

Backpacking with Code: Software Portability for DHTC

Thursday morning, 9:00 am

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Motivation

running a piece of software is like cooking a
meal in a kitchen

The problem



Running
software on
your own
computer =
cooking in your
own kitchen

The problem

In your own kitchen:

- You have all the pots and pans you need
- You know where everything is
- You have access to all the cupboards

On your own computer:

- The software is installed, you know where it is, and you can access it.

The problem



Running on a shared computer =
cooking in someone else's kitchen.

The problem

In someone else's kitchen:

- You are guaranteed some things...
- ...but others may be missing
- You don't know where everything is
- Some of the cupboards are locked

On a shared computer:

- Your software may be missing, unfindable, or inaccessible.

The solution

- Think like a backpacker
- Take your software with you
 - Install anywhere
 - Run anywhere
- This is called making software *portable*



Software

- How do we make software portable?
- First we have to understand:
 - What software is and how it works
 - Where software lives
 - How we run it

How software works

- A software program can be thought of as a list of instructions or tasks that can be run on a computer
- A launched program that is running on your computer is managed by your computer's operating system (OS)
- The program may make requests (access this network via wireless, save to disk, use another processor) that are mediated by the OS
- A single program may also depend on other programs besides the OS

How software works*

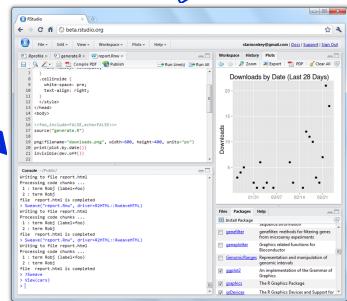
*Not to scale

Program
(software, code,
executable, binary)



launches to

runs
own
tasks



depends on



Running Program
(process, instance)

Operating
System



makes
requests

monitors
running
programs

translates
program's
request to
computer
hardware



Hardware
(processors,
memory, disk)

