Backpacking with Code: Software Portability for DHTC

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Goals For This Session

- Understand the basics of...
  - how software works
  - where software is installed
  - how software is accessed and run
- ...and the implications for Distributed High Throughput Computing (DHTC)
- Describe what it means to make software “portable”
- Learn about and use software portability techniques

An Analogy

Running software on your own computer is like cooking in your own kitchen.

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On Your Computer

- You know what you already have.
  - All the software you need is already installed.
- You know where everything is (mostly).
- You have full control.
  - You can add new programs when and where you want.

The Problem

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

On Someone Else's Computer

- What's already there?
  - Is R installed? Or Python? What about the packages you need?
- Do you know where anything is?
- Are you allowed to change whatever you want?

The Solution

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

PRELIMINARY CONCEPTS

Software Programs Are Files

- Principle
  - Software is a set of files.
  - These files have instructions for the computer to execute.
- Implications for DHTC
  - Isolate the specific software files needed for a job and bring them along.

How Software Works*

*Not to scale

Program

(software, code, executable, binary)

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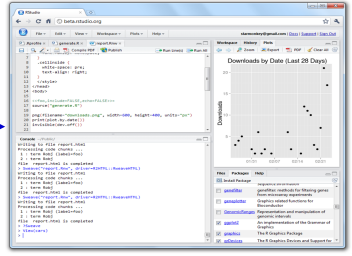
launches to

Running Program

(process, instance)



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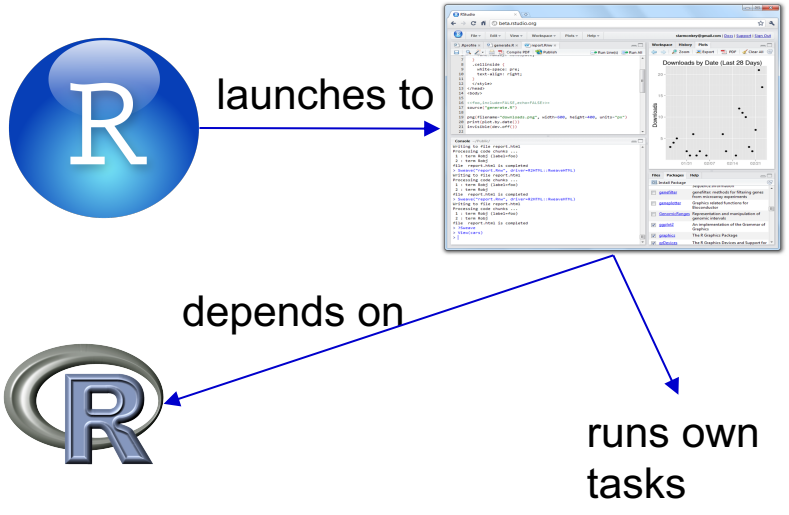

How Software Works*

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Program
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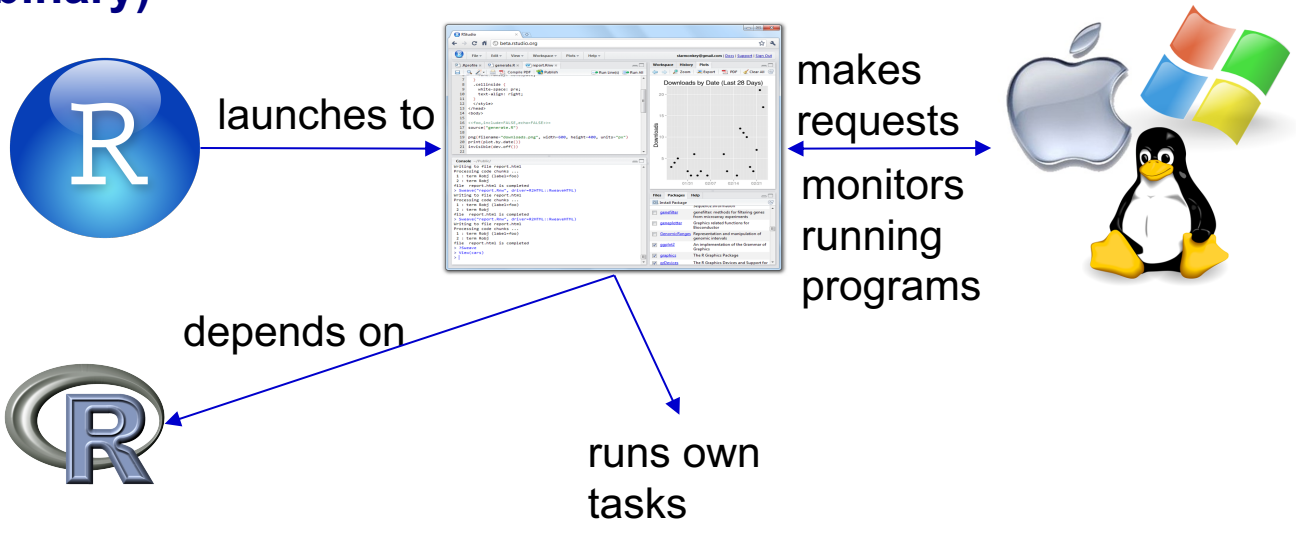
Running Program
(process, instance)

Operating System



How Software Works*

*Not to scale

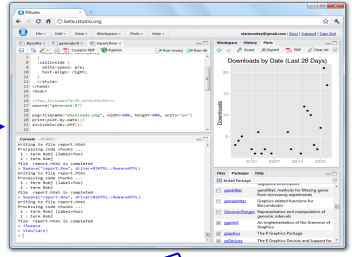
Program
(software, code, executable, binary)

Running Program
(process, instance)

Operating System

Hardware
(processors, memory, disk)

