

Computational Physics

Prof. J.L. Sievers
sieversj@ukzn.ac.za

Course Goals

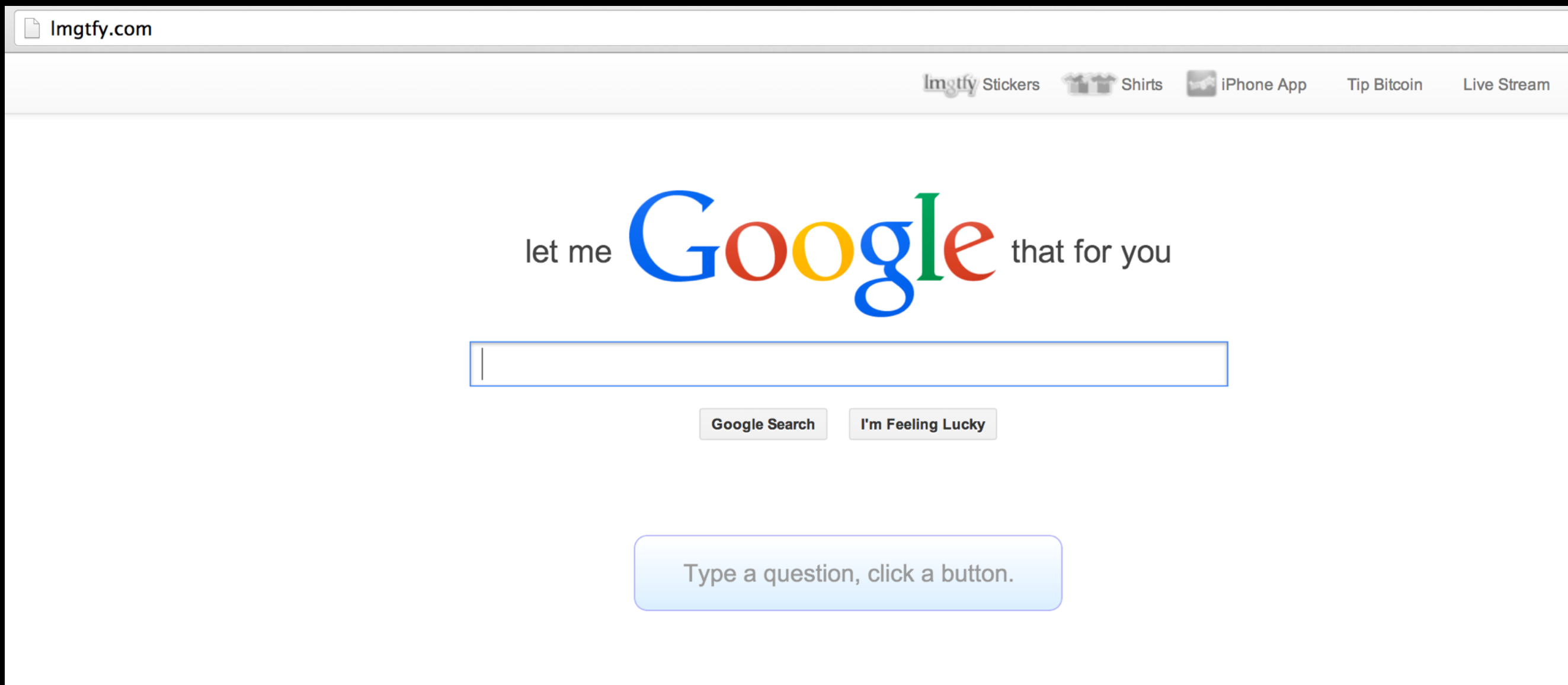
- If you go on in physics, most work likely to be at computer
- The computer will do work for you. It will **not** think for you.
- The only way to learn how to write code is by writing code.
- The goal of this course is to be practical. Focus on tools you'll (likely) need to get things done.
- Lectures/tutorial will be in lab. Try out commands right away.
- What do you want to learn about?

Marking

- 60% practical - half tutorial problems, half final project.
 - Projects to be announced later, If there's something you would like to do for it, let me know.
- 40% theory - test at end of term.

Course Rule

- If you continue in school or get a nice job, reason you will be getting paid is for you to figure things out.
- Do your results make sense? Computer cannot decide that for you. If they don't, say so - grading will be much kinder.
- Feel free to email/ask me questions **after** you have tried to figure it out on your own. Include the 3 things you searched for. Otherwise...