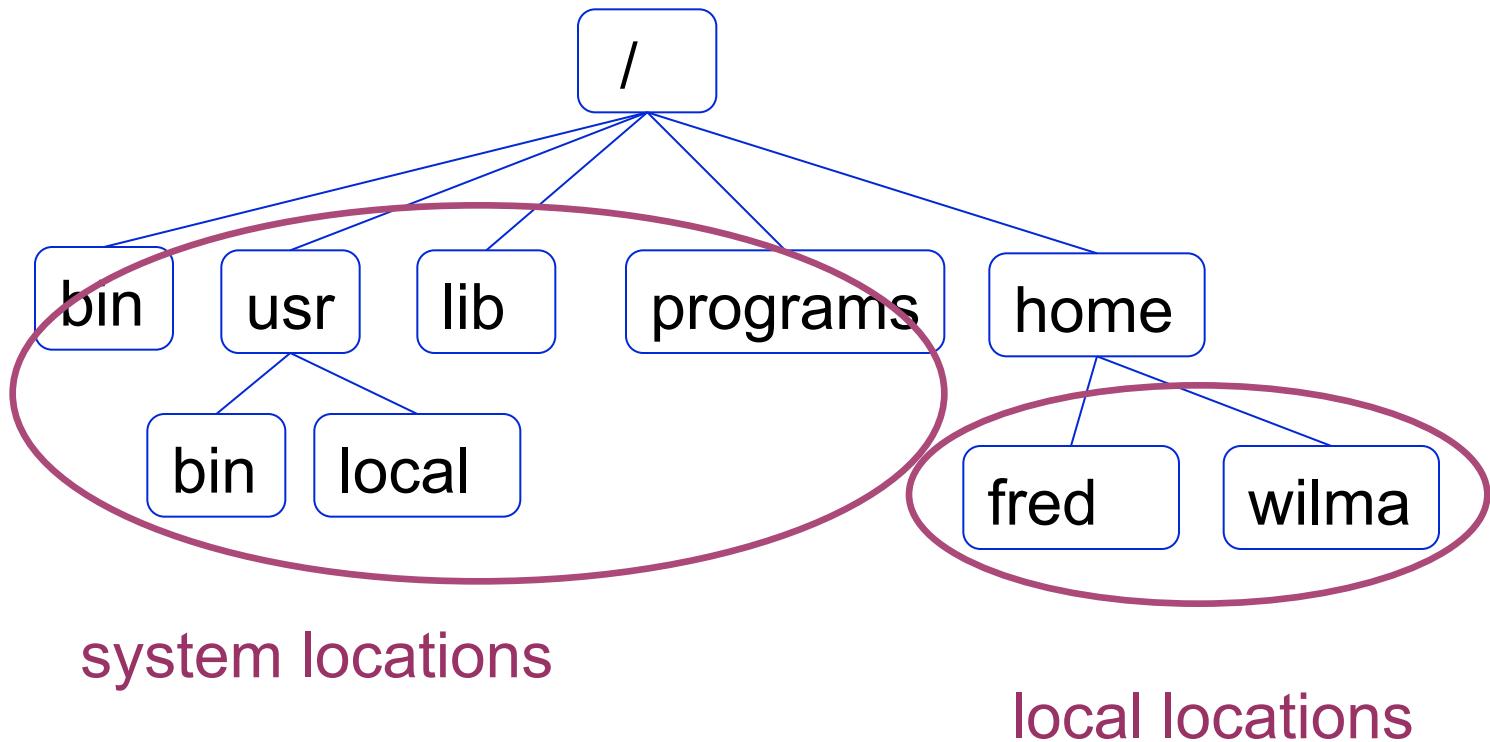
How software works

Implications for DHTC:

- Software must be able to run on target operating system (usually Linux)
- Request specific OS as job requirement
- Know what else your software depends on

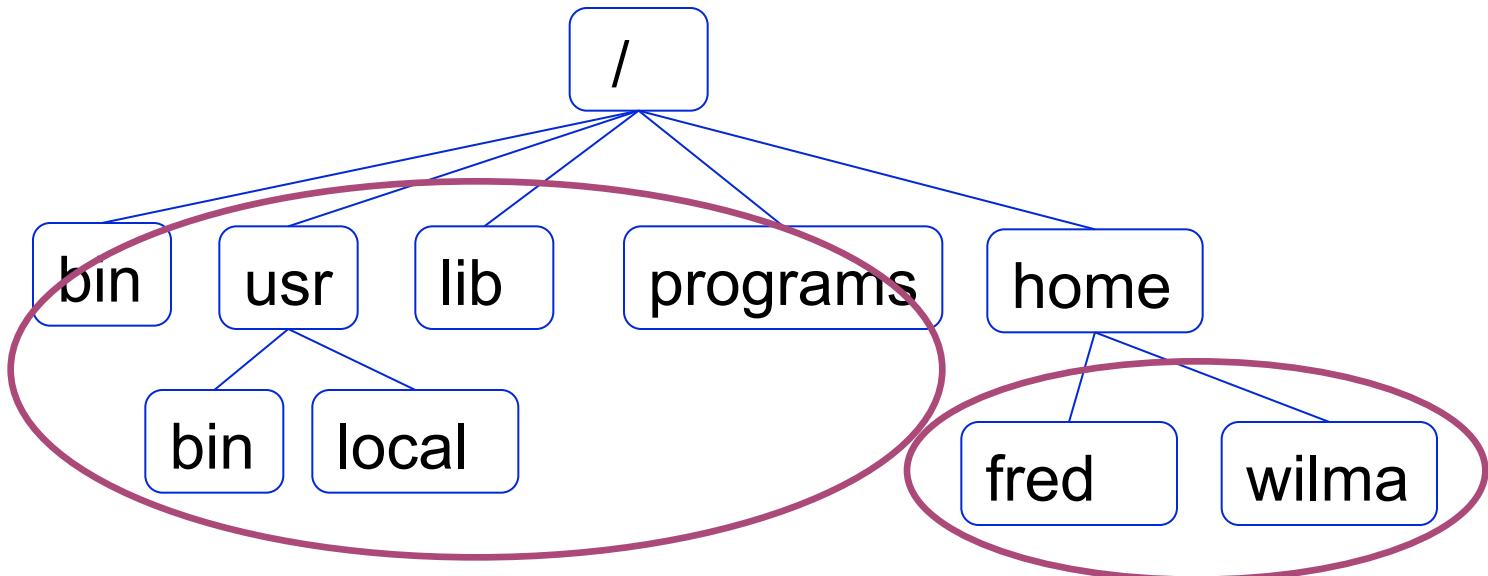
Location, location, location

- Where can software be installed?



Location, location, location

- Who can install the software?