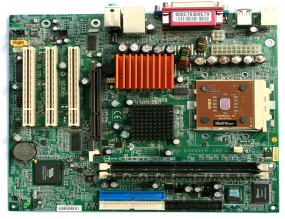
launches to



makes requests

monitors running programs

translates program's request



depends on

runs own tasks

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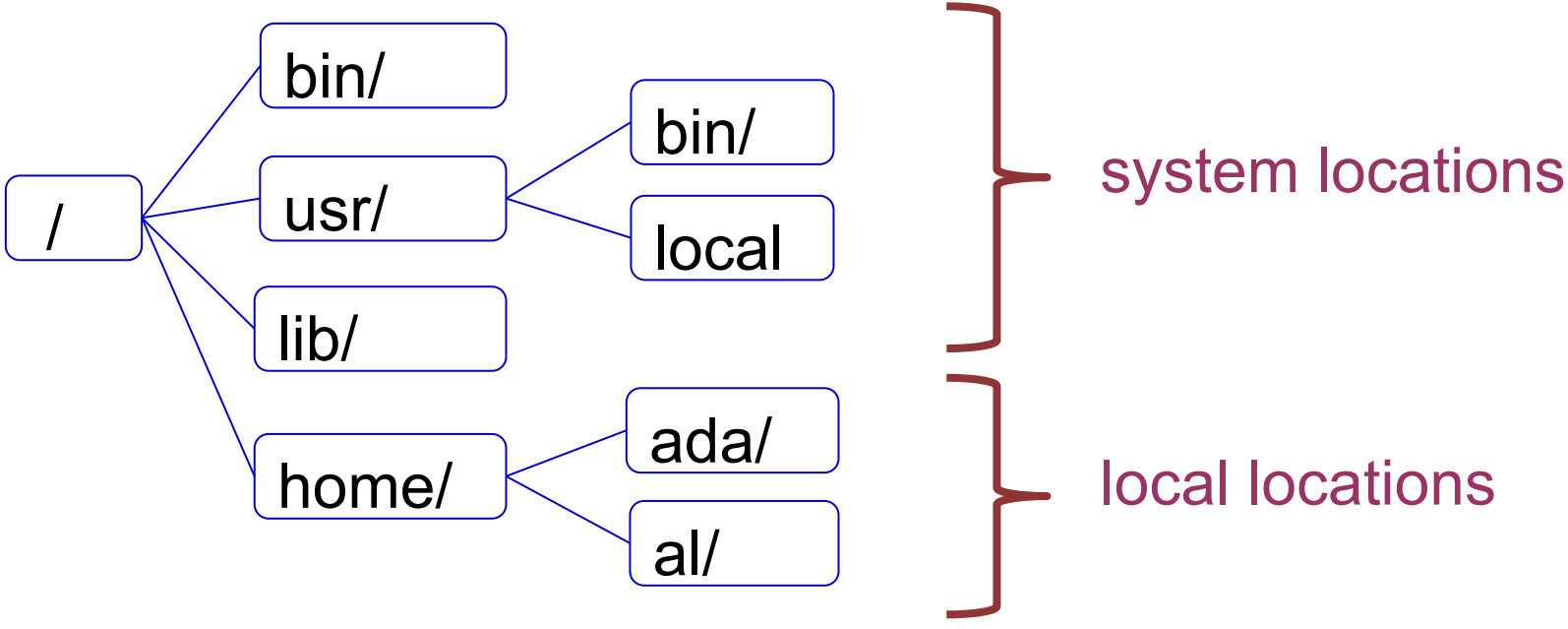
How Software Works

- Principle:
  - Software depends on the operating system, and other installed programs.
- Implications for DHTC:
  - Software must be able to run on target operating system (usually Linux).
  - Know what else your software depends on.

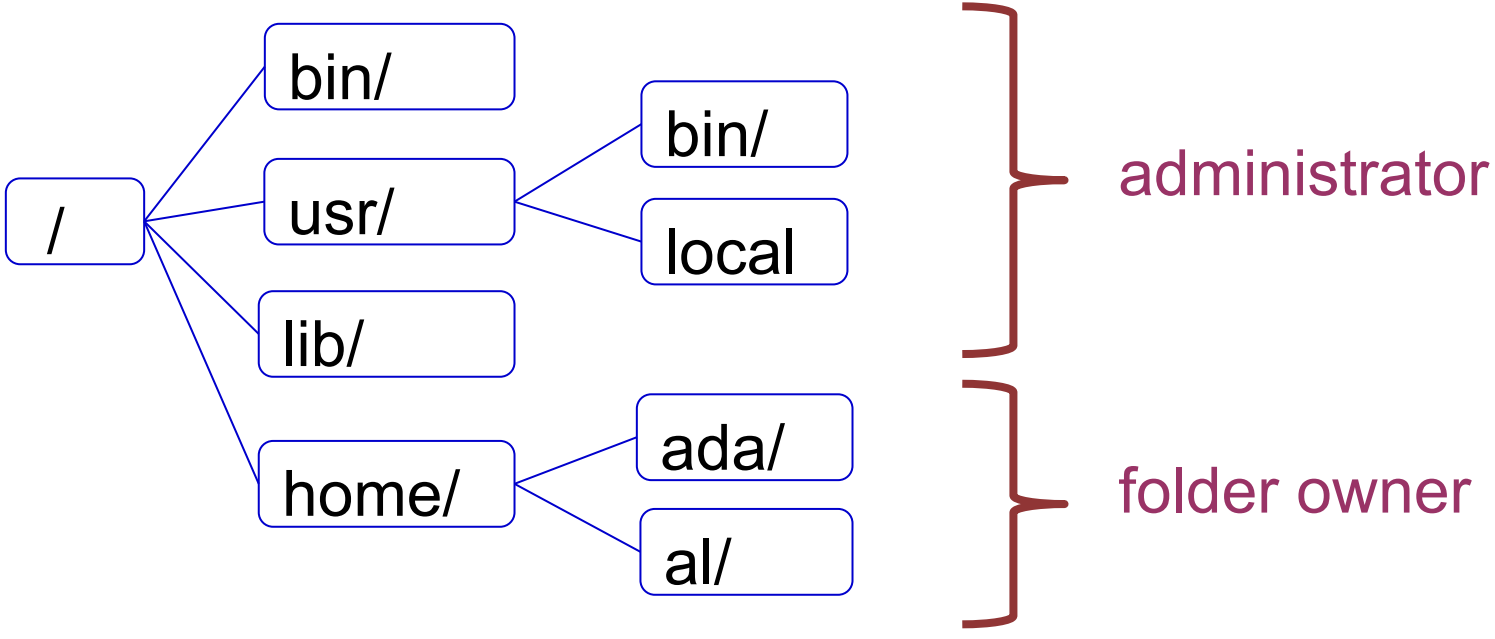
Location, Location, Location

- Where can software be installed?