90% chance that's all I'll be doing anyways

Corollary

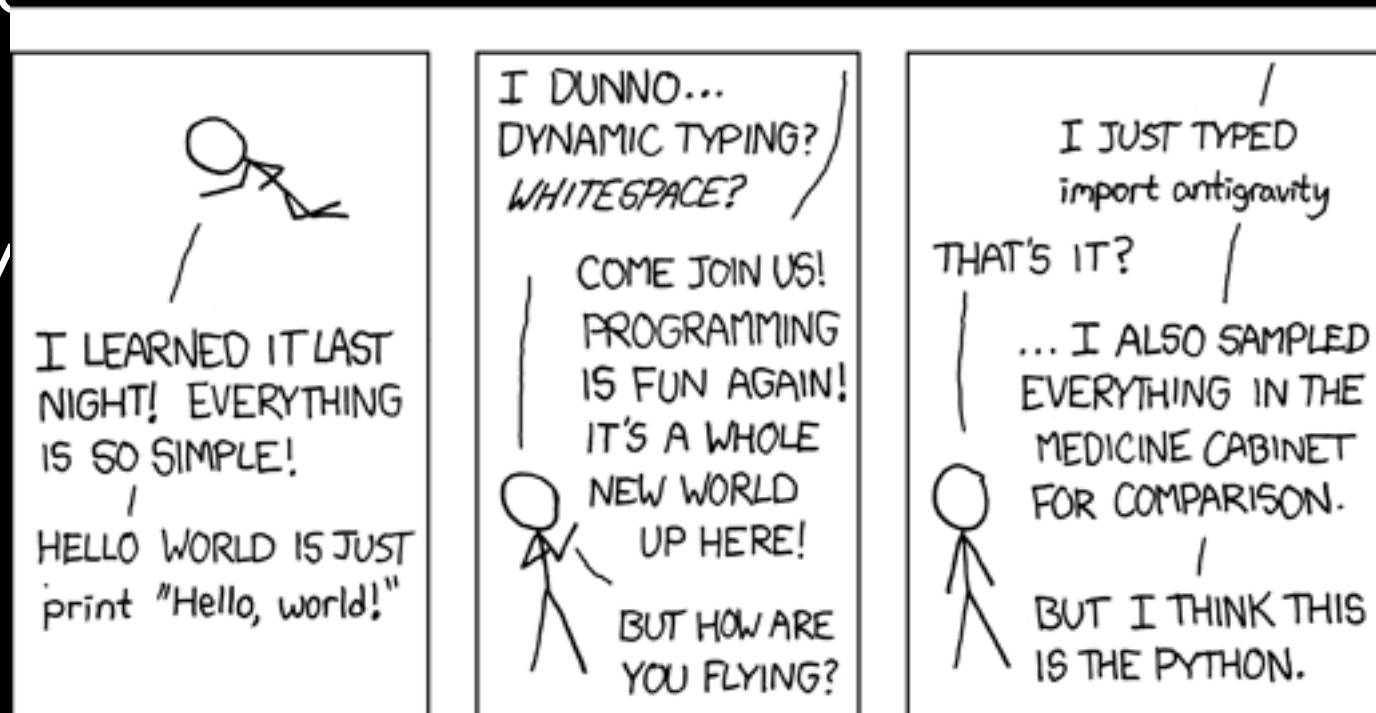
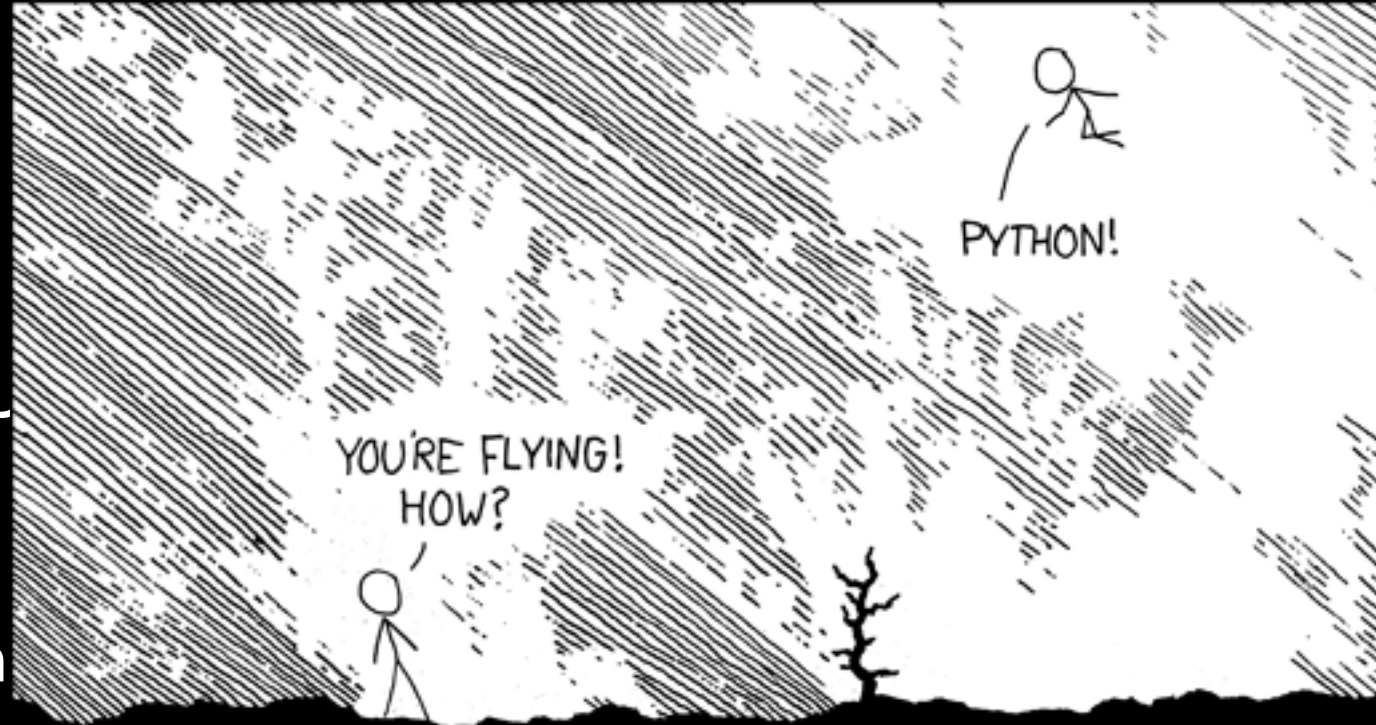
- First rule of coding: Don't!
- Someone has probably spent their career doing (almost) exactly what you're trying to do. Go use what they did!
- Your code will (almost certainly) be slower, buggier, less flexible, and more painful to use.