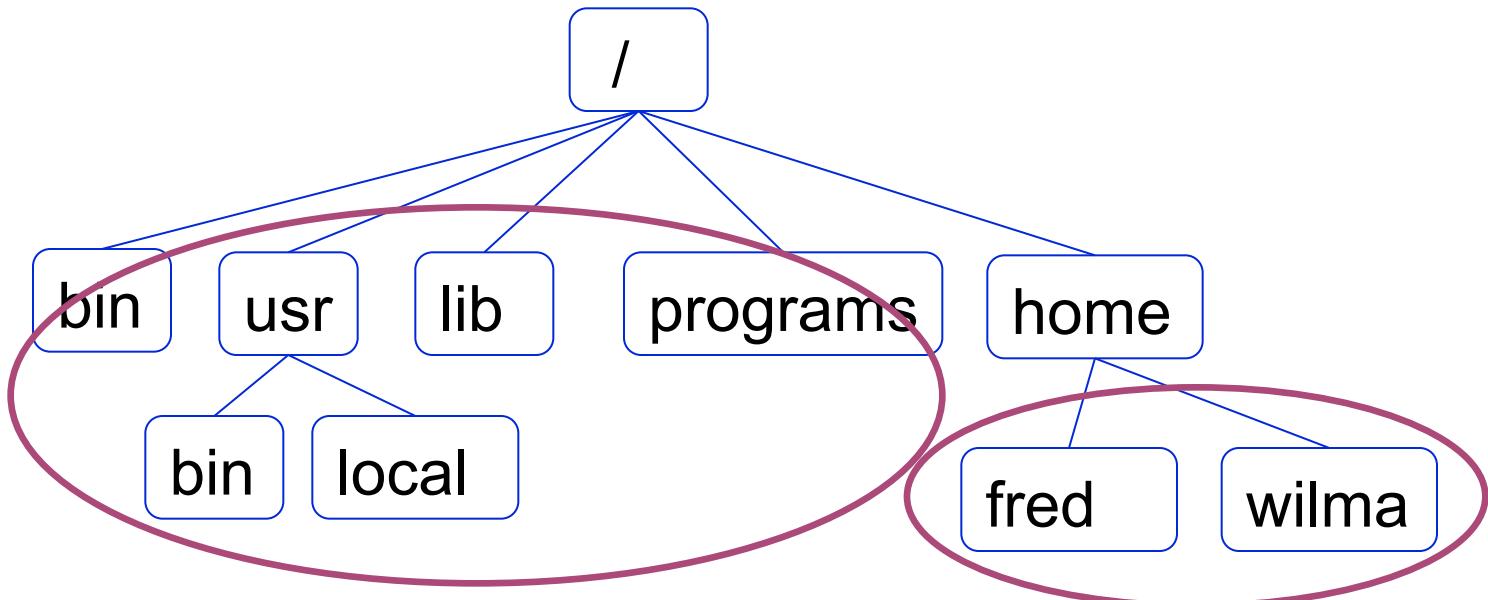


Usually requires
administrative privileges

Owner of the
directory

Location, location, location

- Who can access the software?



Anyone on the system

The local user can control who has access

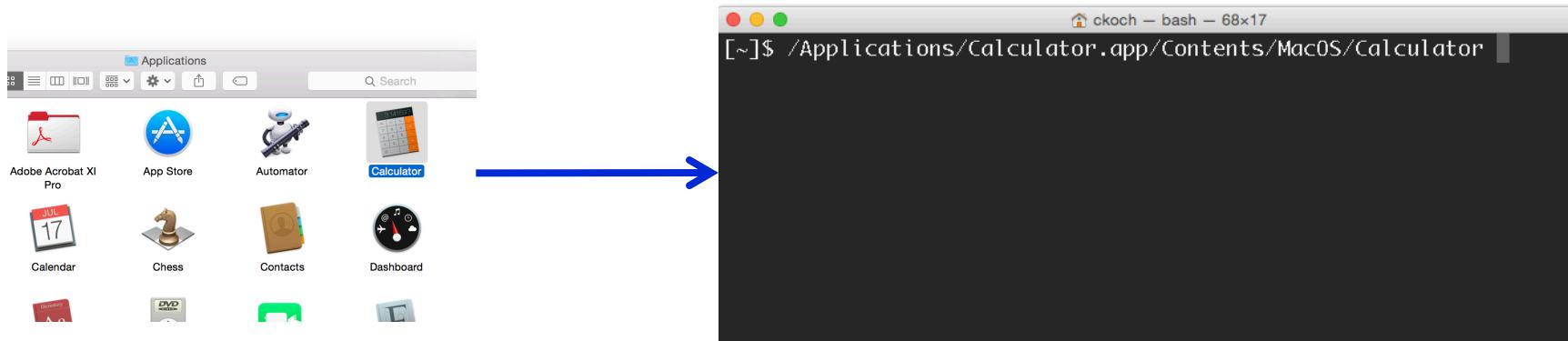
Location, location, location

Implications for DHTC:

- Software MUST be able to install to a local location
- Software must be installable without administrative privileges