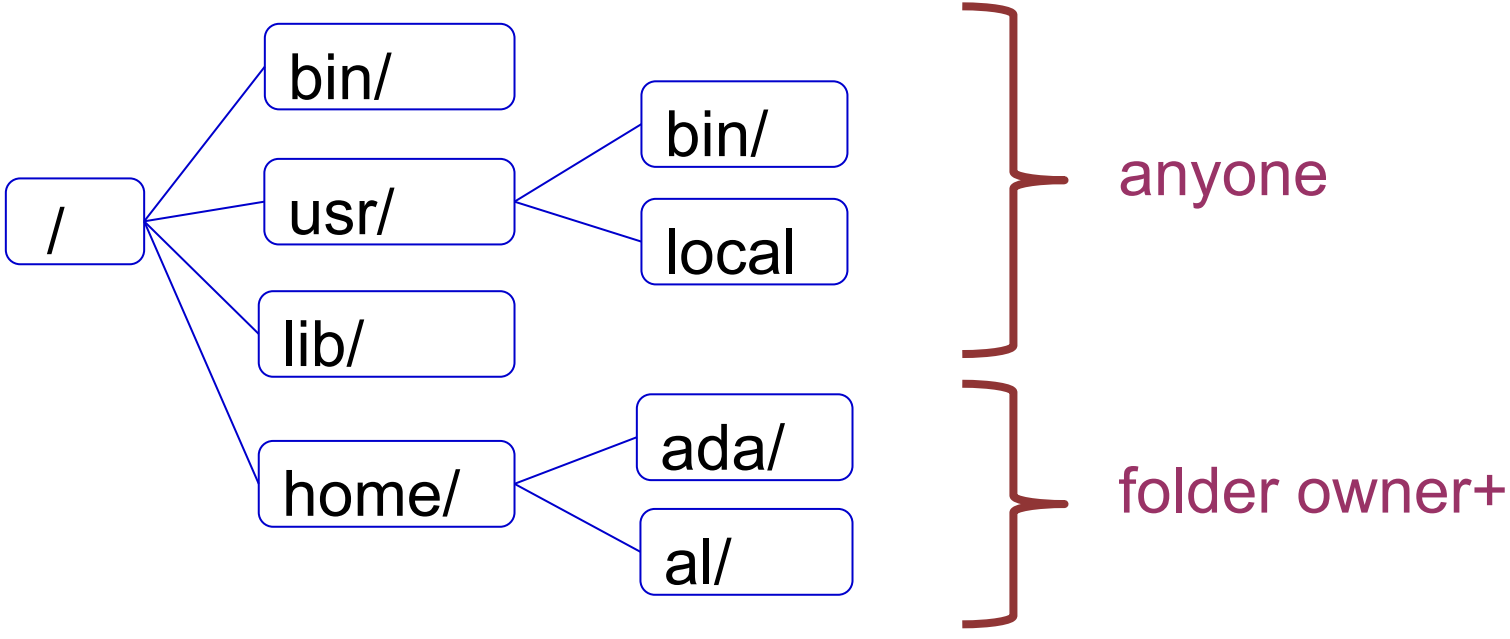
Location, Location, Location

- Who can install the software?



Location, Location, Location

- Who can access the software?

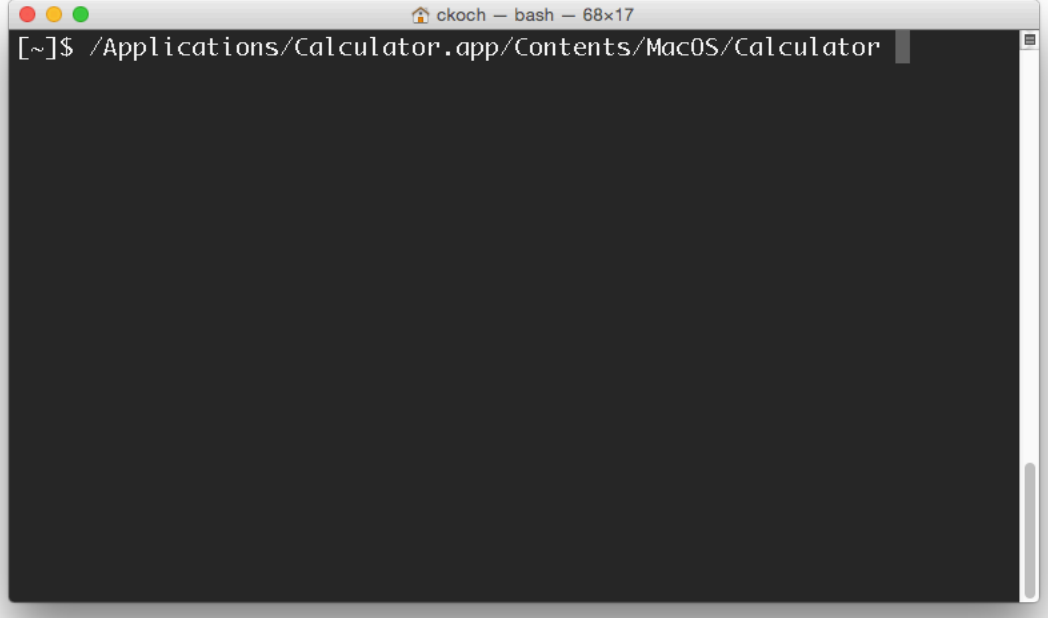


Location, Location, Location

- Principle:
  - Software files have to be installed somewhere in the file system.
- Implications for DHTC:
  - Software must be installable without administrative privileges.
  - The software's location needs to be accessible to you.

Command Line

How to automate programs?



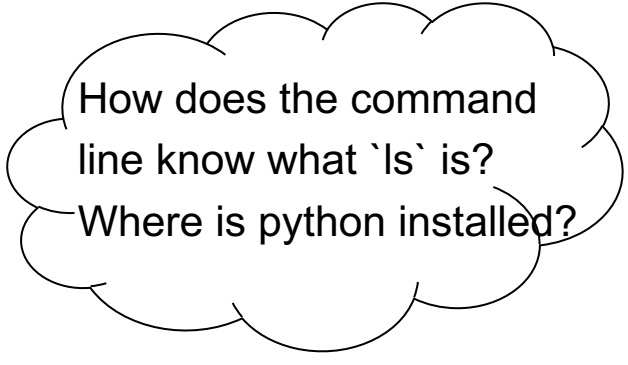
Command Line

- Principle:
  - To automatically run software, need to use text commands (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.

Command Line and Location

- To run a program on the command line, your computer needs to know where the program is located in your computer's file system.

```
$ ls
$ python
$ ~/wrapper.sh
```



Two Location Options

Provide a path (relative or absolute)

```
[~/Code]$ mypy/bin/python --version
Python 2.7.7
```

Use “the” PATH

```
$ export PATH=/Users/alice/Code/mypy/bin:$PATH
$ echo $PATH
/Users/alice/Code/mypy/bin:/usr/local/bin:/usr/bin:/bin:/usr
/sbin:/sbin
$ which python
/Users/alice/Code/mypy/bin/python
```

Command Line

- Principle:
  - To run a program on the command line, the computer has to be able to find it.
- Implications for DHTC:
  - There are different ways to “find” your software on the command line: relative path, absolute path, and PATH variable

