MANCHESTER 1824
The University of Manchester

Deciding on the ideal software environment

Personal experiences with Anaconda, Docker, virtual machines, and servers

Raymond Wan and Patrick Yizhi Cai
Manchester Institute of Biotechnology
4 September 2024

MANCHESTER 1824
The University of Manchester

Outline

MANCHESTER 1824
The University of Manchester

Introduction

Prior to project development, two main considerations:

- operating systems (i.e., Microsoft Windows, MacOS, or Linux)
- programming language (i.e., Python, C/C++, Java, etc.)

A third but equally important consideration is the *environment*. Some options include:

- Anaconda,
- Docker,
- virtual machines, and
- servers

i.e., “inside what” will the program run – the focus of this talk

MANCHESTER 1824
The University of Manchester

Introduction

The decision for operating system, programming language, and environment affects all of this:

- who should be hired to develop the project,
- who can be brought on to the project to help, and
- even how the software will be maintained.

MANCHESTER 1824
The University of Manchester

Outline

Describe

1. briefly, what each of them are,
2. pros and cons of each, and
3. what has gone wrong?

MANCHESTER 1824
The University of Manchester

Motivation for this talk

Each promises reproducibility and ease of software maintenance. Including:

- Reproducing a system from backups on to the same or other system.
- Long-term support of a piece of software, possibly by someone who was not the original developer.

But are they all equal? If they each promise the same thing, how would an RSE choose one over another?

MANCHESTER 1824
The University of Manchester

Motivation for this talk

Each promises reproducibility and ease of software maintenance. Including:

- Reproducing a system from backups on to the same or other system.
- Long-term support of a piece of software, possibly by someone who was not the original developer.

But are they all equal? If they each promise the same thing, how would an RSE choose one over another?

MANCHESTER 1824
The University of Manchester

About me

Obtained a computer science degree in the 1990s and a PhD in computer science in 2004.

Relevance? My degrees pre-date all of these:

- Anaconda,
- Docker, and
- virtual machines

Like many of us, I had to learn them myself. Regrettably, it means I might not know them very well.

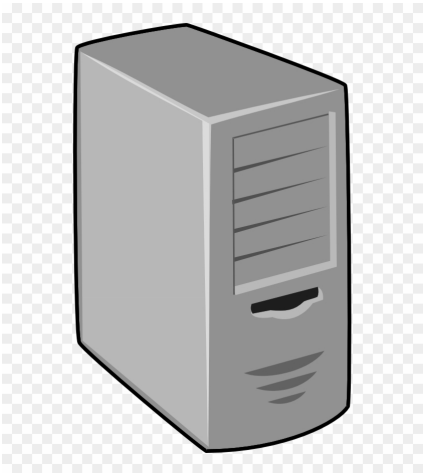
MANCHESTER 1824
The University of Manchester

Outline

Servers

Physical computer (or server):

- It can be networked to another computer both inside (intranet) or outside (Internet) a workplace.
- Otherwise, no dependencies (or interferences) from other computers.



MANCHESTER 1824
The University of Manchester

Servers

Pros:

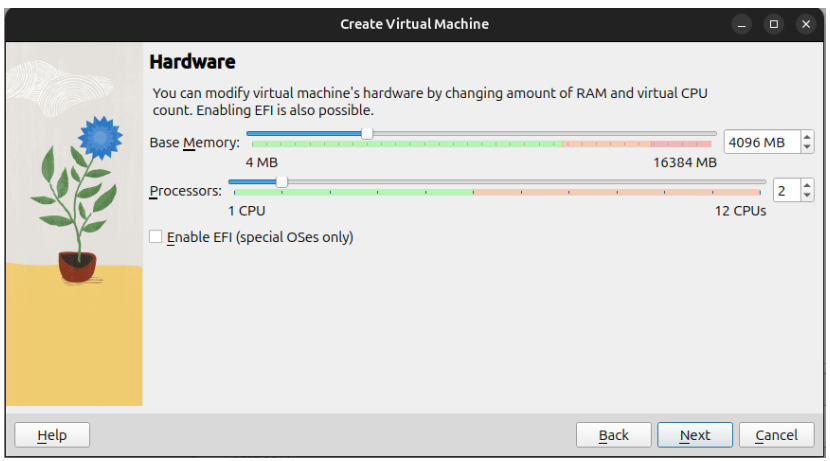
- Reproducible if you buy a similar computer and install the same software.
- Possible to purchase with a research budget since it is a fixed cost.