Preliminary Outline

- Lecture 1: Linux/unix intro, filesystems, git
- Lecture 2: Python intro
- Lecture 3: Numpy/matplotlib/ more python
- Lecture 4: Linear Algebra
- Lecture 5: Model fitting, MCMC
- Lecture 6: FFTs
- Lecture 7: Diffusion, 1-d PDEs
- Lecture 8: Fluid simulations, multi-d PDEs
- Lecture 9: N-body
- Lecture 10: Programming style, testing
- Lecture 11: Speeding up python - cython/C library interfaces
- Lecture 12: Test

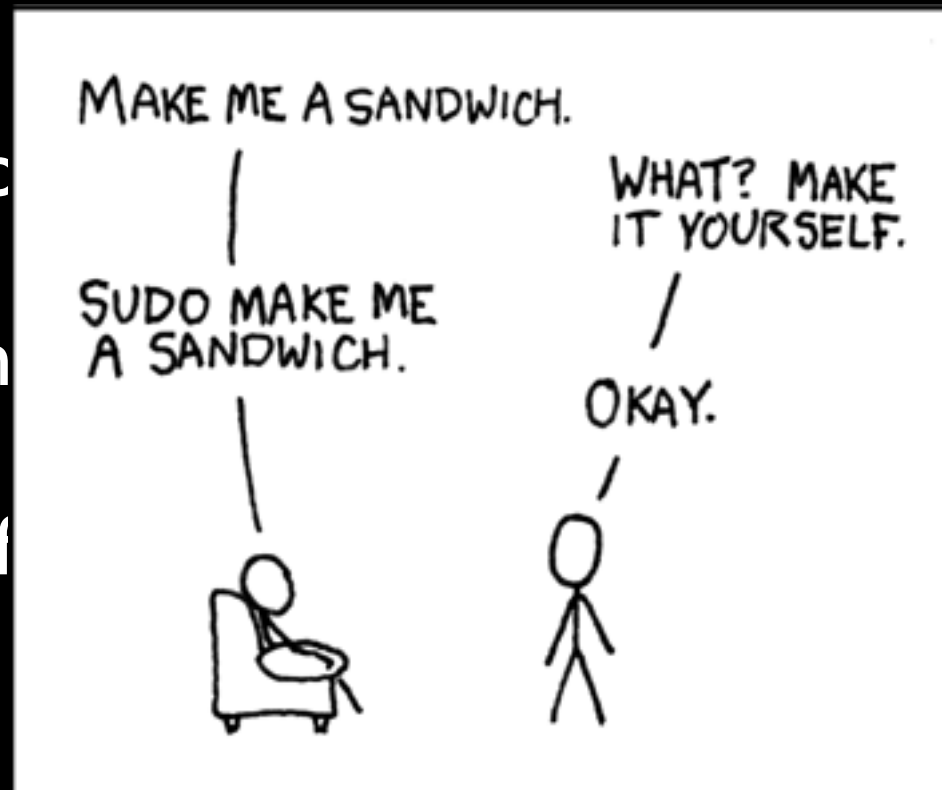
Unix & Python

- Course will be in a Linux (a variety of Linux distributions) environment
- Course will mainly use python programming language
- Why python? Flexible language, open source, lots of things already written for it.
- Open source means wherever you go, you can find it and follow.



Unix Intrinsically Multi-User

- Individual people have accounts in unix, with identifying user names. Each account has a password with it.
- Guiding principle - you aren't allowed to muck up someone else's account
- Every file has an owner. You own your own.
- Once you have a user name, you choose wisely...
- root is a special, all-powerful user. Be very careful when root. Don't break the OS. Be
- sudo (super-user do) executes commands as root. You will not have root/sudo access on these computers.