Portability

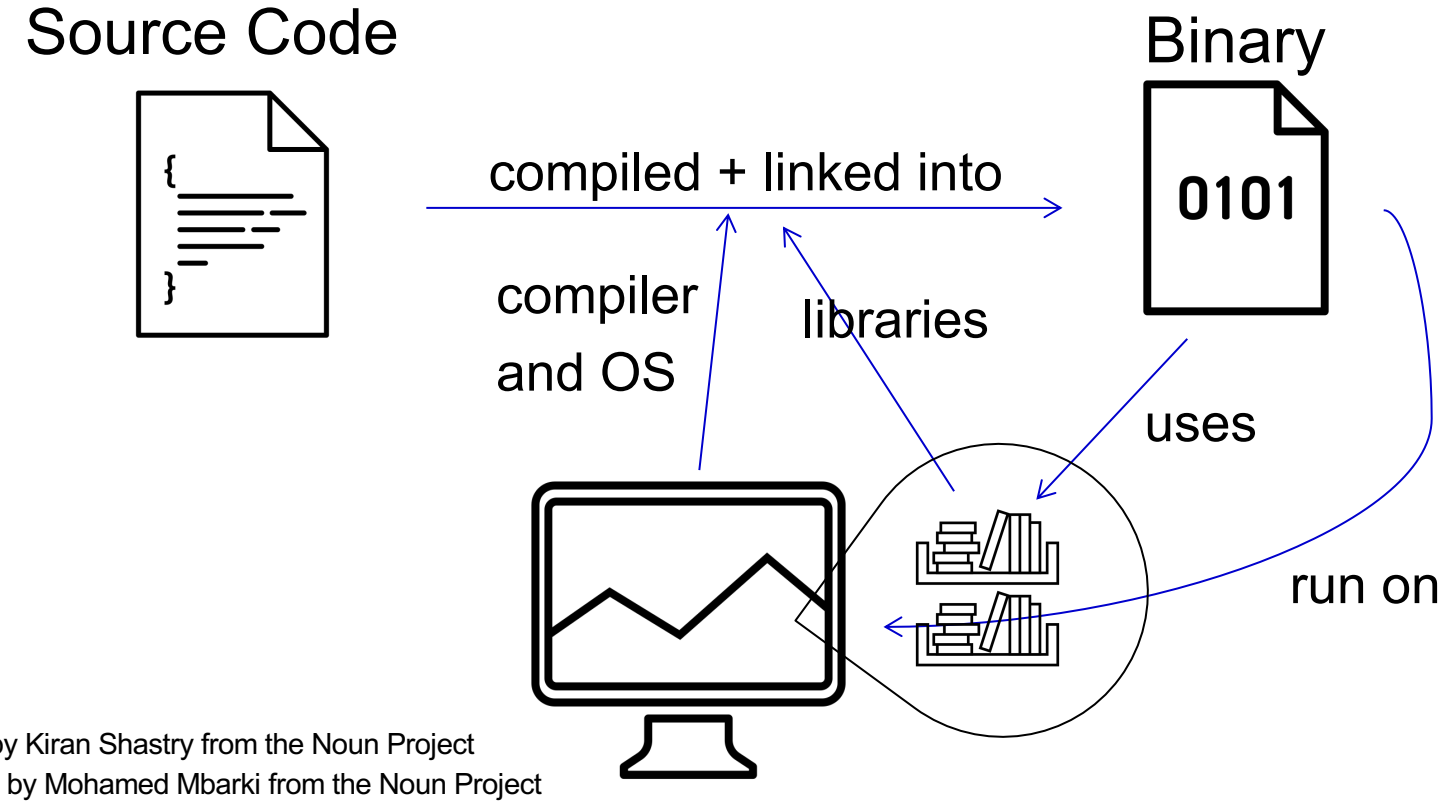
- Run “anywhere” by:
  - bringing along the software files you need…
  - to a location you can access/control…
  - using the command line to run…
  - by providing the correct software location…
  - (on Linux).

BRING ALONG SOFTWARE FILES

Ways to Prepare Software Files

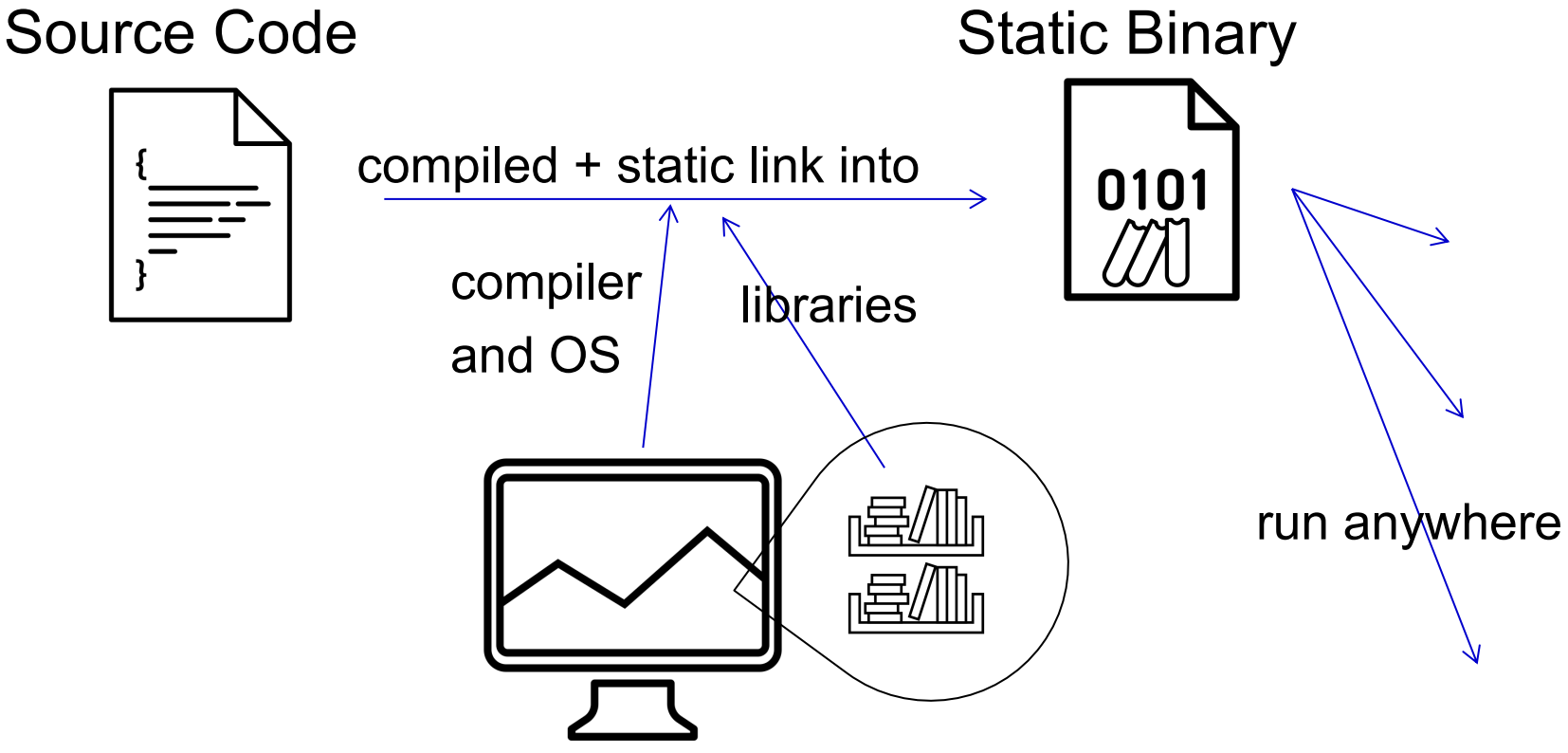
- Download pre-compiled software
- Compile yourself
  - Single binary file
  - Installation contained in a single folder

What is Compilation?



binary code by Kiran Shastry from the Noun Project
Source Code by Mohamed Mbarki from the Noun Project
Computer by rahmat from the Noun Project
books by Viral faisalovers from the Noun Project

Static Linking



Book by Aleksandr Vector from the Noun Project

Compilation Process

- Use a compiler (like gcc) directly
  - Can use options to control compilation process
- More common:

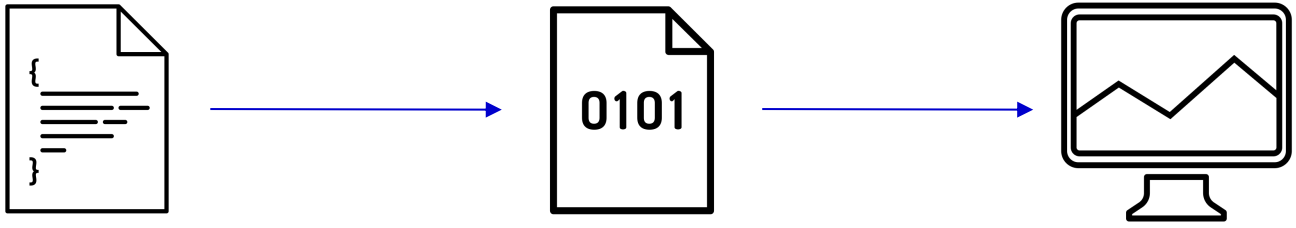
  ./configure # can also include options

  make

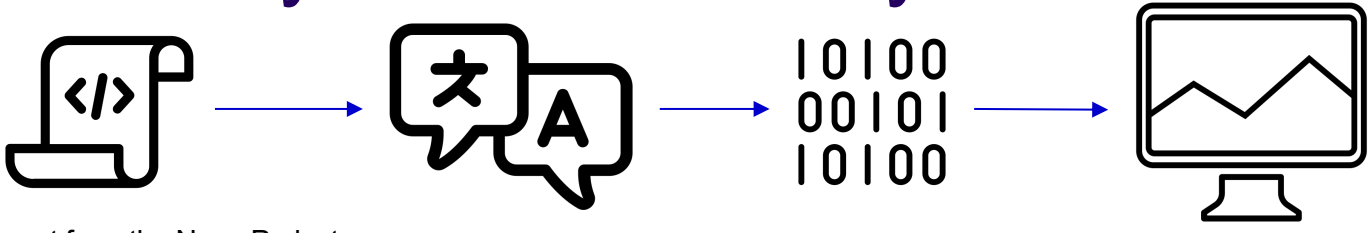
  make install

Interpreted code

- Instead of being compiled and then run…



- …interpreted languages are translated into binary code “on the fly.”



script by Adrien Coquet from the Noun Project
translate by Adrien Coquet from the Noun Project
coding by Vectorstall from the Noun Project

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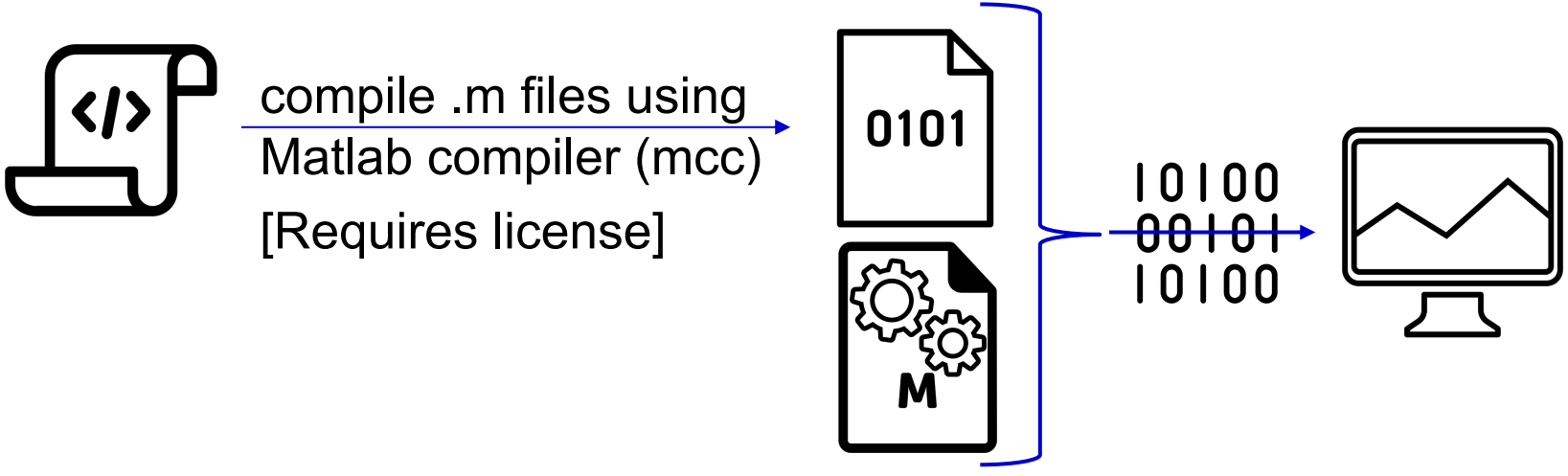
What Kind of Code?

- Programs written in C, C++ and Fortran are typically compiled.
- For interpreted (scripting) languages like perl, Python, R, or Julia:
  - Don’t compile the scripts, but *do* use a compiled copy of the underlying language interpreter.

Matlab

- Matlab is a scripting language…but can also be compiled.



compiled file and Matlab Runtime work together to run program.

[no license needed]

M File by Viktor Vorobyev from the Noun Project
Gears by Trevor Dsouza from the Noun Project

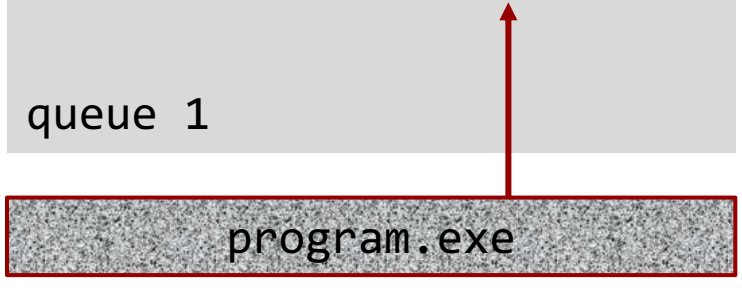
Ways to Run Software

Executable

- Software must be a single compiled binary file.

```
executable = program.exe

queue 1
```