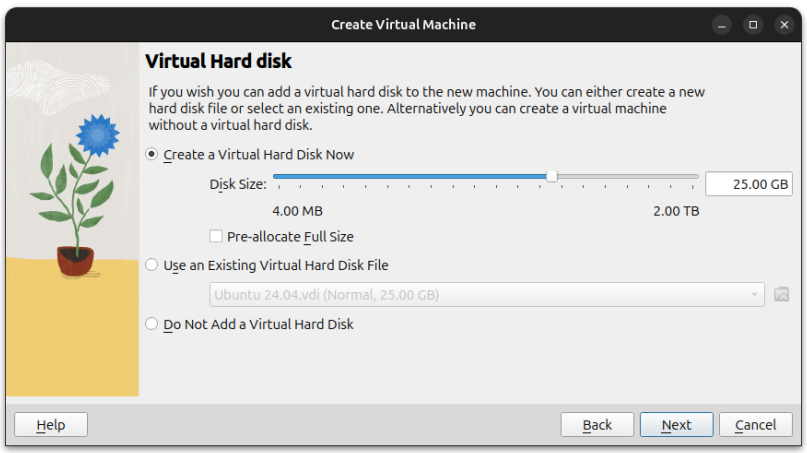
Cons:

- Buying an entire server is a big investment.
- Keeping it requires physical space as well as electricity, cooling, physical security, etc.
- Someone in-house needs to look after it and act as system administrator.

Virtual machines

- Virtualisation[1] at the level of the physical computer.
- Host multiple virtual computers on one computer.
- On the virtualisation program, you allocate how much memory should be used, disk space, network, etc.
- Some programs: Oracle VirtualBox or Microsoft Windows Hyper-V. Amazon AWS employs the same approach.