Location and running software

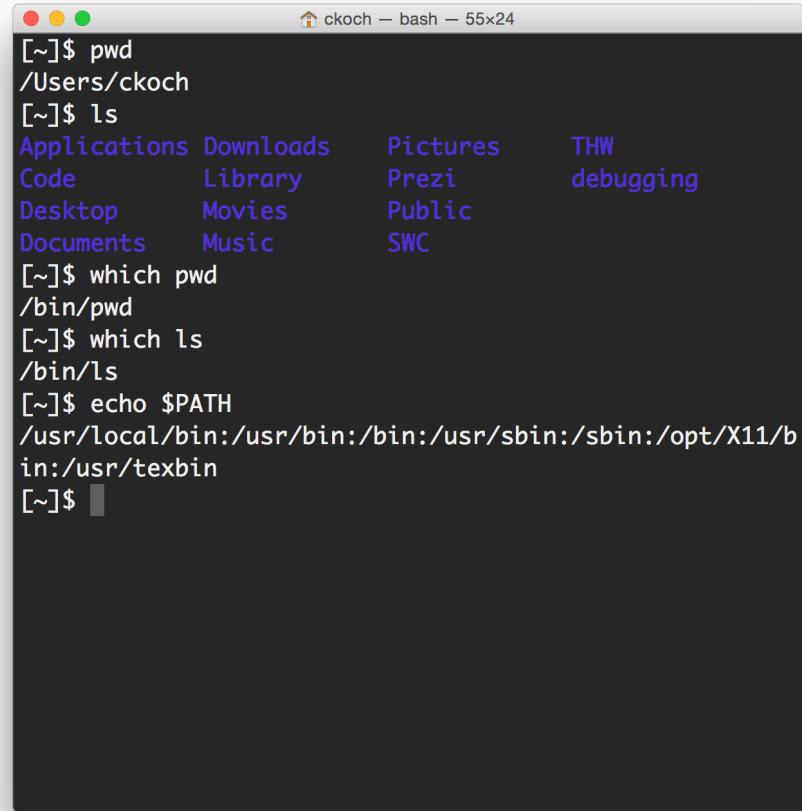
Instead of graphic interface... command line



- All DHTC jobs must use software that can be run from the command line.
- To run a program on the command line, your computer needs to know where the program is located in your computer's filesystem.

Common programs on command line

- Common command line programs like `ls` and `pwd` are in a system location called `/bin`
- Your computer knows their location because `/bin` is included in your `PATH`
- The PATH is a list of locations to look for programs

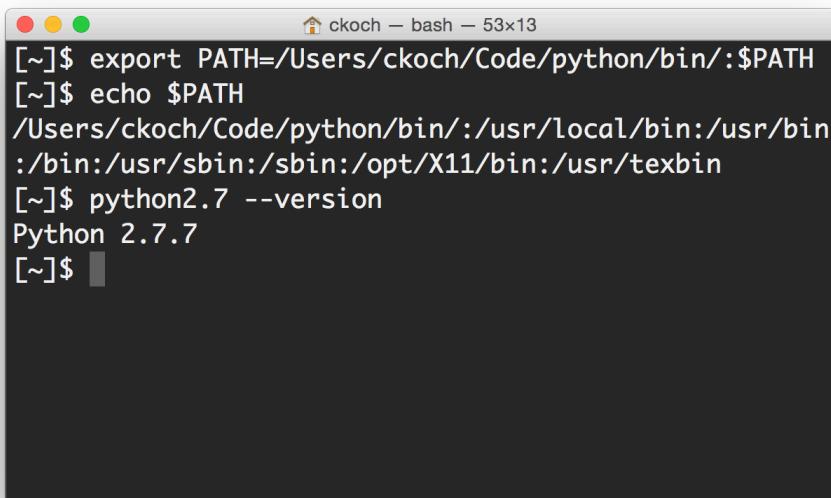


```
[~]$ pwd  
/Users/ckoch  
[~]$ ls  
Applications Downloads Pictures THW  
Code Library Prezi debugging  
Desktop Movies Public  
Documents Music SWC  
[~]$ which pwd  
/bin/pwd  
[~]$ which ls  
/bin/ls  
[~]$ echo $PATH  
/usr/local/bin:/usr/bin:/bin:/usr/sbin:/sbin:/opt/X11/bin:/usr/texbin  
[~]$
```