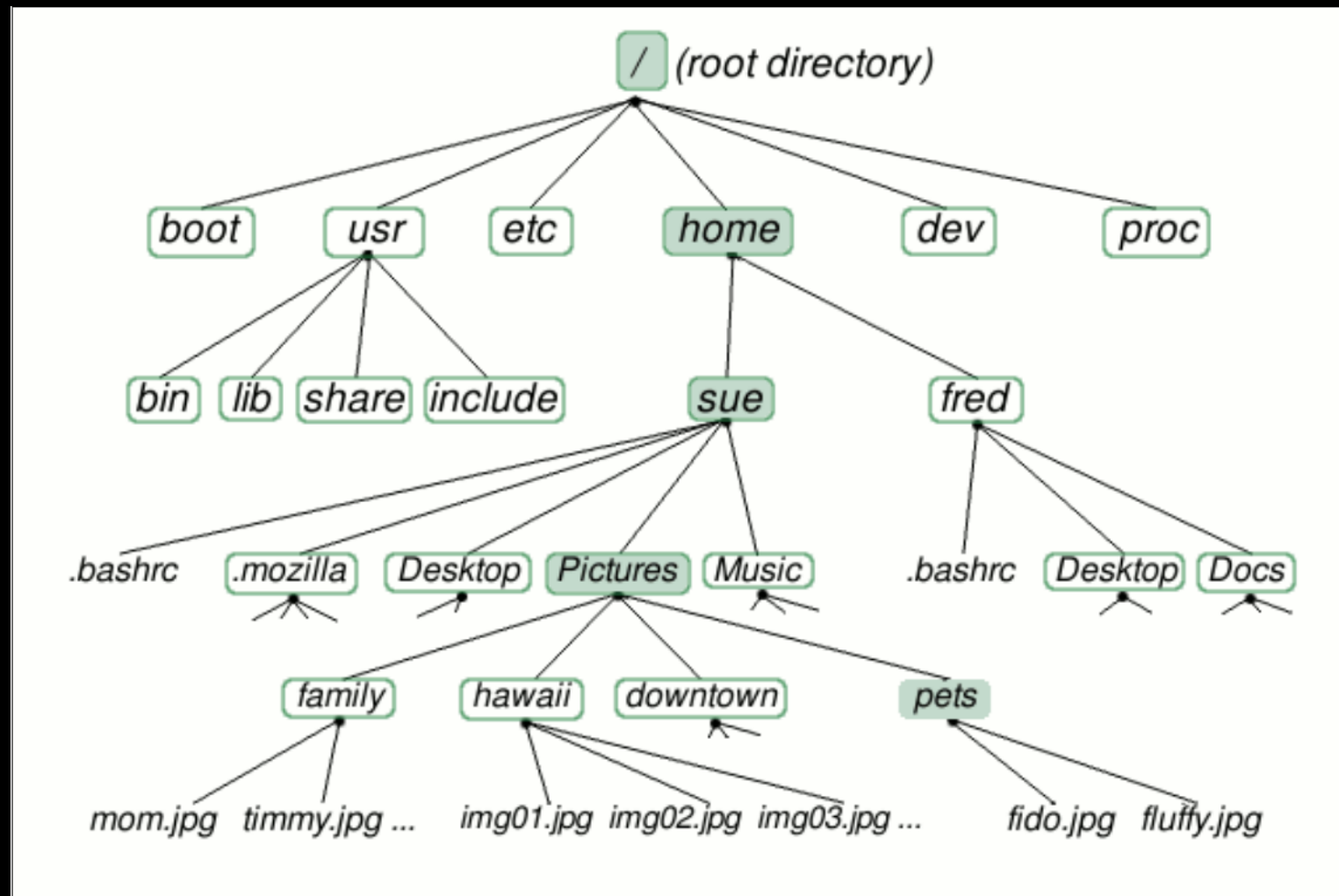
Let's Get Everyone Accounts

- Think of a user name and password.
- Let me know when you're ready and I'll make the account.
- Since accounts only on one machine, you should expect to sit at the same computer during the term.
- We'll wait until everyone is logged in as themselves.

Terminal Time

- Unix's power lies in the command line. You can tell the computer to do most anything there.
- Let's all get a terminal started:
- Click on upper left ("dash"). Should get a search box.
- Type in "terminal" in the search box. Click to start.
- You might want to pin terminal to the sidebar.

File Heirarchy



- All regular files live in directories.
- Directories arranged in trees.
- Every directory has a parent directory (except for the root directory)
- Directories help keep you organized. Use them!

First Commands

- Your command line always has a location in the directory tree. Type “pwd” (print working directory) to find out where it is.
- See what files live in the directory - “ls” (list).
- Change directory of command lines - “cd <arg>” (change directory) where <arg> is the desired new directory.
- “..” always points to the parent directory. “cd ..” says “go up one level in the directory heirarchy.” “.” always points to the current directory.

Commands are Flexible

- Many commands can do a variety of tasks through *options*.
- example: “ls -l” lists long-form information on files in directory
- “ls -a” lists hidden files.
- Commands can (usually) be combined: “ls -alh” says “list files (including hidden ones) in long-form. Report the sizes in human-readable format.
- Can you remember all the magic options? Me neither. man (manual) pages are installed on the system. Just type “man <command>” to learn about it.
- So, to learn more about the “man” command, type “man man”

Looking at Files

- “cat” will dump the contents of a file to the screen.
- “more” will do the same thing, but one page at a time.
- “head” and “tail” will dump the first (or last) 10 lines of a file to the screen.

Copying/moving/deleting

- “rm” (remove) will delete a file `rm foo.txt`
- “cp” (copy) will make an identical copy of a file: `cp foo.txt fwee.txt`
- `mkdir` will create a directory: `mkdir fwee`
- `rmdir` remove an empty directory.