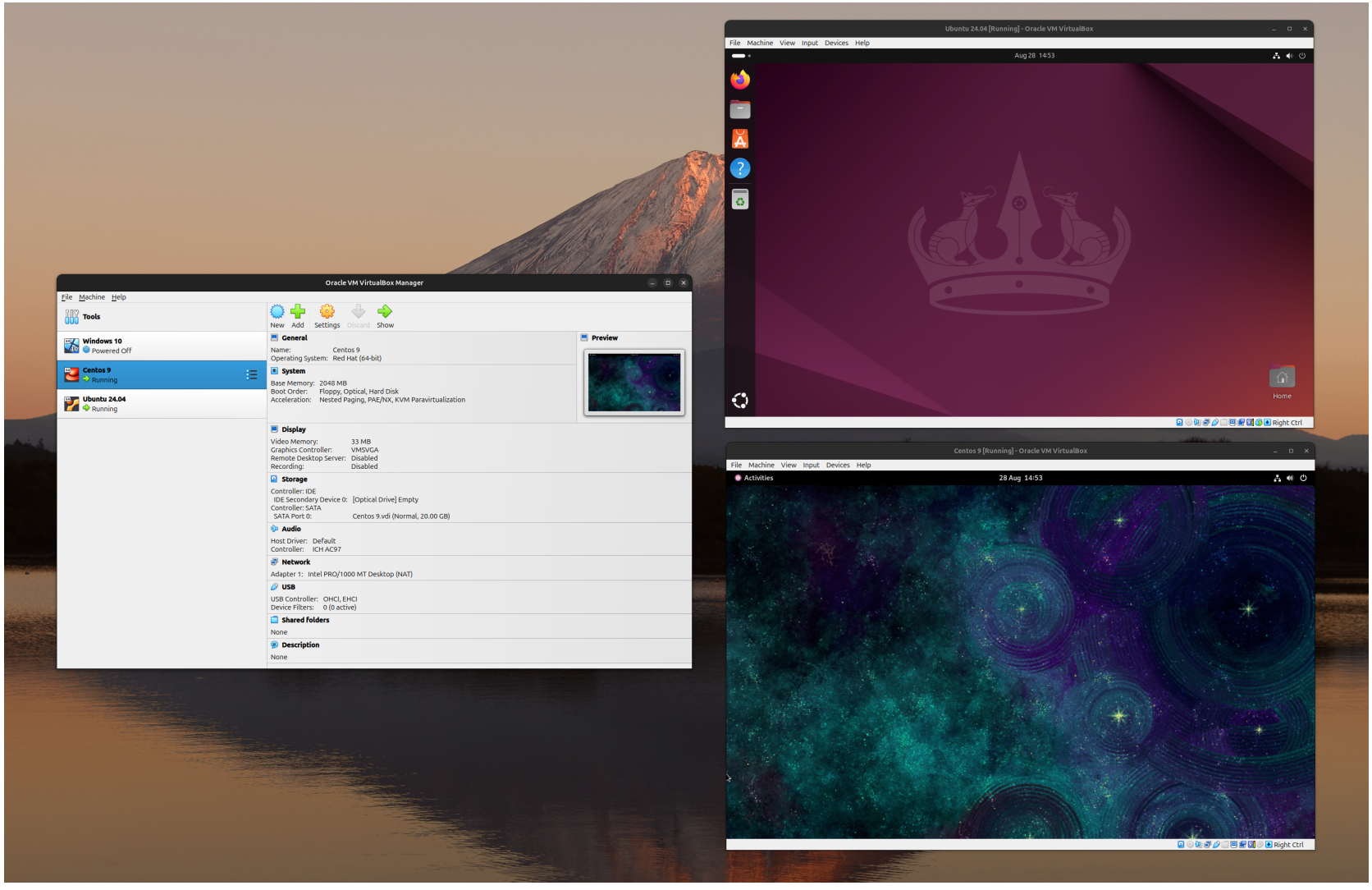




[1] Dividing of physical computer resources into separate units

MANCHESTER 1824
The University of Manchester

Virtual machines



MANCHESTER 1824
The University of Manchester

Virtual machines

Pros:

- Each VM exists independently of other VMs.
- Virtual hard disks can be backed up, copied, and restored on another system.
- A snapshot on a live system is possible (with some caveats).

Cons:

- Common memory, hard disk, and network means that a computationally intensive VM can take up resources from other VMs and the host system.
- Some projects require the location of the server and data to be known. This might rule out Amazon AWS.

MANCHESTER 1824
The University of Manchester

Docker

- Virtualisation at the level of the operating system, one level above virtual machines.
- Unlike before, one physical computer running one operating system. On this operating system, Docker Engine is continuously running.
- Docker Engine hosts various containers, which are “self-contained” software and configuration files.
- Multiple Docker containers can be running simultaneously that can communicate with each other.

Docker

Example `docker-compose.yml` for starting up applications based on multiple containers:

```
version: '3.0'
services:
    helloworld:
        container_name: hello-world
        working_dir: /hello
        volumes:
            - /var/logs/helloworld:/myapp/logs
...
```

- `/hello` and `/var/logs/helloworld` are directories on the host computer
- `/myapps/logs` is from the point of view of the application

MANCHESTER 1824
The University of Manchester

Docker

Pros:

- Good for programs that start up, run, and end (i.e., for data processing/analysis, etc.).
- Some developers use it to write web applications.

Cons:

- With less separation from the host compared to virtual machines, diagnosing problems (i.e., why does it work on this computer but not that one) can be frustrating.
- Personally, a steeper learning curve than the other options.

