developers.

Also useful for single user, e.g. to:

- Keep track of history and changes to files,
- Be able to revert to previous versions,
- Keep many different versions of code well organized,
- Easily archive exactly the version used for results in publications,
- Keep work in sync on multiple computers.
Server-client model:

Original style, still widely used (e.g. CVS, Subversion)

One central repository on server.

Developers’ workflow (simplified!):

- Check out a working copy,
- Make changes, test and debug,
- Check in (commit) changes to repository (with comments). This creates new version number.
- Run an update on working copy to bring in others’ changes.

The system keeps track of diffs from one version to the next (and info on who made the changes, when, etc.)

A changeset is a collection of diffs from one commit.

Notes:

Server-client model:

Only the server has the full history.

The working copy has:

- Latest version from repository (from last checkout, commit, or update)
- Your local changes that are not yet committed.

Note:

- You can retrieve older versions from the server.
- Can only commit or update when connected to server.
- When you commit, it will be seen by anyone else who does an update from the repository.

Often there are trunk and branches subdirectories.

Notes:

Distributed version control

Git uses a distributed model:

When you clone a repository you get all the history too,

All stored in .git subdirectory of top directory.

Usually don’t want to mess with this!

Ex: (backslash is continuation character in shell)

```
$ git clone \n  https://bitbucket.org/rjleveque/uwhpsc \n  mydirname
```

will make a complete copy of the class repository and call it mydirname. If mydirname is omitted, it will be called uwhpsc.

This directory has a subdirectory .git with complete history.

Notes:
Distributed version control

Git uses a distributed model:
- **git commit** commits to your clone's .git directory.
- **git push** sends your recent changesets to another clone by default: the one you cloned from (e.g. bitbucket), but you can push to any other clone (with write permission).
- **git fetch** pulls changesets from another clone by default: the one you cloned from (e.g. bitbucket)
- **git merge** applies changesets to your working copy

Note: pushing, fetching, merging only needed if there are multiple clones.

Next lecture: simpler example of using git in a single directory.

Advantages of distributed model:
- You can commit changes, revert to earlier versions, examine history, etc. without being connected to server.
- Also without affecting anyone else's version if you're working collaboratively. *Can commit often while debugging.*
- No problem if server dies, every clone has full history.

For collaboration will still need to push or fetch changes eventually and **git merge** may become more complicated.

Bitbucket

You can examine class repository at:
[https://bitbucket.org/rjleveque/uwhpsc](https://bitbucket.org/rjleveque/uwhpsc)

Experiment with the "Source", "Commits" tabs...

See also class notes bibliography for more git references and tutorials.

Notes:
Github

https://github.com

Another repository for hosting git repositories.
Many open sources projects use it, including Linux kernal.
(Git was developed by Linus Torvalds for this purpose!)

Many open source scientific computing projects use github, e.g.
- IPython
- NumPy, Scipy, matplotlib

Other tools for git

The gitk tool is useful for examining your commits.
This is not installed on the VM, but you can install it via:

```bash
$ sudo apt-get install gitk
```

Demo...

Many other tools, e.g.
- SmartGit / SmartHg
- GitHub for Mac