HCS7004 – Session 13

Software and containers

September 16th, 2020

CFAES

THE OHIO STATE UNIVERSITY

COLLEGE OF FOOD, AGRICULTURAL, AND ENVIRONMENTAL SCIENCES

Agenda for today

- Some commands and concepts:
  `sudo` recap, the **`$PATH`** environment variable, and remote file transfer

- Avoiding dependency hell

- Increasing reproducibility and portability of software environments
  using **conda** and **containers**

sudo **recap**

- Use **sudo** to temporarily gain administrative rights
  for tasks such as software installation with a package manager

- To run a command in sudo mode, simply prepend “sudo”:

```
jelmer@jpi:~$ apt-get update
Reading package lists... Done
E: Could not open lock file /var/lib/apt/lists/lock - open (13: Permission denied)
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```
jelmer@jpi:~$ sudo apt-get update
[sudo] password for jelmer:
Hit:1 http://us.archive.ubuntu.com/ubuntu focal InRelease
```

sudo **recap**

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[sudo] password for jelmer:
Hit:1 http://us.archive.ubuntu.com/ubuntu focal InRelease
```

- At OSC, you will **not** be able to use sudo

The $PATH environment variable

- **$PATH** is one of several *environment variables*.

- It lists the directories that will be searched when you type a program's name. This allows you to run programs without specifying the full path to the executable.

```
jelmer@jpi:~$ vcftools


VCFtools (0.1.16)
© Adam Auton and Anthony Marcketta 2009
```

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jelmer@jpi:~$ vcftools


VCFtools (0.1.16)
© Adam Auton and Anthony Marcketta 2009
```

```
jelmer@jpi:~$ which vcftools          # "which" to check location
/usr/bin/vcftools
```

The $PATH environment variable

- To check which dirs are in your **$PATH**:

```
jelmer@jpi:~$ echo $PATH
/home/jelmer/.local/bin:/home/jelmer/bin:/home/jelmer/.yarn/bin:/usr/local/go/bin
```

The $PATH environment variable

- To check which dirs are in your **$PATH**:

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jelmer@jpi:~$ echo $PATH
/home/jelmer/.local/bin:/home/jelmer/bin:/home/jelmer/.yarn/bin:/usr/local/go/bin
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- **$PATH** is a *variable* (hence the dollar sign) and can be modified directly.
  To add a dir to your path:

```
jelmer@jpi:~$ PATH=$PATH:~/new-dir-with-software
```

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  To add a dir to your path:

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```

- For *lasting* changes, edit your bash configuration files (like **~/.bashrc**),
  from which **$PATH** is loaded whenever you open a terminal

Remote file transfer

- Use `sftp` to establish contact between a local and a remote (OSC) computer:

```
jelmer@jpi:~$ sftp jelmer@sftp.osc.edu
Connected to sftp.osc.edu.
sftp>
```

Remote file transfer

- Use `sftp` to establish contact between a local and a remote (OSC) computer:

```
jelmer@jpi:~$ sftp jelmer@sftp.osc.edu
Connected to sftp.osc.edu.
sftp>
```

- Use "`put` <file> [target-dir]" to upload to remote:

```
sftp> put multiqc_1.9--py_1.sif          # No target dir specified: goes to home
Uploading multiqc_1.9--py_1.sif to /users/PAS0471/jelmer/multiqc_1.9--py_1.sif
```

Remote file transfer

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```

```
sftp> put multiqc_1.9--py_1.sif /fs/scratch/PAS1752/jelmer/
Uploading multiqc_1.9--py_1.sif to /fs/scratch/PAS1752/jelmer/multiqc_1.9--py_1.sif
```

Remote file transfer

- Use `sftp` to establish contact between a local and a remote (OSC) computer.

- Other, even simpler methods include the command “`scp`” (and “`rsync`”), but OSC prefers you to use `sftp` so as to use nodes specifically reserved for file transfer.

Dependency hell

- As you heard in the previous session, many pieces of software have several **dependencies**, sometimes so many that installation can become tricky

- It gets worse: different (versions of) software can have mutually exclusive dependencies – “**dependency hell**”

Software management in Ubuntu

- In Ubuntu, the Advance Package Tool automatically handles dependencies and updates – for instance with the **apt-get** command.

```
jelmer@jpi:~$ sudo apt-get update          # Update package index first
```

```
jelmer@jpi:~$ sudo apt-get install -y vcftools bcftools   # Install
```

Software management in Ubuntu

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-y: don't prompt for confirmation

>1 package at once works

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jelmer@jpi:~$ sudo apt-get install -y vcftools bcftools   # Install
```

