Installing common programs/applications on a research computer

Rob Porritt, G. G. USArray short course, 2016

If on



first install the command line tools

From finder, open /Applications/Utilities/Terminal.app

Enter: xcode-select --install and follow the graphical prompts

Then install XQuartz windowing system via .dmg from web

If or



then you should be good to go.

Check your distro for whether you should use yum, apt-get, rpm, or something new to me

If on



look into Matlab or Python as cross-platform working environments. You may need to dual-boot with Linux or install cyg-win

Your computer needs a "path" variable.

This is a list of directories, separated by: which the operating system searches for executable files

On the macs I set it by editing a file called:

~/.profile

and add lines in bash syntax such as:

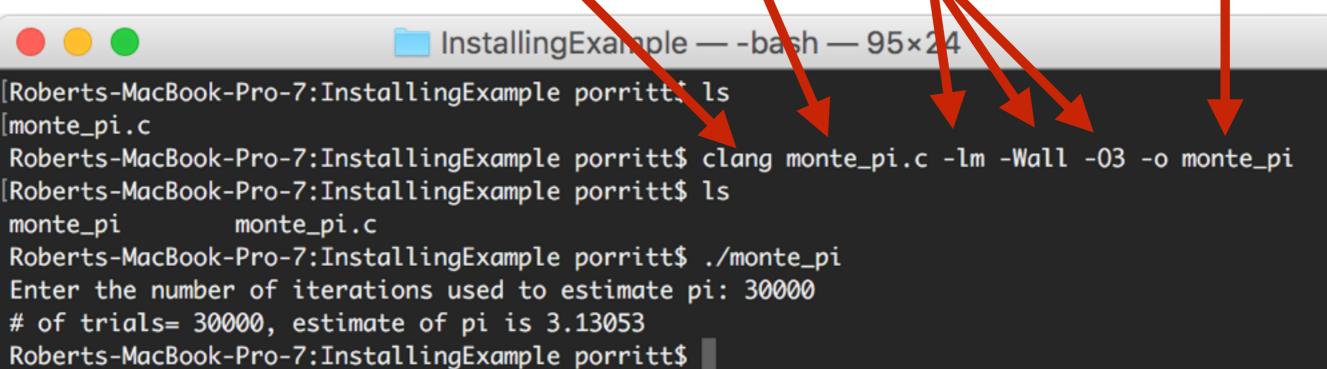
export PATH=~/bin/:\${PATH}

Alternatively you could use ~/.bashrc

If using a tcsh shell, you'd edit your ~/.tcshrc with lines like: setenv PATH ~/bin:\${PATH}

```
c monte_pi.c
```

```
/* Program to compute Pi using Monte Carlo methods */
   /* http://www.dartmouth.edu/~rc/classes/soft_dev/C_simple_ex.html */
  #include <stdlib.h>
6 #include <stdio.h>
7 #include <math.h>
8 #include <string.h>
9 #include <time.h>
10 #define SEED 35791246
11
12 int main(int argc, char *argv[])
13 {
      int niter=0;
14
      double x,y;
15
      int i,count=0; /* # of points in the 1st quadrant of unit circle */
16
      double z:
17
      double pi;
18
      time_t t;
19
20
      printf("Enter the number of iterations used to estimate pi: ");
21
      scanf("%d",&niter);
22
23
      /* initialize random numbers */
24
  // srand(SEED);
25
      srand((unsigned) time(&t));
26
      count=0;
27
      for ( i=0; i<niter; i++) {
28
         x = (double)rand()/RAND_MAX;
29
         y = (double)rand()/RAND_MAX;
30
         z = x*x+y*y;
31
         if (z<=1) count++;
32
33
      pi=(double)count/niter*4;
34
      printf("# of trials= %d, estimate of pi is %g \n", niter, pi);
35
      return 0;
36
37
   }
38
39
```