Wrapper Script

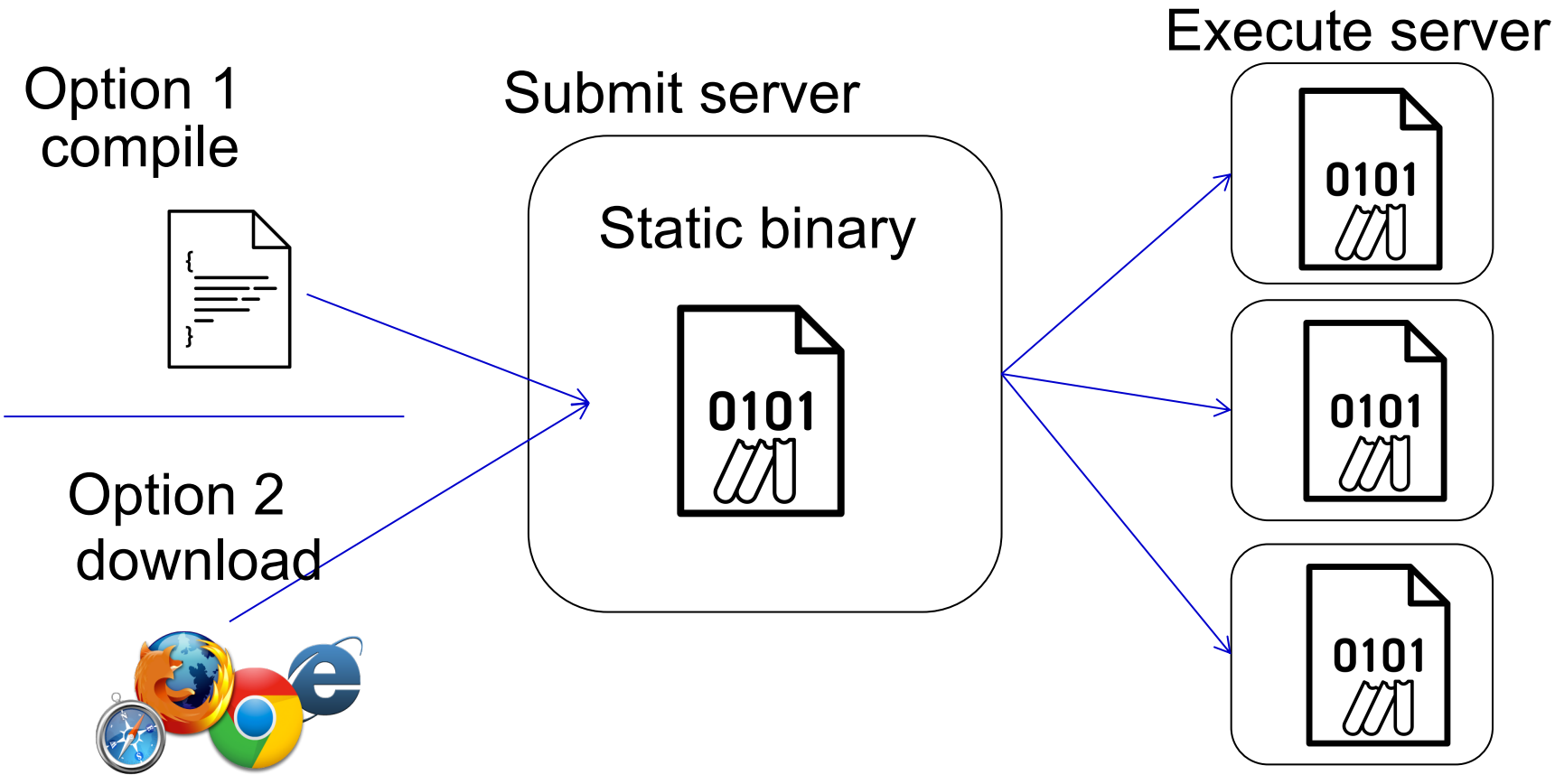
- Software can be in any compiled format.

```
executable = run_program.sh
transfer_input_files =
            program.tar.gz
queue 1
```

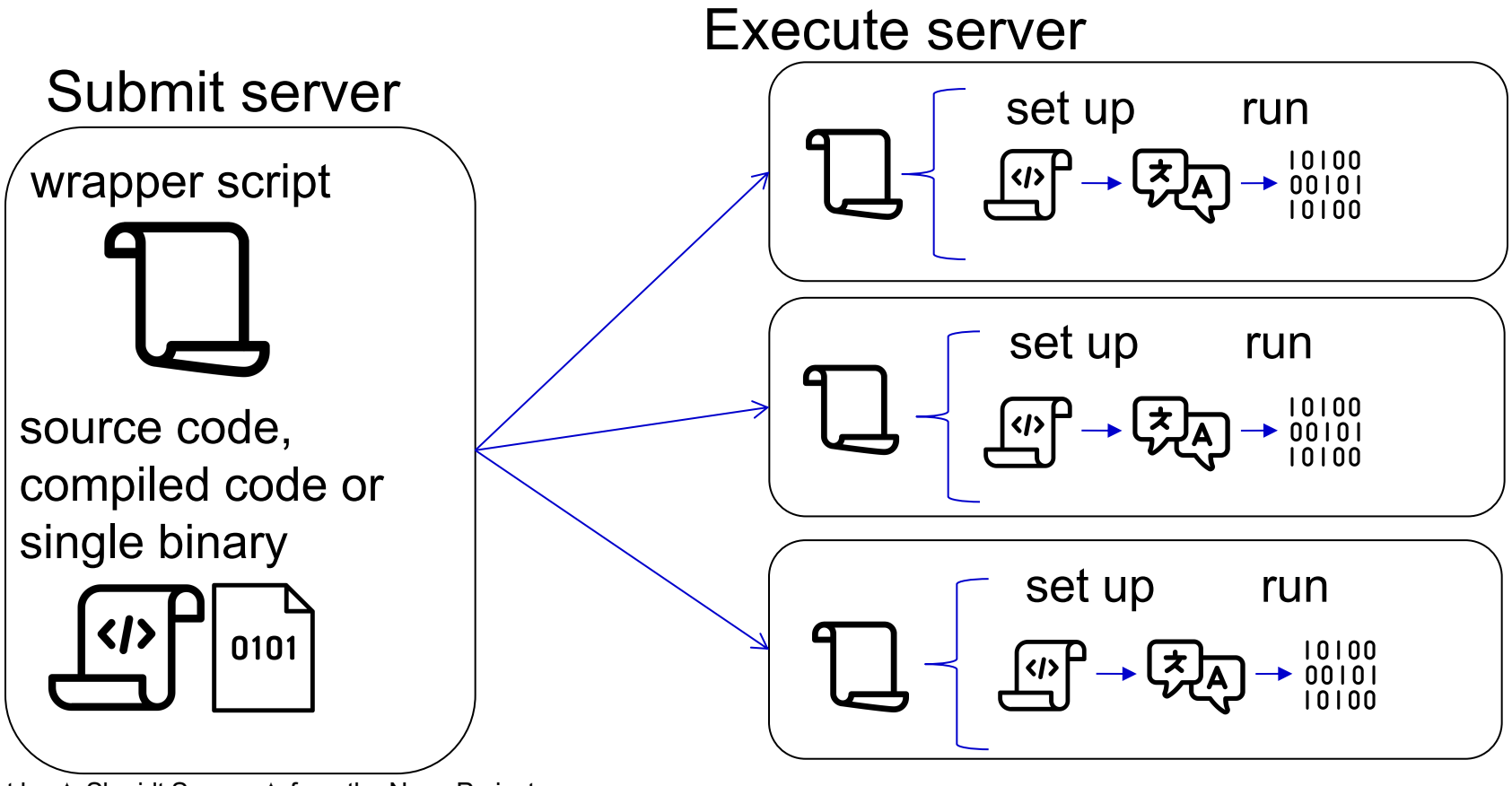
```
#!/bin/bash
# run_program.sh

tar –xzf program.tar.gz
program/bin/run in.dat
```