```
jelmer@jpi:~$ sudo apt-get upgrade vcftools   # Update a package
```

```
jelmer@jpi:~$ sudo apt-get upgrade            # Update all packages
```

```
jelmer@jpi:~$ apt-cache search vcftools       # Search for a package
vcftools - Collection of tools to work with VCF files
```

Software management in Ubuntu

- In Ubuntu, the Advance Package Tool automatically handles dependencies and updates – for instance with the **apt-get** command.

- This is very useful, **but what if**:
  - Software isn’t available in the package manager?
  - You need a specific (older) version of software?
  - You need different versions at different times?
  - There are mutually exclusive dependencies for software you all want?

Similarly, at OSC

- Using specific versions & version switching is made easy with `module`
- But, when software isn’t installed, lack of admin rights makes software installation at OSC even more challenging than usual...

The alternatives

- Two main alternatives:
    - **conda**
    - **containers** (*Docker* and *Singularity*)

- These alternatives are useful *not only* at OSC – but more generally, for:
    - Reproducible environments
    - Portable environments (especially containers)
    - Avoidance of dependency hell

conda: a software and environment manager

- Creates *environments* with one (= best-practice) or more software packages
- Lots of bioinformatics software is available as a conda package
- Handles dependencies but does not require admin rights
- Environments are activated and deactivated – much like *Lmod* at OSC

conda: benefits and limits

- **Benefits of conda**:
  - Easy to use specific software versions
  - Easy to have multiple versions of the same software available
  - Easy to use mutually incompatible software
  - Save and share environment instructions
  - Not much of a learning curve
  - Available at OSC

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- **Limits of conda** – it does not:
  - Create an isolated environment that can be exported and used anywhere
  - Allow running software requiring a different OS / OS version

Using conda

- To create a new environment for `multiqc`, activate it, and install `multiqc`:

```
[jelmer@owens-login01 ~]$ module load python/3.6-conda5.2  # Load Python+conda module
[jelmer@owens-login01 ~]$ conda create -n multiqc          # Create a new environment
```

arbitrary environment name

Using conda

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```
[jelmer@owens-login01 ~]$ conda activate multiqc                # Activate the environment
(multiqc) [jelmer@owens-login01 ~]$ conda install -c bioconda multiqc  # Install multiqc
Solving environment: /
```

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```

Tells us the conda environment we're in

specify "channel" – bioconda has bioinformatics software

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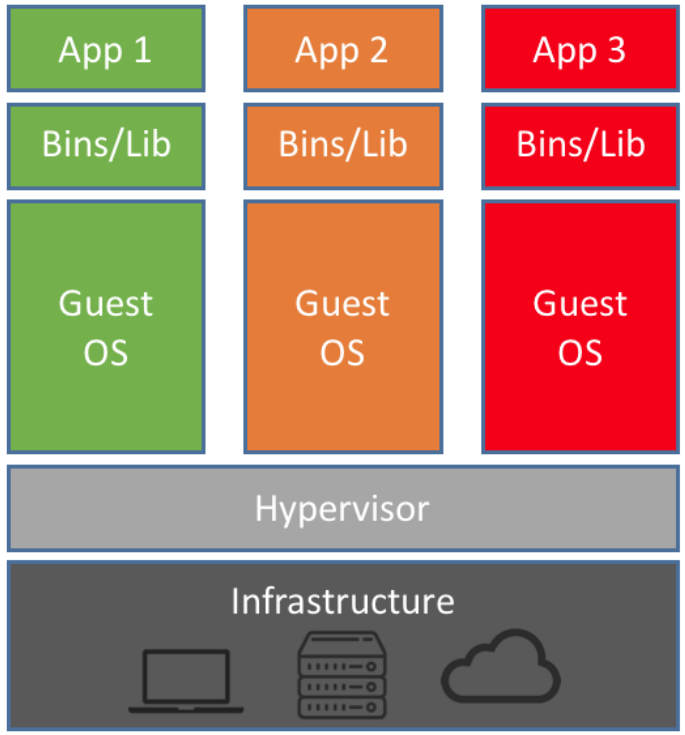
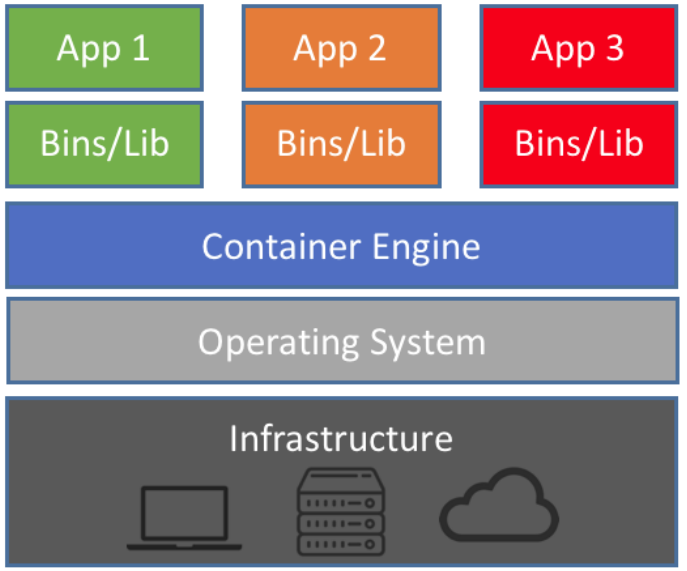
Solving environment: /
```