c monte_pi2.c

```
器 〈 〉 c monte_pi2.c 〉 No Selection
    /* Edit of monte_pi to use a subroutine */
 2
 3 #include <stdlib.h>
  4 #include <stdio.h>
 5 #include <math.h>
  6 #include <string.h>
 7 #include <time.h>
 8
    int count_it(int count);
 9
 10
 11
    int main(int argc, char *argv[])
 12
    {
        int niter=0;
 13
        int i,count=0; /* # of points in the 1st quadrant of unit circle */
 14
        double pi;
 15
 16
        time_t t;
 17
        printf("Enter the number of iterations used to estimate pi: ");
 18
        scanf("%d",&niter);
 19
 20
        /* initialize random numbers */
 21
             srand(SEED);
 22
        srand((unsigned) time(&t));
 23
        count=0;
 24
        for ( i=0; i<niter; i++) {
 25
 26
            count=count_it(count);
        }
 27
 28
        pi=(double)count/niter*4;
 29
        printf("# of trials= %d, estimate of pi is %g \n", niter, pi);
        return 0;
 30
 31 }
 32
 33
```

Contents of subroutine

```
c monte_sub.c

int count_it(int count) {
    double x, y, z;
    x = (double)rand()/RAND_MAX;
    y = (double)rand()/RAND_MAX;
    z = x*x+y*y;
    if (z<=1) count+;
    return count;
}</pre>
```

Separately compile the subroutine with -c and .o extension. Then compile together

```
InstallingExample — -bash — 125×24
[Roberts-MacBook-Pro-7:InstallingExample porritt$ ls
                               monte_pi2.c
monte_pi
               monte_pi.c
                                               monte_sub.c
Roberts-MacBook-Pro-7:InstallingExample porritt$ clang monte_sub.c -c -o monte_sub.o
[Roberts-MacBook-Pro-7:InstallingExample porritt$ ls
               monte_pi.c __ monte_pi2.c
monte_pi
                                               monte_sub.c
                                                               monte_sub.o
[Roberts-MacBook-Pro-7:InstallingExample porritt$ clang monte_pi2.c monte_sub.o -lm -Wall -O3 -o monte_pi2
[Roberts-MacBook-Pro-7:InstallingExample porritt$ ls
monte_pi
               monte_pi.c
                               monte_pi2
                                               monte_pi2.c
                                                               monte_sub.c
                                                                               monte_sub.o
Roberts-MacBook-Pro-7:InstallingExample porritt$ ./monte_pi2
Enter the number of iterations used to estimate pi: 3000
# of trials= 3000, estimate of pi is 3.15467
Roberts-MacBook-Pro-7:InstallingExample porritt$
```

```
CC = clang
```

```
FLAGS = -lm -Wall -03
INSTALL_DIR = ~/bin/
BIN = monte_pi
SUBS = monte_sub.c
SRC = monte_pi2.c
```

```
all :: $(BIN)
```

```
install ::
    install -s $(BIN) $(INSTALL_DIR)
```

clean :: rm subs.o \$(BIN)



```
[Roberts-MacBook-Pro-7:InstallingExample porritt$ ls
                monte_pi.c
                                monte_pi2.c
Makefile
                                               monte_sub.c
[Roberts-MacBook-Pro-7:InstallingExample porritt$ make
clang monte_sub.c -c -lm -Wall -03 -o subs.o
clang: warning: -lm: 'linker' input unused
clang monte_pi2.c subs.o -lm -Wall -03 -o monte_pi
[Roberts-MacBook-Pro-7:InstallingExample porritt$ ls
                                monte_pi.c
Makefile
                monte_pi
                                               monte_pi2.c
                                                                monte_sub.c
                                                                                subs.o
[Roberts-MacBook-Pro-7:InstallingExample porritt$ ./monte_pi
Enter the number of iterations used to estimate pi: 3000
# of trials= 3000, estimate of pi is 3.12933
[Roberts-MacBook-Pro-7:InstallingExample porritt$ make install
install -s monte_pi ~/bin/
[Roberts-MacBook-Pro-7:InstallingExample porritt$ monte_pi
Enter the number of iterations used to estimate pi: 3000
# of trials= 3000, estimate of pi is 3.184
[Roberts-MacBook-Pro-7:InstallingExample porritt$ make clean
rm subs.o monte_pi
[Roberts-MacBook-Pro-7:InstallingExample porritt$ ./monte_pi
-bash: ./monte_pi: No such file or directory
[Roberts-MacBook-Pro-7:InstallingExample porritt$ monte_pi
Enter the number of iterations used to estimate pi: 3000
# of trials= 3000, estimate of pi is 3.15067
Roberts-MacBook-Pro-7:InstallingExample porritt$
```

```
TIME_DOMAIN_VS_FREQUENCY_DOMAIN_CONVOLUTION — vi Makefile — 125×24
BIN = convolutionTests
CC = gcc
OBJ = convolutionTests.c
LIBS = -L/usr/local/lib -lfftw3 -lm
FLAGS = -Wall -02 -I/usr/local/include
INSTALL_DIR = ~/bin
all ::
       $(CC) $(OBJ) $(LIBS) $(FLAGS) -o $(BIN)
install ::
       install -s $(BIN) $(INSTALL_DIR)
clean ::
       rm $(BIN)
"Makefile" 17L, 271C
```