Wildcards

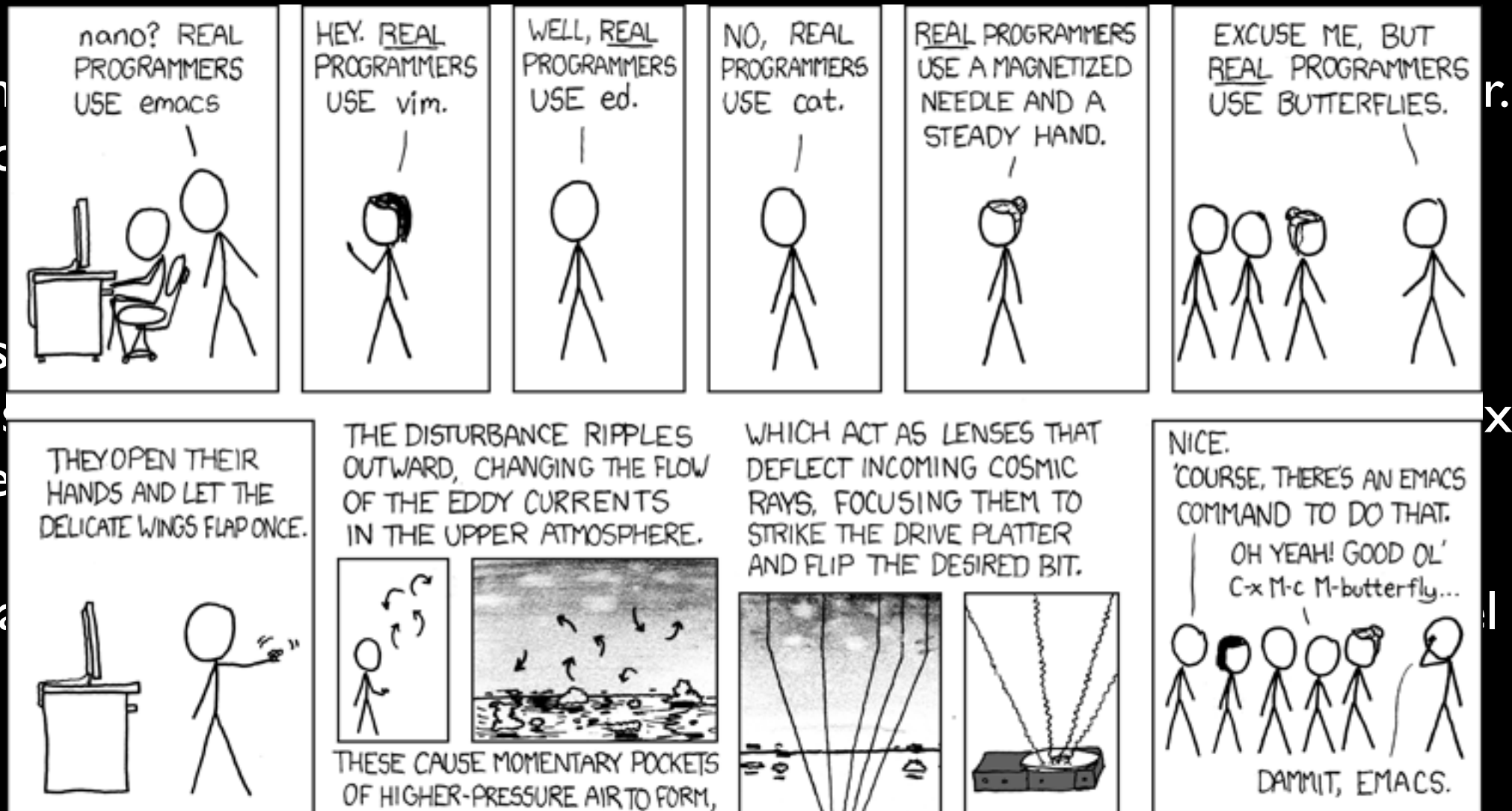
- The command line will let you specify subsets of files.
- “*” matches any set of characters: “ls *.txt” lists all files whos names end in “.txt”
- “?” matches any single character: “ls crud.?” will list all files that start with crud. followed by a single character. crud.9 would match, crud.l0 would not.
- [] matches any character inside the brackets. “ls set_[0123].txt” would match set_0.txt and set_3.txt, but **not** set_4.txt.
- {} lists comma separated tags that will match. “ls *.{txt,jpg}” will list all files whos names end in .txt *or* in .jpg

Redirection

- A magic power of unix is the ability to redirect output into files or other commands.
- “|” (pipe) sends the output of one command into the next. “wc” (word count) will count the # of words in something. So, “ls -l *.txt | wc” will tell you how many .txt files you have in a directory.
- “>” redirects output into a file. So, “ls -l > foo.txt” will list extended info about each file into the file “foo.txt”, which you can look at.
- “>>” is similar to “>”, but puts things at the end of the file. What would “echo thats all folks >> foo.txt” do?

Text Editors

- At some point, one person says to others, "emacs changed, followed by..."
- There are a lot of people free to...



Environment Variables

- Normally you will have variables defined that guide what happens at the command line.
- “env” or “printenv” will normally print them to the screen.
- Some important ones include :“PATH” - tells the command line where to search for commands to execute. “HOME” - tells you where your home directory is - this is where your files live. (Note that environment variables are case sensitive.)
- values of variables can be accessed with a “\$” sign. “echo” is like a print command, so to see the location of your home directory, type “echo \$HOME”.
- At UKZN, “http_proxy” is another important one - this tells the system how to get through the proxy server.