MANCHESTER 1824
The University of Manchester

Anaconda

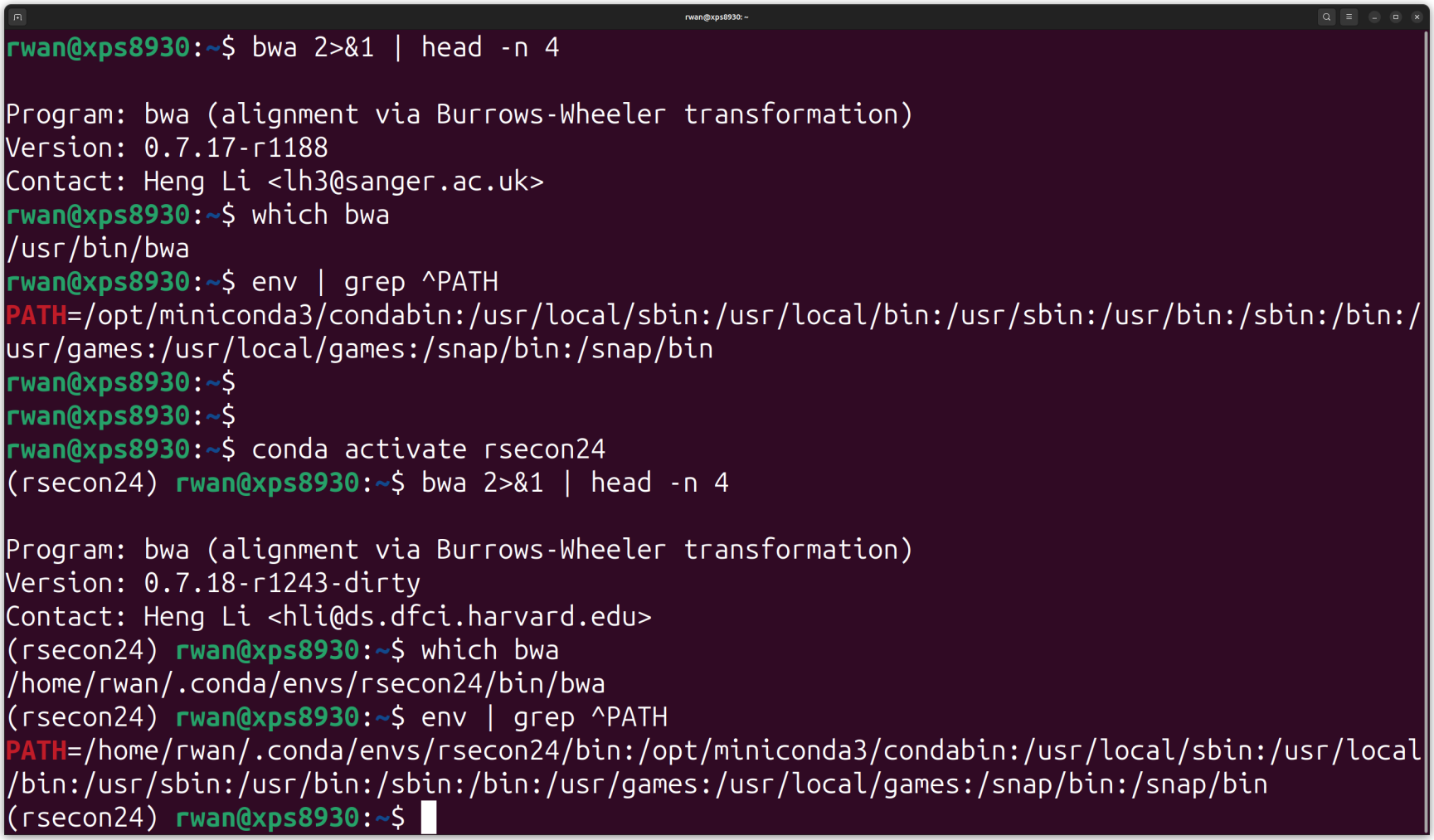
- Able to manage separate instances of Python and R, as well as other open source programs.
- Software packages are grouped together into Anaconda environments.
- Same program at different versions can be installed in multiple environments by the same user.

Example setup on Ubuntu host:

Command	What it does
`sudo apt-get install bwa`	Install `bwa` on host
`conda create --name rsecon24`	Create an environment
`conda activate rsecon24`	Activate environment
`conda install bwa`	Install `bwa` in environment

MANCHESTER 1824
The University of Manchester

Anaconda



MANCHESTER 1824
The University of Manchester

Anaconda

```
rwan@xps8930:~$ bwa 2>&1 | head -n 4

Program: bwa (alignment via Burrows-Wheeler transformation)
Version: 0.7.17-r1188
Contact: Heng Li <lh3@sanger.ac.uk>
rwan@xps8930:~$ which bwa
/usr/bin/bwa
rwan@xps8930:~$ env | grep ^PATH
PATH=/opt/miniconda3/condabin:/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/
usr/games:/usr/local/games:/snap/bin:/snap/bin
rwan@xps8930:~$
rwan@xps8930:~$
rwan@xps8930:~$ conda activate rsecon24
(rsecon24) rwan@xps8930:~$ bwa 2>&1 | head -n 4

Program: bwa (alignment via Burrows-Wheeler transformation)
Version: 0.7.18-r1243-dirty
Contact: Heng Li <hli@ds.dfci.harvard.edu>
(rsecon24) rwan@xps8930:~$ which bwa
/home/rwan/.conda/envs/rsecon24/bin/bwa
(rsecon24) rwan@xps8930:~$ env | grep ^PATH
PATH=/home/rwan/.conda/envs/rsecon24/bin:/opt/miniconda3/condabin:/usr/local/sbin:/usr/local
/bin:/usr/sbin:/usr/bin:/sbin:/bin:/usr/games:/usr/local/games:/snap/bin:/snap/bin
(rsecon24) rwan@xps8930:~$
```