Mailing List

Introduction

FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data (as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST). We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

Features

fftw.org

C

FAQ

Feedback

Documentation

The latest official release of FFTW is version 3.3.4, available from our download page. Version 3.3 introduced support for the AVX x86 extensions, a distributed-memory implementation on top of MPI, and a Fortran 2003 API. Version 3.3.1 introduced support for the ARM Neon extensions. See the release notes for more information.

Benchmark

The FFTW package was developed at MIT by Matteo Frigo and Steven G. Johnson.

Download

GitHub

Our <u>benchmarks</u>, performed on on a variety of platforms, show that FFTW's performance is typically superior to that of other publicly available FFT software, and is even competitive with vendor-tuned codes. In contrast to vendor-tuned codes, however, FFTW's performance is *portable*: the same program will perform well on most architectures without modification. Hence the name, "FFTW," which stands for the somewhat whimsical title of "Fastest Fourier Transform in the West."

Subscribe to the fftw-announce mailing list to receive release announcements (or use the web feed ...).

Features

FFTW 3.3.4 is the latest official version of FFTW (refer to the release notes to find out what is new). Here is a list of some of FFTW's more interesting features:

```
Roberts-MacBook-Pro-7:FFTW porritt$ ls
fftw-3.3.4.tar
Roberts-MacBook-Pro-7:FFTW porritt$ tar -xvf fftw-3.3.4.tar
\times fftw-3.3.4/
x fftw-3.3.4/mpi/
x fftw-3.3.4/mpi/f03api.sh
x fftw-3.3.4/mpi/Makefile.am
x fftw-3.3.4/mpi/genf03-wrap.pl
x fftw-3.3.4/mpi/transpose-alltoall.c
x fftw-3.3.4/mpi/rdft2-rank-geq2.c
x fftw-3.3.4/mpi/mpi-dft.h
x fftw-3.3.4/mpi/fftw3-mpi.h
x fftw-3.3.4/mpi/fftw3-mpi.f03.in
x fftw-3.3.4/mpi/rdft2-problem.c
x fftw-3.3.4/mpi/dft-rank1.c
x fftw-3.3.4/mpi/block.c
x fftw-3.3.4/mpi/rdft2-serial.c
x fftw-3.3.4/mpi/rdft-problem.c
x fftw-3.3.4/mpi/mpi-rdft2.h
x fftw-3.3.4/mpi/testsched.c
x fftw-3.3.4/mpi/rdft2-solve.c
x fftw-3.3.4/mpi/any-true.c
```

```
Roberts-MacBook-Pro-7:FFTW porritt$ ls
fftw-3.3.4
                fftw-3.3.4.tar
[Roberts-MacBook-Pro-7:FFTW porritt$ cd fftw-3.3.4
Roberts-MacBook-Pro-7:fftw-3.3.4 porritt$ ls
                Makefile.am
AUTHORS
                                                 configure
                                                                 genfft
                                                                                 missing
                                api
                                                                                                 tests
CONVENTIONS
                Makefile.in
                                                 configure.ac
                                                                 install-sh
                                bootstrap.sh
                                                                                 mpi
                                                                                                 threads
COPYING
                                                                 kernel
                                                                                 rdft
                                compile
                                                depcomp
                NEWS
                                                                                                 tools
COPYRIGHT
                                config.guess
                                                                                 reodft
                README
                                                 dft
                                                                 libbench2
ChangeLog
                TOD0
                                config.h.in
                                                                                 simd-support
                                                 doc
                                                                 ltmain.sh
                                                 fftw.pc.in
INSTALL
                                confia.sub
                aclocal.m4
                                                                                 support
Roberts-MacBook-Pro-7:fftw-3.3.4 porr
                                        General install from source:
                                        1. tar -xvf software.tar.gz
                                       2. cd {software directory}
                     config.status: creatin
                                       3. ./configure
                     config.status: creatin
                     config.status: creatin
                                       4. make
                     config.status: creatin
                     config.status: creatin
                     config.status: creatin
                     config.status: creatin
                                       5. make install
                     config.status: creatin
                     config.status: creatin
                                                             Voila!
                     config.status: creatin
                     config.status: creatin
                     config.status: creatin
                     config.status: creating tests/makerile
                     config.status: creating doc/Makefile
                     config.status: creating doc/FAQ/Makefile
                     config.status: creating tools/Makefile
```