Other programs on command line

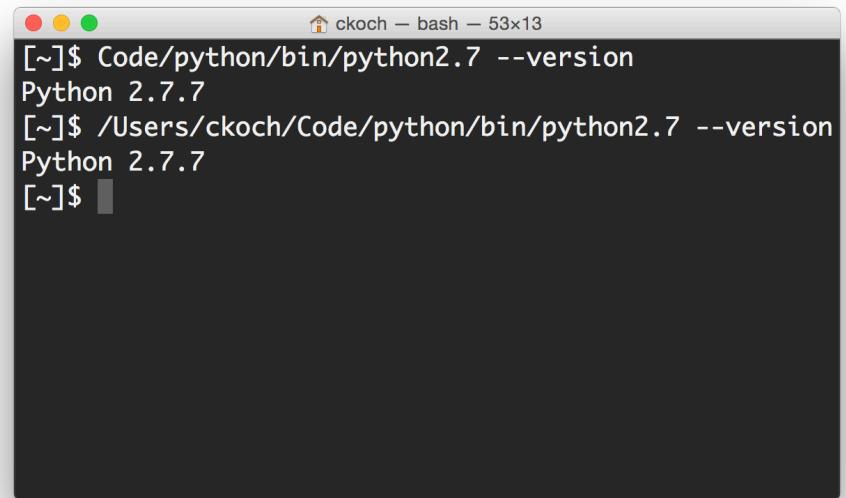
- Other programs may be installed in locations not listed in the PATH. You can access them by:

Adding their location to the PATH, then running



```
[~]$ export PATH=/Users/ckoch/Code/python/bin/:$PATH
[~]$ echo $PATH
/Users/ckoch/Code/python/bin:/usr/local/bin:/usr/bin
:/bin:/usr/sbin:/sbin:/opt/X11/bin:/usr/texbin
[~]$ python2.7 --version
Python 2.7.7
[~]$
```

Using an relative or absolute path to the software



```
[~]$ Code/python/bin/python2.7 --version
Python 2.7.7
[~]$ /Users/ckoch/Code/python/bin/python2.7 --version
Python 2.7.7
[~]$
```

Command line

Implications for DHTC:

- Software must have ability to be run from the command line
- Multiple commands are okay, as long as they can be executed in order within a job

Portability requirements

Based on the previous slides, we now know that in order to make software portable for DHTC, the software:

- Must work on target operating system (probably Linux)
- Must be accessible to your job (placed or installed in job's working directory)
- Must be able to run without administrative privileges
- Must be able to run from the command line, without any interactive input from you

Returning to our scenario:

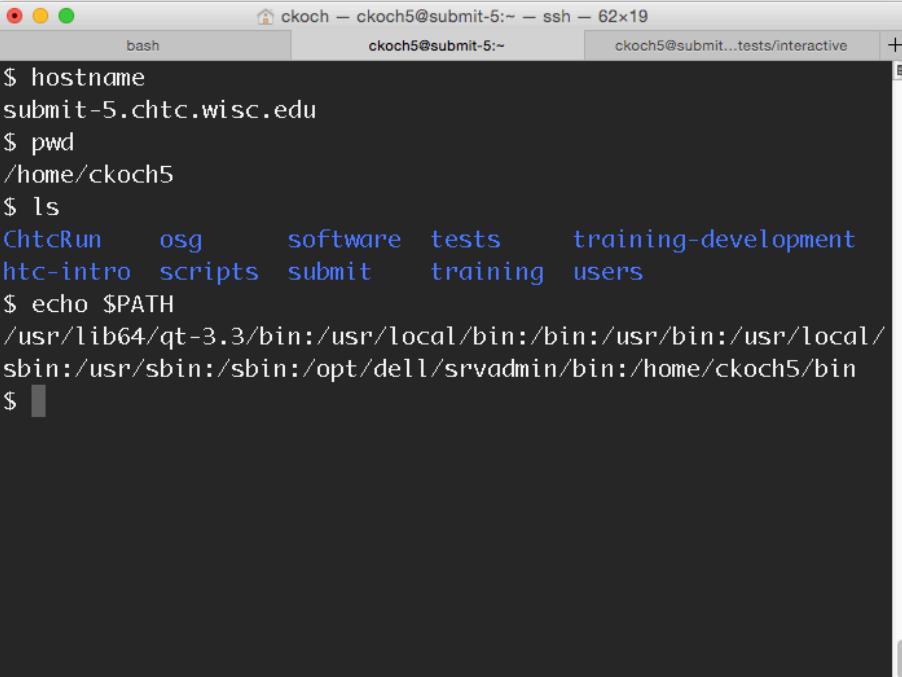
In a DHTC situation, we are:

- Using someone else's computer
 - Software may not be installed
 - The wrong version may be installed
 - We can't find/run the installed software

Therefore:

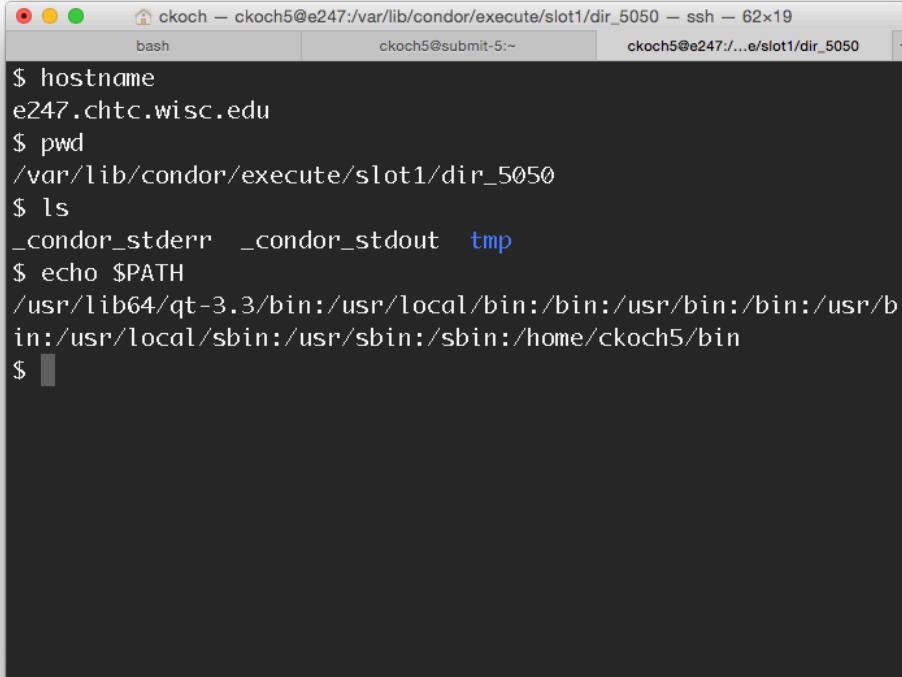
- We need to bring along and install/run software ourselves

Home server vs job server



```
ckoch - ckoch5@submit-5:~ - ssh - 62x19
bash                                ckoch5@submit-5:~                                ckoch5@submit...tests/interactive +
```

```
$ hostname
submit-5.ctc.wisc.edu
$ pwd
/home/ckoch5
$ ls
ChtcRun    osg      software  tests      training-development
htc-intro   scripts  submit     training   users
$ echo $PATH
/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/
sbin:/usr/sbin:/sbin:/opt/dell/srvadmin/bin:/home/ckoch5/bin
$
```



```
ckoch - ckoch5@e247:/var/lib/condor/execute/slot1/dir_5050 - ssh - 62x19
bash                                ckoch5@submit-5:~                                ckoch5@e247:...e/slot1/dir_5050 +
```

```
$ hostname
e247.ctc.wisc.edu
$ pwd
/var/lib/condor/execute/slot1/dir_5050
$ ls
._condor_stderr  ._condor_stdout  tmp
$ echo $PATH
/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/b
in:/usr/local/sbin:/usr/sbin:/sbin:/home/ckoch5/bin
$
```

Portability methods

There are two primary methods to make code portable:

- Use a compiled binary
 - Typically for code written in C, C++ and Fortran
- “Install” with every job
 - Can’t be compiled into a single binary
 - Interpreted languages (Matlab, Python, R)



Open Science Grid

Method 1

USE A COMPILED BINARY

What is compilation?

Source code

```
1<?php
2    $tPass;
3    $users = file("login.dat");
4    $i = 0; $i < count($users); $i++
5    $line = $users[$i];
6    if (eregi("^$username:", $line))
7        // User gevonden, password is nu
8        $pass = $regs[1]; trim($line)
9        break; // stop met de 'for'-loop
10   }
11   return $pass;
12 }
13 function IsLoggedIn() {
14     global $username, $password;
15     if ($username && $password)
16         $pass = md5($password);
17     return ($password == $pass);
18 }
19 return FALSE;
```

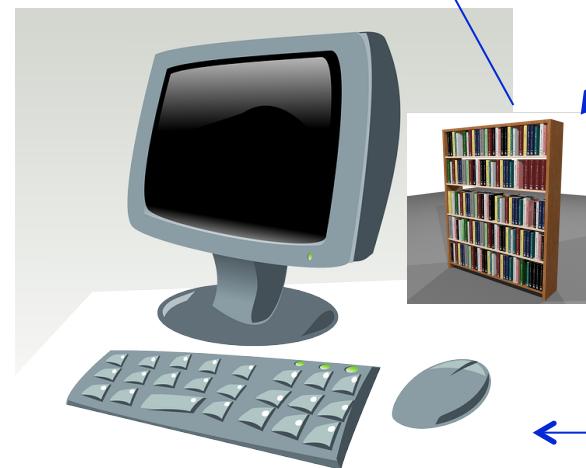
Binary

```
11100110011100100000000
1011001010111001010101
100000110000101110000
00100110000101110000
10110111001100111001
111100101011100111011
101000000111000001100
100000110100101101111
101100001011100000110
110001100111001000000
1011001010111001010101
```