Single Binary Workflow



Wrapper Script Workflow

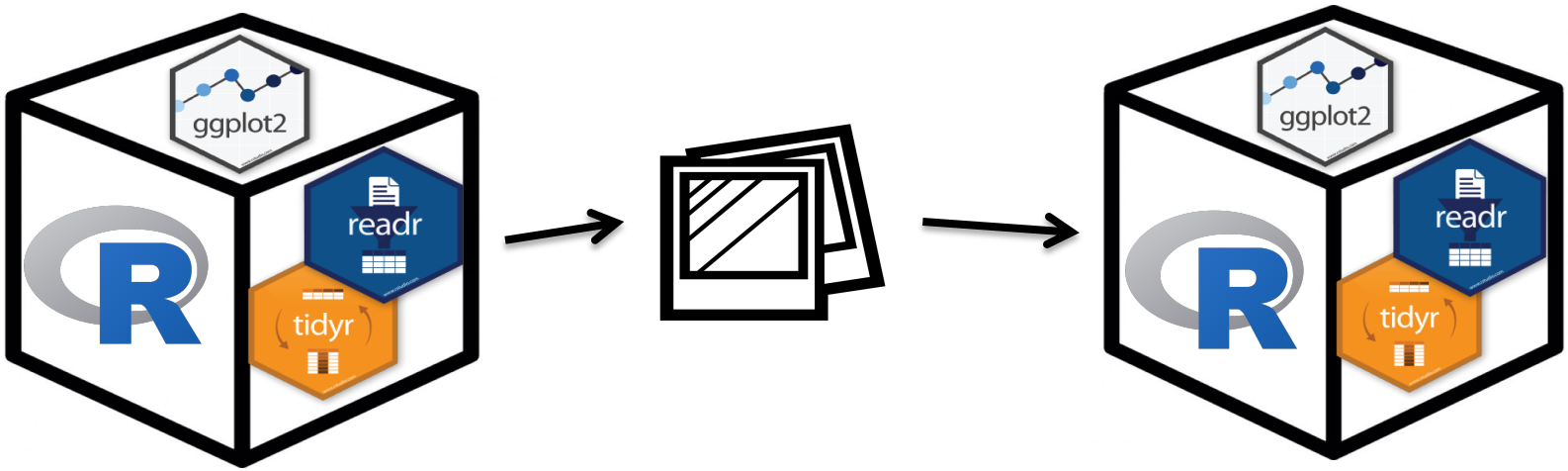


script by ✦ Shmidt Sergey ✦ from the Noun Project

BRING ALONG CONTAINERS

Containers

- Containers are a tool for capturing an entire job “environment” (software, libraries, operating system) into an “image” that can be used again.



Credit: polaroid photos by Nick Bluth from the Noun Project

Returning to Our Analogy…

- Using a container is kind of like bringing along a whole kitchen…

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Why Containers?

Why use containers
instead of the methods
we just discussed?

Why Containers?

- Complex installations: software that has a lot of dependencies or components.

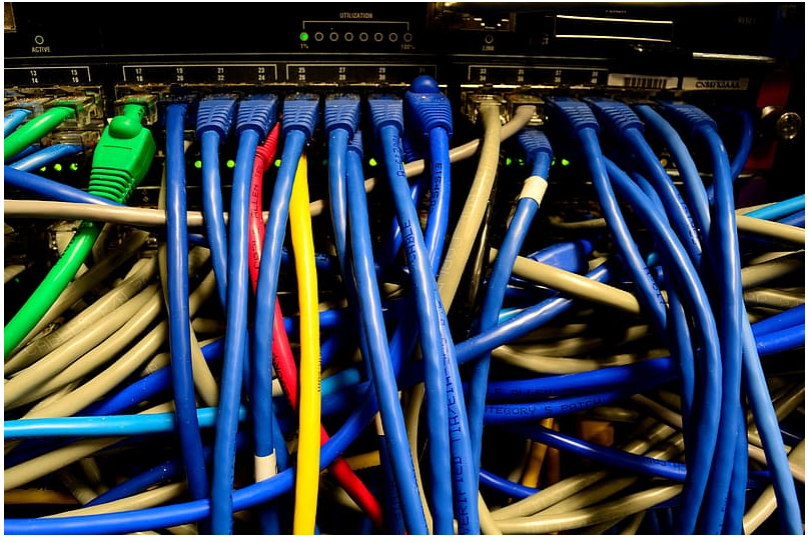


Photo on pikrepo

Why Containers?

- Software that can't be moved: do files or libraries have to be at a specific path?

Why Containers?

- Sharing with others:
  one container can be used by a whole group that's doing the same thing.

Why Containers?

- Reproducibility: save a copy of your environment.

Using Containers

- To use a container as your software portability tool, need to either:
  - Find a pre-existing container with what you need.
  - Build your own container.*

* not covered today

Container Types

- Two common container systems:

Docker	Singularity
https://www.docker.com/	https://sylabs.io/

The container itself will always be some version of Linux - but can be run on Linux / Mac / Windows if Docker or Singularity is installed

Submit File Requirements

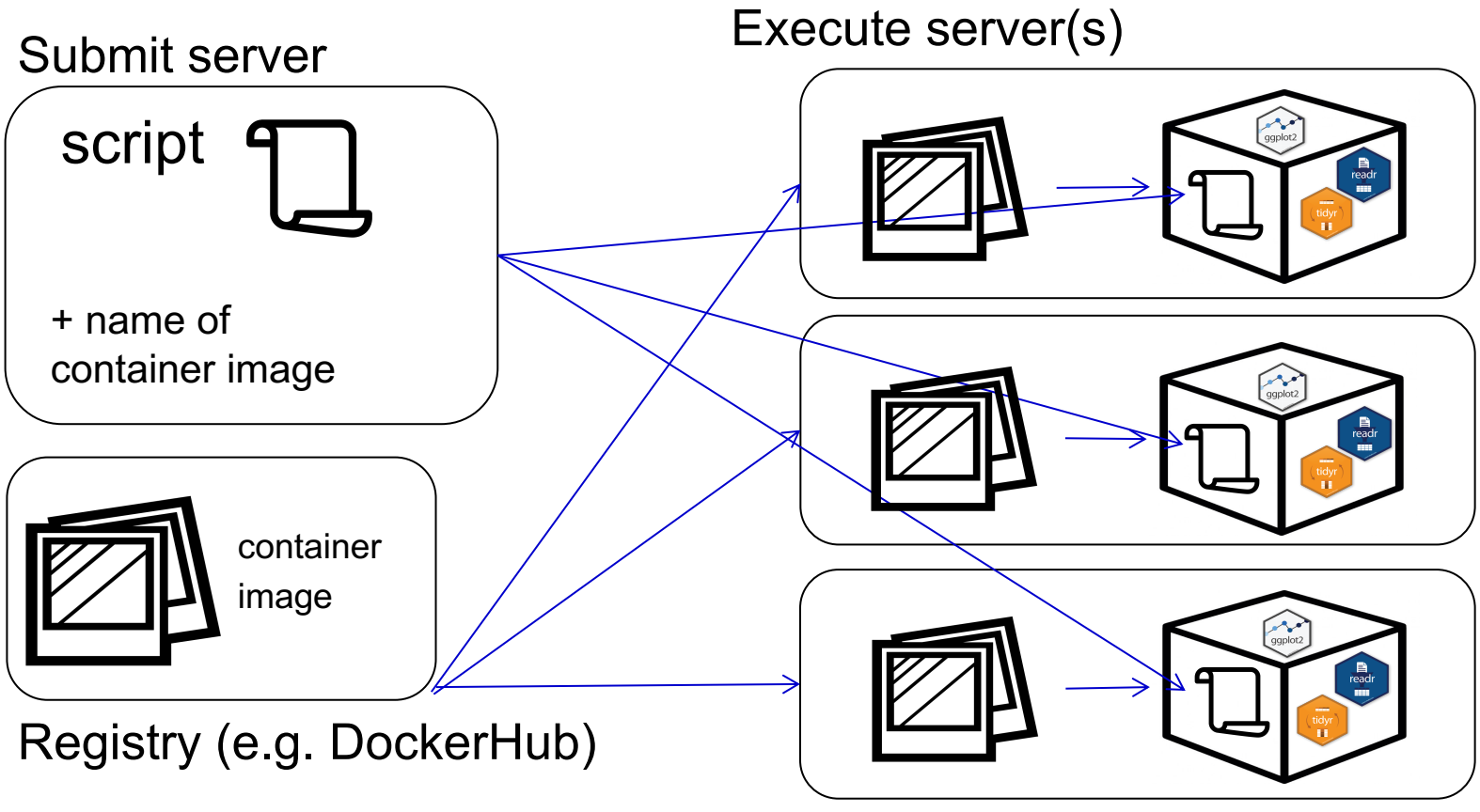
- Docker (from CHTC submit server)

```
universe = docker
docker_image = python:3.7.0
requirements = (HasDocker == true)
```