config.status: creating tools/Makefile
config.status: creating tools/fftw_wisdom.1
config.status: creating tools/fftw-wisdom-to-conf
config.status: creating m4/Makefile
config.status: creating fftw.pc
config.status: creating config.h
config.status: executing depfiles commands
config.status: executing libtool commands
Roberts-MacBook-Pro-7:fftw-3.3.4 porritt\$

Some packages installed this way...

- mseed2sac
- evalresp
- sac (also pre-compiled versions are available)
- seismic unix
- Computer Programs in Seismology (slightly modified)

Package Management

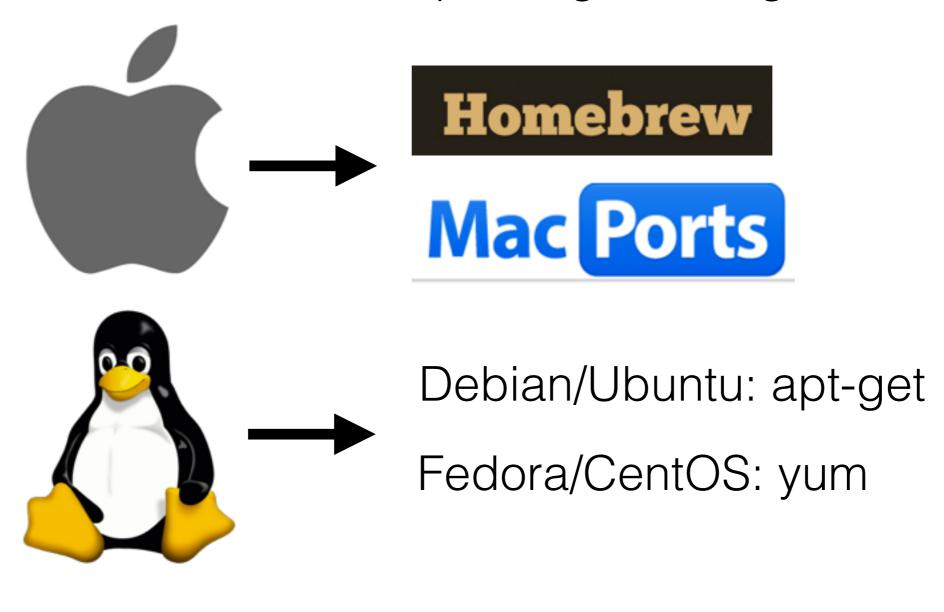
How do you deal with software dependencies?

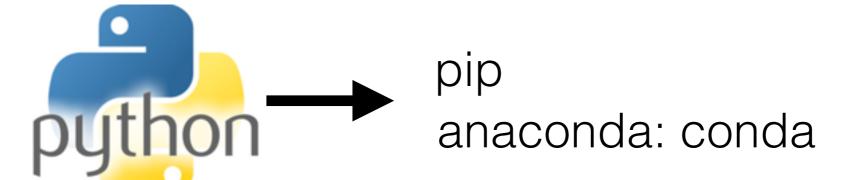
How do you deal with hardware dependencies?