compiled into

compiler
and OS

libraries



run on

Static compilation

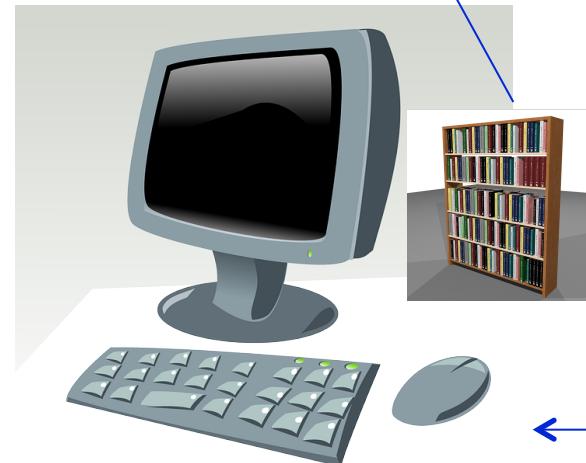
Source code

```
1<?php
2    $tPassw
3    <?
4    = file("login.dat");
5    $i = 0; $i < count($users); $i++
6    $line = $users[$i];
7    if (eregi("^$usernames(.*)", trim($line))
8        // User gevonden, password is nu
9        $pass = $regs[1]; $pass is nu
10       break; // stop met de 'for'-loop
11   }
12   return $pass;
13 }
14 function IsLoggedIn() {
15     global $username, $password;
16     if ($username && $password)
17         $pass = md5($password);
18     return ($password == $pass);
19 }
20 return FALSE;
```

statically compiled into

compiler
and OS
libraries

Static binary



run anywhere

Compilation (command line)

```
ckoch — ckoch5@submit-5:~/osg/code/compile — ssh — 69x21
$ ls
hello.c
$ gcc hello.c -o hello_dynamic
$ ls
hello.c  hello_dynamic
$ file hello_dynamic
hello_dynamic: ELF 64-bit LSB executable, x86-64, version 1 (SYSV), d
ynamically linked (uses shared libs), for GNU/Linux 2.6.18, not strip
ped
$ gcc -static hello.c -o hello_static
$ ls
hello.c  hello_dynamic  hello_static
$ file hello_static
hello_static: ELF 64-bit LSB executable, x86-64, version 1 (GNU/Linux
), statically linked, for GNU/Linux 2.6.18, not stripped
$
```

Static compilation workflow

Option 1
compile

```
1<file>
2<file>
3<file>
4<file>
5<file>
6<file>
7<file>
8<file>
9<file>
10<file>
11<file>
12<file>
13<file>
14<file>
15<file>
16<file>
17<file>
18<file>
19<file>
20<file>
21<file>
22<file>
23<file>
24<file>
25<file>
26<file>
27<file>
28<file>
29<file>
30<file>
31<file>
32<file>
33<file>
34<file>
35<file>
36<file>
37<file>
38<file>
39<file>
40<file>
41<file>
42<file>
43<file>
44<file>
45<file>
```

Option 2
download



Submit server

Static binary

```
111001100111001000000
0011001010110010■01
100000110000101110000
001000110000101110000
1011001101100110011001
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
01100000011100001100
101100110011001011011
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
```

Execute server

```
111001100111001000000
0011001010110010■01
100000110000101110000
001000110000101110000
1011001101100110011001
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
01100000011100001100
101100110011001011011
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
```

```
111001100111001000000
0011001010110010■01
100000110000101110000
001000110000101110000
1011001101100110011001
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
01100000011100001100
101100110011001011011
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
```

```
111001100111001000000
0011001010110010■01
100000110000101110000
001000110000101110000
1011001101100110011001
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
01100000011100001100
101100110011001011011
01110010■01110111011
00100000011100001100
100000010100101101111
001100110011001011011
10100000011100001100
```