Let's Make a Useful File

- Whenever you start a new shell, a resource file is used. For us, that will be “\${HOME}/.bashrc” (bourne-again shell resources).
- Let's make it so we can get through the proxy. Let's set “http_proxy” so we can get out from the command line.
- “export http_proxy=http://<username>:<password>@bcproxy.ukzn.ac.za:8080”.
- NEVER write your password in plain text. Proxy forcing us now, though.
- You can put this in your .bashrc. How would you check if new terminals register this?
- ftp_proxy and https_proxy should also be set to the same value.

Finally, Version Control

- Let's role play.

Version Control ctd.

- What did we just learn? It's important to be able to undo changes
- Merging changes from different places/different people important. Should be done in a systematic way. If I change one part of a file while you change another, would like to combine those changes automatically.
- What happens if someone steals your computer? The more places code lives, the safer you are.

Version Control 3

- Several version control (VC) systems exist, 3 most common are CVS, SVN, and git. We will use git.
- VC lets many people edit files. A set of files being tracked is called a “repository.” A VC system can keep your local files in a repository synced with the central repository.
- When you are done making changes, you “commit” them to your local repository, then “push” them to the central repository. When someone else makes changes, you “pull” them from the central repository.
- If you both edited the same part of a file, the VCS will throw an error and tell you to fix the conflict by hand.
- VCSs usually require your local repository to be up-to-date with the central one before you’re allowed to push changes.

Git

- git was developed by Linux Torvalds (the “Li” in linux)
- very powerful/flexible VCS.
- Basic commands: “git init” will initialize an empty repository. “git add <files>” will add those files to the repository.
- When ready, “git commit -a -m “<message>” “ will commit your changes to your repository.
- “git history” will tell you the messages you saved in your commits.
- “git revert” will let you go to a previous version of the repository.

Github

- Github provides free repository support. Much of the code released today is done on github.
- You can make an account, then github will walk you through the steps you need to do what you want.
- “git clone” will copy a repository. I have made a github page for this class - you can get the slides plus a linux tutorial cheat sheet there.
- In the browser, go to “<https://github.com/ukzncompphys>”

Click on lecture 1

GitHub

Search or type a command

ExploreFeaturesEnterpriseBlog

Sign upSign in

Contributions

Repositories

Public Activity

Follow

Popular repositories

welcome

This contains a welcome message for UKZN computational physics students.

0

lecture1

Slides from Lecure 1

0

Public contributions

AprMayJunJulAugSepOctNovDecJanFebMar

M

W

F

Summary of Pull Requests, issues opened and commits. [Learn more.](#)

LessMore

0 Total

Mar 31 2013 - Mar 31 2014

Year of Contributions

0 days

Rock - Hard Place

Longest Streak

0 days

Rock - Hard Place

Current Streak

Contribution Activity

Period: 1 Week

ukzncompphys

Joined on Mar 31, 2014

0

followers

0

starred

0

following

PUBLIC



ukzncompphys / lecture1



Star

0



Fork

0

Slides from Lecure 1



1 commit



1 branch



0 releases



1 contributor



branch: master ▾

lecture1 / +

initial commit



sievers authored 7 minutes ago

latest commit 8a8fb868a6



compphys_1.key

initial commit

7 minutes ago



linux_boot_camp.pdf

initial commit

7 minutes ago



Code



Issues

0



Pull Requests

0



Pulse



Graphs



Network

HTTPS clone URL

https://github.com/



You can clone with [HTTPS](#) or [Subversion](#). ?



Clone in Desktop



Download ZIP



Then Clone the Repository

- “git clone <link from github>” will get you the slides.
- <https://github.com/ukzncompphys/lecture1.git> is the link in case you can't get to it.
- If this doesn't work, your proxy settings haven't been set correctly.

Tutorial Problems

- How can you list all files in a directory, with the most recent one displayed last?
- How can you display the first 25 lines of a file? How can you display just lines 16 through 25?
- How can you search for all commands relating to python? Hint - it will be a use of “man”.
- Make a new text file with your name, email address, what you’re working on for your honours project, plus a few things you’d like to learn in the course. Initialize a git repository and commit this file.
- Put your answers to the other tutorial questions into another text file. Add this to the repository also.
- Make a github account and push the repository onto github. Email me your github name so I can have a look at your file/answers.