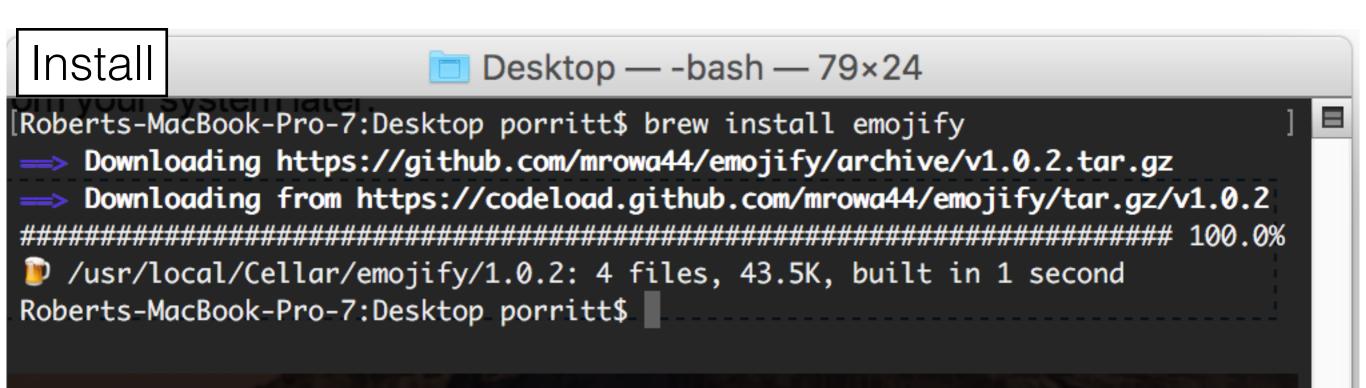
How do you build new programs with old tools?

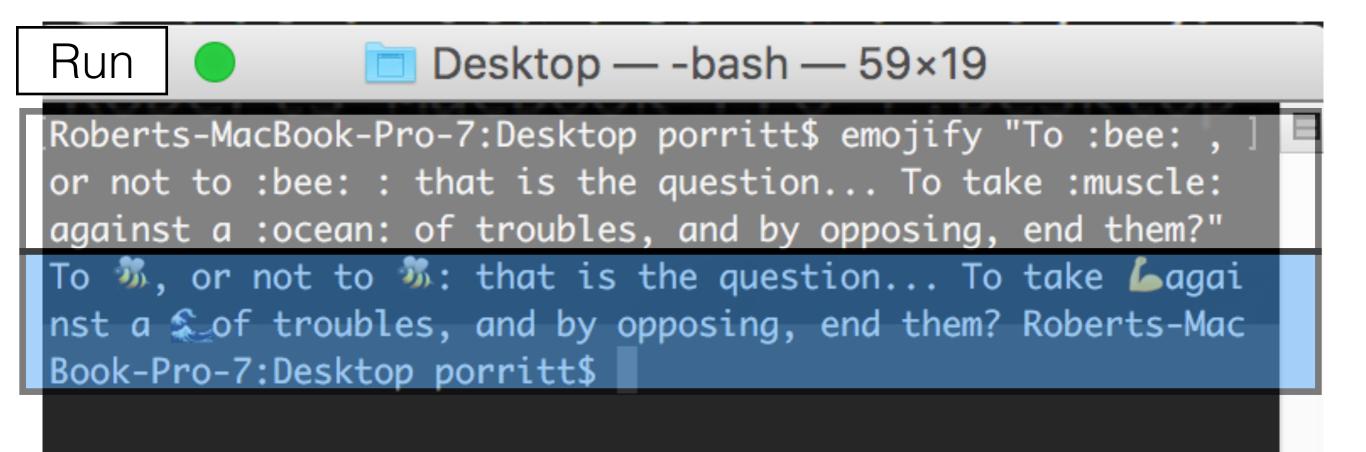


Command-line package managers









Example, installing GMT5

Red Hat, CentOS, Fedora:

\$ sudo yum install GMT gshhg-gmt-nc4-all dcw-gmt

Mac OSX

Download installer and add to path

Or

- \$ sudo port install gdal +curl +geos +hdf5 +netcdf
- \$ sudo port install gmt5

or

\$ sudo fink install gmt5

Or

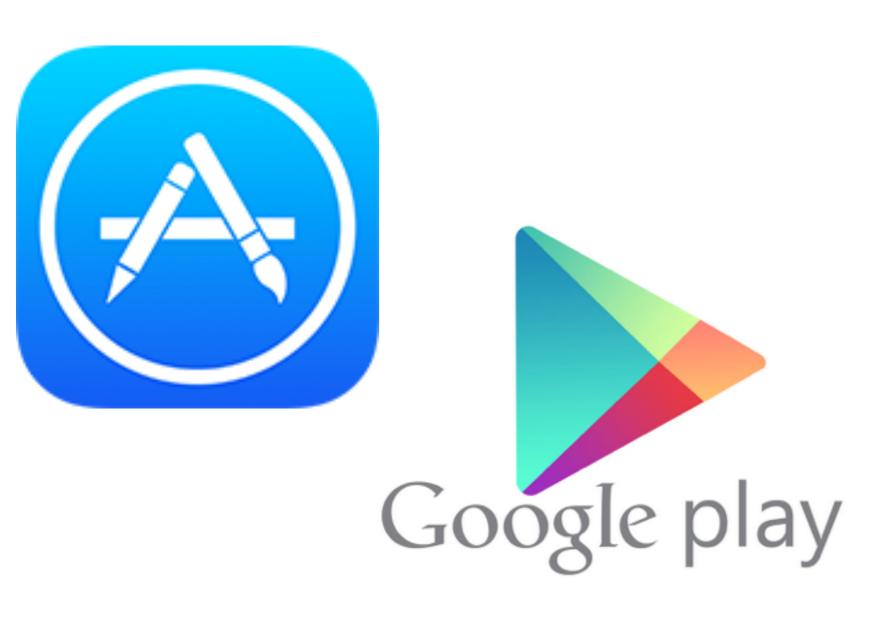
\$ brew install homebrew/science/gmt

Windows

Download and run installer

Seems uncomfortable to use package managers?

You already use them everyday...