MANCHESTER 1824
The University of Manchester

Anaconda

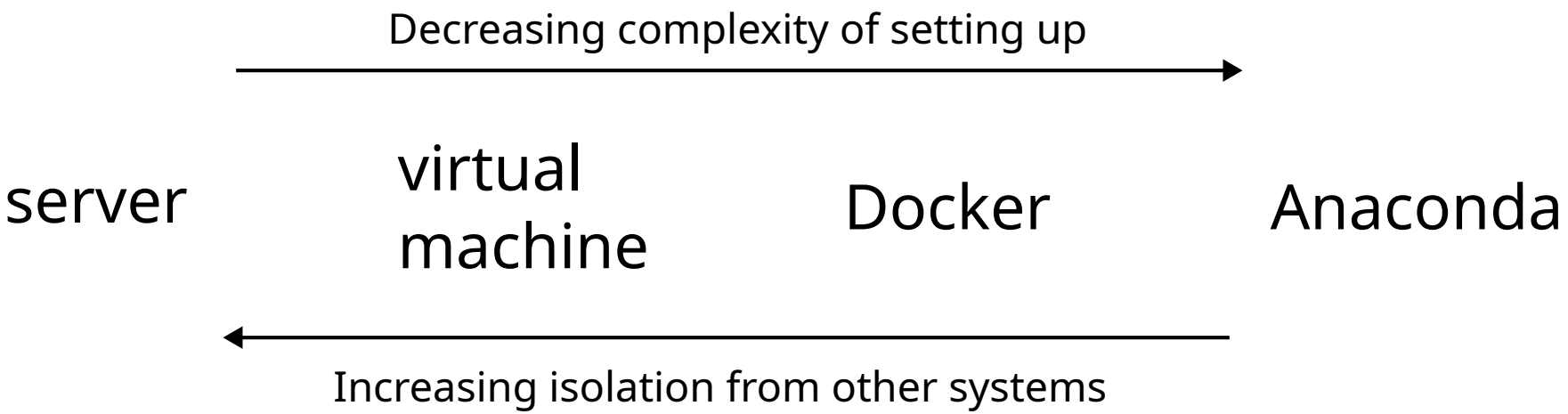
Pros:

- Relatively very little setup. Anaconda can be installed by a user or the system administrator. Then, the user can create and delete their own Anaconda environments.
- Neither Oracle VirtualBox nor a Docker Engine-like system is running.
- Conceptually easier to understand; it's "just" updating the user's `PATH`.
- Ideal for data analysis; not useful for writing a web application.

Cons:

- No separation between environments and between environments and the host system.

Summary



We all want less complexity:

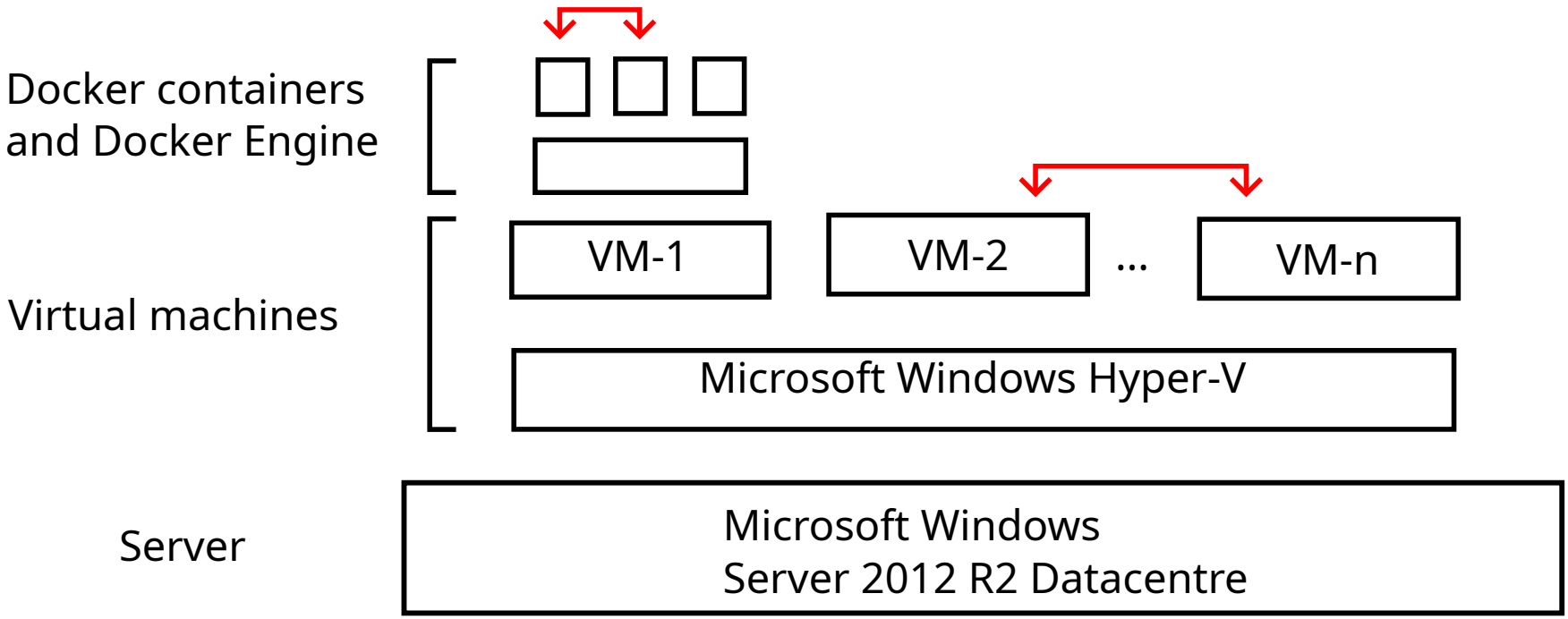
- Lower financial costs
- Anaconda environments can be created and maintained without system administrator access