- Singularity (from OSG submit server)

```
+SingularityImage =
"/cvmfs/singularity.opensciencegrid.org/cent
os/python-34-centos7:latest"
requirements = (HAS_SINGULARITY == true)
```

Container Workflow



Conclusion

To use any software in a DHTC system:

1. Create/find software package:
   - download pre-compiled code, compile your own, create/find a container
2. Account for all dependencies, files, and requirements in the submit file.
3. If needed, write a script to set up the environment when the job runs.

PRE-INSTALLED SOFTWARE

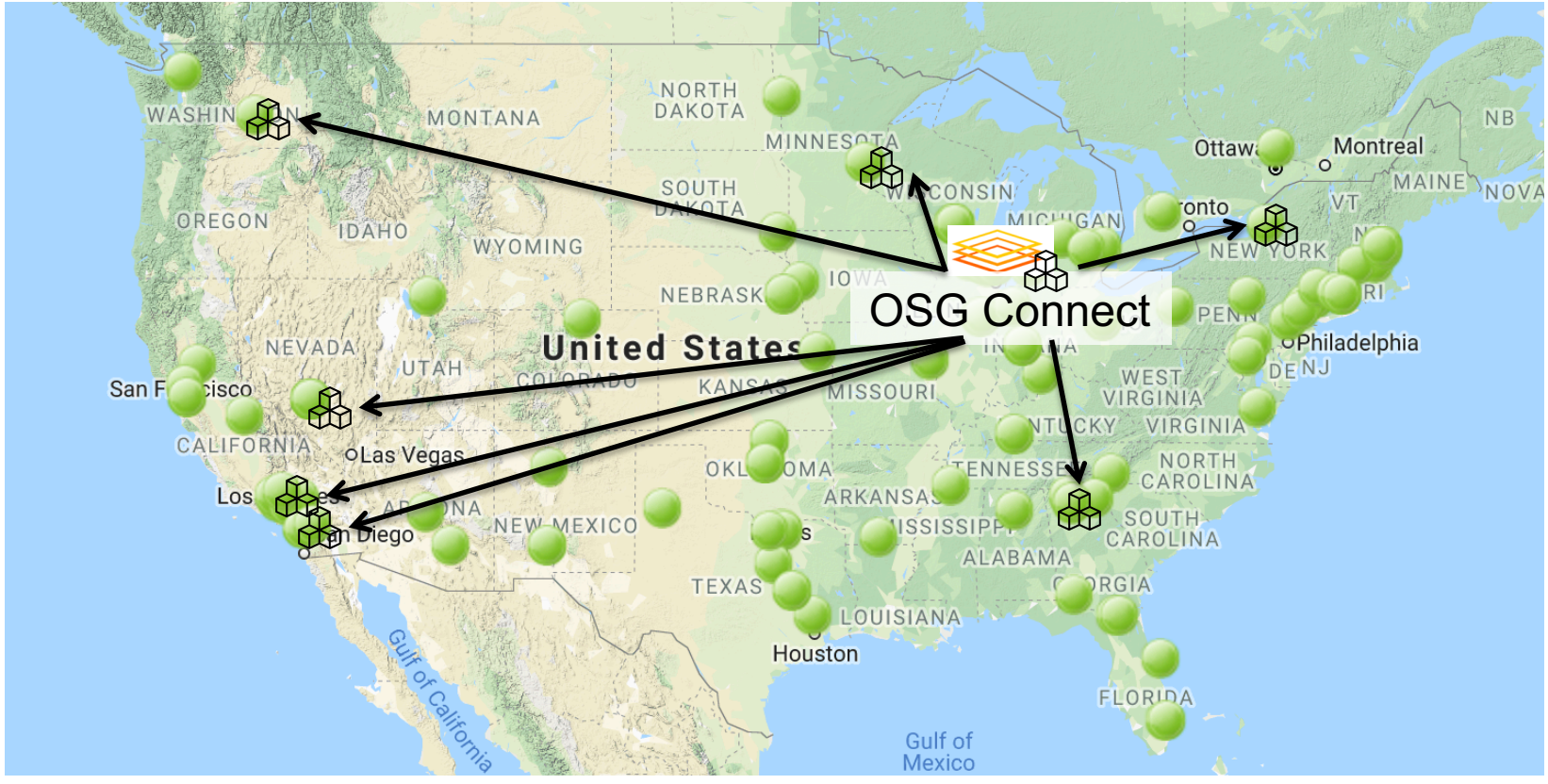
Pre-existing Software

- The ideal for DHTC is to package and bring along your own software, but…
- You can use pre-existing software installations **if** the computers you're running on have your software installed (or access to a repository with the software).

Pre-existing Software via OSG Connect

- On the Open Science Grid, jobs submitted from OSG Connect have access to a software repository maintained by OSG Connect staff.
- The software repository is available across the OSG.
- Software is accessed using “modules”.

Software Across the OSG



Module Commands

- See what modules are available

```
[~]$ module avail

[~]$ module spider lammps
```

- Load a module

```
[~]$ module load lammps/20180822
```

- See loaded modules

```
[~]$ module list
```

Module Workflow

1. Find a module for your software.
2. Write a wrapper script that loads the module and runs your code.
3. Include requirements to ensure that your job has access to modules.

```
requirements = (HAS_MODULES =?= true) &&
(OSGVO_OS_STRING == "RHEL7") && (OpSys == "LINUX")
```

Module Workflow