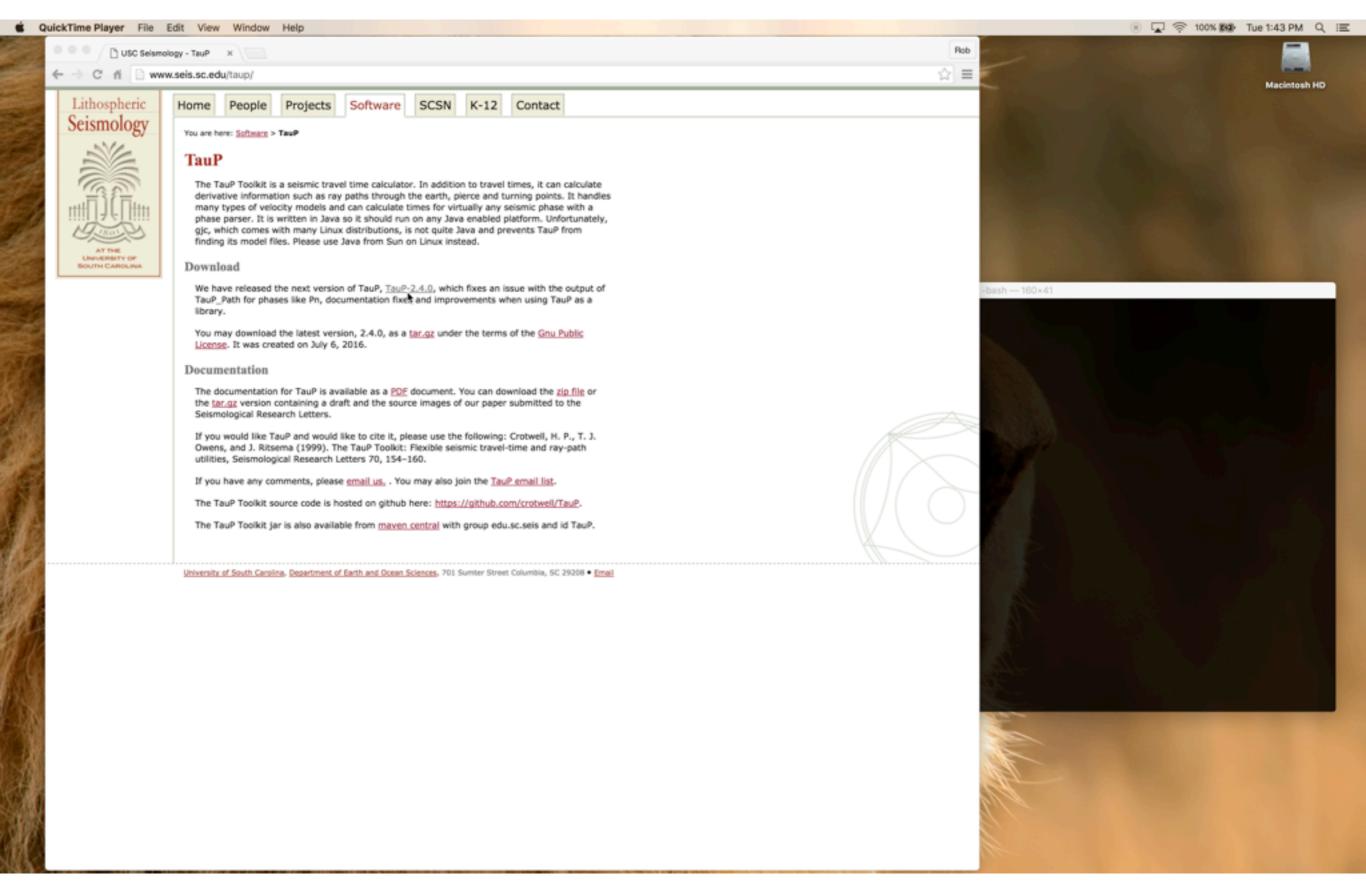




Some packages installed this way...

- obspy (also installs numpy, matlibplot, etc...)
- gmt
- git

Installing scripts or pre-compiled software (SOD, TauP, Fetch scripts, etc...)



Installing scripts or pre-compiled software (SOD, TauP, Fetch scripts, etc...)

```
[guest-wireless-upc-1606-10-120-106-164:~ porritt$ ls -lh FetchData
-rw-r----@ 1 porritt staff 72K Jul 14 12:36 FetchData
[guest-wireless-upc-1606-10-120-106-164:~ porritt$ head FetchData
#!/usr/bin/perl
                                   Tells shell what program to run this under
# FetchData
# Find the most current version at http://service.iris.edu/clients/
# Fetch data and related metadata from web services. The default web
# service are from the IRIS DMC, other FDSN web services may be
# specified by setting the following environment variables:
                                                                  Adds permission to execute
[guest-wireless-upc-1606-10-120-106-164:~ porritt$ ./FetchData
-bash: ./FetchData: Permission denied
[guest-wireless-upc-1606-10-120-106-164:~ porritt$ chmod +x FetchData
[guest-wireless-upc-1606-10-120-106-164:~ porritt$ ./FetchData
FetchData: collect time series and related metadata (version 2015.246)
http://service.iris.edu/clients/
Usage: FetchData [options]
 Options:
                   Increase verbosity, may be specified multiple times
 -v
                   Be quiet, do not print anything but errors
                   Network code, list and wildcards (* and ?) accepted
 -N,--net
                   Station code, list and wildcards (* and ?) accepted
 -S,--sta
```

Installing programs for Matlab

Check the file exchange:

https://www.mathworks.com/matlabcentral/fileexchange/

Hope the authors include an install or setup script

Add executable scripts to matlab path (ie pathtool or addpath)

Add jar files (ie group of java software files) to either the dynamic java path (javaaddpath) or the static class path edit ~/.matlab/{Version}/classpath.txt

Thanks! Any questions?