Open Science Grid

Method 2

INSTALL WITH EVERY JOB

Install software with every job

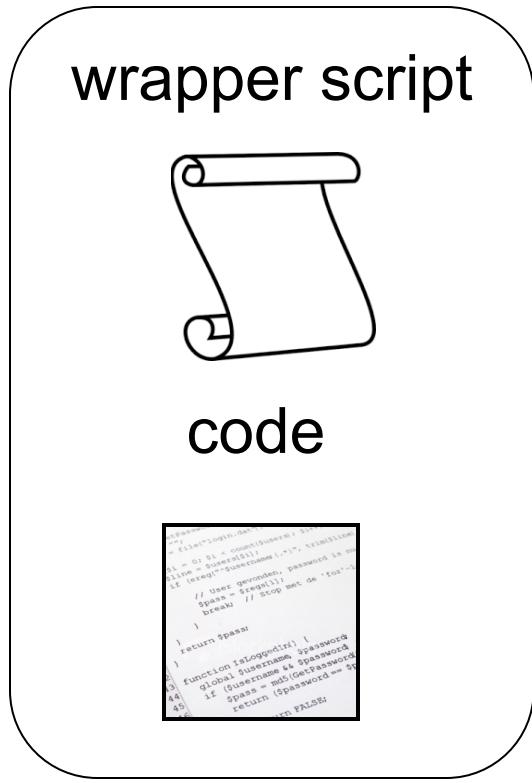
- Good for software that:
 - Can't be statically compiled
 - Uses interpreted languages (Matlab, Python, R)
 - Any software with instructions for local installation
- Method: write a wrapper script
 - Contains a list of commands to execute
 - Typically written in bash or perl (usually common across operating systems/versions)

Wrapper scripts

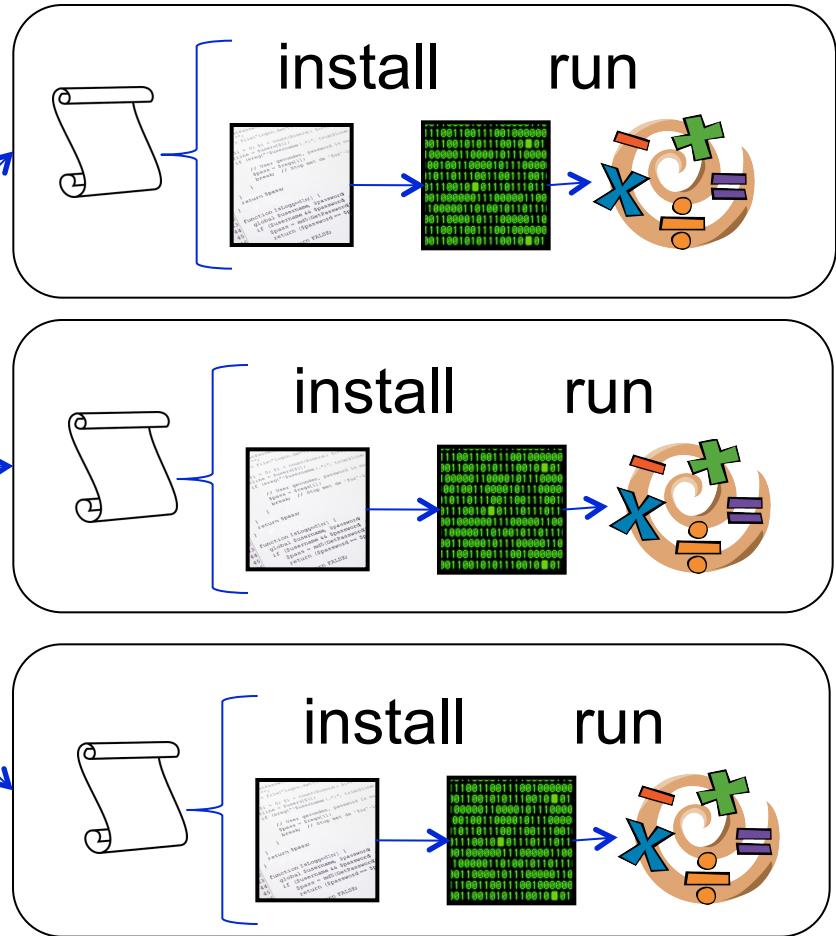
- Install software in the working directory
 - Bring along pre-built software
 - or
 - Install a fresh copy
- Run software
- Besides software: manage data/files in the working directory
 - Move or rename output
 - Delete installation files before job completion

Wrapper script workflow

Submit server



Execute server



Preparing your code

- Where do you compile code? Pre-build code? Test your wrapper script installation?
- Guiding question: how computationally intensive is the task?
 - Computationally intensive (takes more than a few minutes, as a rule of thumb)
 - Run as interactive job, on a private computer/server, or with a queued job
 - Computationally light (runs in few minutes or less)
 - Run on submit server (or above options, if desired)

Exercises

- Software is a compiled binary
 - Exercise 1.1: statically compile code and run (C code)
 - Exercise 1.2: download and run pre-compiled binary (BLAST)
- Install software with each job
 - Exercise 1.3: write a wrapper script to install and run software (GROMACS)

Questions?

- Feel free to contact me:
 - ckoch5@wisc.edu
- Now: Hands-on Exercises
 - 9:30-10:30am
- Next:
 - 10:30-10:45am: Break
 - 10:45am-12:15pm: Other research software considerations: licenses and interpreted languages
 - 12:15-1:15pm: Lunch