```
(multiqc) [jelmer@owens-login01 ~]$ multiqc --help
Usage: multiqc [OPTIONS] <analysis directory>
```

Containers: isolated environment for software



Machine Virtualization



Containers

VMs versus containers:

- Containers don't virtualize entire Operating Systems:
  - Containers are smaller
  - Containers are more lightweight to run
- Use a VM for long interactive sessions with multiple programs
- Use a container to run one or a few programs non-interactively

What can I do with containers

- Run an application with complicated stack dependencies in a few keystrokes.
- Package a workflow so that it can run on your laptop, in the cloud, and at OSC.
- Publish a paper and include a link to a container with all of the data and software.
- Create a workflow where different programs run on different operating systems.

After https://github.com/ArangoGutierrez/Singularity-tutorial

Docker versus Singularity

- Docker and Singularity are two different container platforms
- Docker is by far the most widely used

Docker versus Singularity

- Docker and Singularity are two different container platforms
- Docker is by far the most widely used
- However, Singularity:
  - Was specifically designed for HPCs & available at OSC
  - Needs no admin rights to run containers
  - Can work with Docker images but not vice versa
  - Integration with several host directories by default
  - Has single-file container images
  - Is open-source

Getting a container

- Container images for most software can be found at these registries:
  - Docker Hub: https://hub.docker.com/
  - Sylabs Cloud Library: https://cloud.sylabs.io/
  - Biocontainers (for bioinformatics software): https://biocontainers.pro/

- If no suitable image is available, you can build your own!

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Container terminology

• *Image*	File(s) containing the container application
• *Container*	A *running* container image
• *Definition file* (Singularity) *Dockerfile* (Docker)	Recipe to build a container image

Downloading a container image

- Download (“`pull`”) a container with multiqc:

```
(base) jelmer@jpi:~$ singularity pull docker://quay.io/biocontainers/multiqc:1.9--py_1
INFO:    Converting OCI blobs to SIF format
```

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Library://user/project/image-name/image-tag (version)

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Library://user/project/image-name/image-tag (version)

Conversion necessary because it is a Docker image

Downloading a container image

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```

```
jelmer@jpi:~$ ls multiqc_1.9--py_1*          # Now we have a ".sif"
multiqc_1.9--py_1.sif                        # container image
```

Downloading a container image

- Download ("`pull`") a container with multiqc:

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INFO:    Converting OCI blobs to SIF format
```

- Download a container from Singularity hub ("shub"):

```
(base) jelmer@jpi:~$ singularity pull shub://singularityhub/hello-world
INFO:    Downloading shub image
 59.75 MiB / 59.75 MiB [============================================================] 100.00%
```

Running a container

- “run” the container (= run the default script):

```
jelmer@jpi:~$ singularity run multiqc_1.9--py_1.sif     # In this case, we get a
Singularity>                                            # terminal inside the container
```

Running a container

- “run” the container (= run the default script):

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jelmer@jpi:~$ singularity run multiqc_1.9--py_1.sif     # In this case, we get a
Singularity>                                            # terminal inside the container
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```
Singularity> multiqc --help
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```

- The `shell` sub-command always opens a terminal in the container:

```
jelmer@jpi:~$ singularity shell multiqc_1.9--py_1.sif
Singularity>
```

Running a container

- "`run`" the container (= run the default script):

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jelmer@jpi:~$ singularity run multiqc_1.9--py_1.sif    # In this case, we get a
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Singularity>
```

- The `exec` sub-command lets you directly execute a shell command – and exits:

```
jelmer@jpi:~$ singularity exec multiqc_1.9--py_1.sif multiqc --help
Usage: multiqc [OPTIONS] <analysis directory>
jelmer@jpi:~$
```

“Containerizing” an analysis / script

- Running a locally installed program:

```
jelmer@jpi:~$ multiqc --help
```

- Run the same program using a container:

```
jelmer@jpi:~$ singularity exec multiqc_1.9--py_1.sif multiqc --help
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“Containerizing” an analysis / script

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>     multiqc --help
```

Building your own container

Building a container does require admin rights –
Need to do this on your own computer or VM with A Linux operating system

1) Download a suitable base image (e.g., Ubuntu 18.04)

```
jelmer@jpi:~$ singularity pull docker://ubuntu:20.04
INFO:    Converting OCI blobs to SIF format
INFO:    Starting build...
```

Building your own container

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Need to do this on your own computer or VM with A Linux operating system

1) Download a suitable base image (e.g., Ubuntu 18.04)
2) Run the image and enter the container in interactive, writeable mode
3) Install the required software
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4) When you exit the container, the image will have been updated

5) Best-practice – next create a Dockerfile:
   - Reproduce commands that worked & were necessary for installation
   - Add some metadata and formalities

Recap

- `sudo`, `$PATH`, and remote file transfer with `sftp`
- Use of `apt-get` and Lmod (`module`)
- Alternatives to package managers and manual installation:
  - `conda`
  - Containers – Singularity for working at HPCs such as OSC