More isolation makes it easier to reproduce an environment and/or troubleshoot.

MANCHESTER 1824
The University of Manchester

Outline

Layered organisation



With communication (in red) between Docker containers and virtual machines.

At first glance, it should help with reproducibility...

MANCHESTER 1824
The University of Manchester

Layered organisation

In practice, when something goes wrong (i.e., network connection failed or one Docker container not communicating with another), finding the cause is difficult...

Occasionally, the server's operating system or a virtual machine's OS should be upgraded. If it fails, then anything that depends on it will be affected. Thus, many systems can fail at the same time.

Also, see this.

MANCHESTER 1824
The University of Manchester

Dependencies

As part of “software reuse”, most software depend on modules, libraries, packages, etc. created by others.

If one of those dependencies is ever removed or made redundant, then restoring the system from backups would be difficult. This is less likely when the system is first completed; and more likely during the software’s maintenance period.

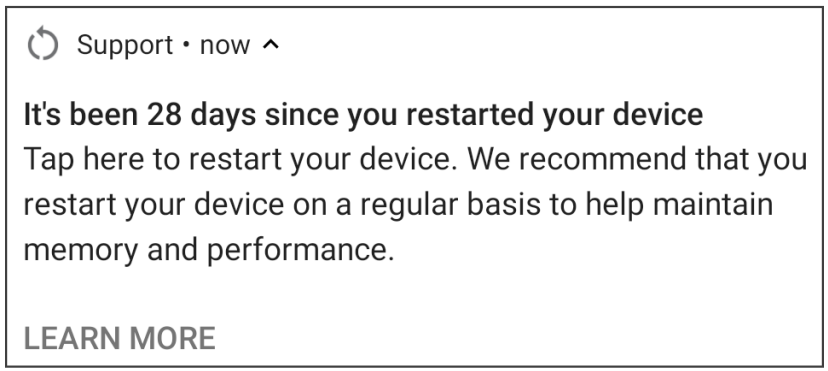
My own experience is that this is less likely at the operating system level (i.e., Debian/Ubuntu packages) and more likely when:

- Re-creating Docker containers
- Re-creating Anaconda environments

See this for some personal examples.

Rebooting systems

Message on my phone:



Restarting computers and software as a solution used to be a punch-line to a joke. Now, it is actually recommended...

Due to the two previous reasons, we avoided restarting the entire system. Ultimately, we were delaying the inevitable.

MANCHESTER 1824
The University of Manchester

Outline

MANCHESTER 1824
The University of Manchester

Which to choose?

- Each has its pros and cons.
- If one option has issues, then it would have disappeared by now.
- Best is to know when to use one over another, instead of using one for everything.

MANCHESTER 1824
The University of Manchester

Which to choose?

- Server – If server or data location is an issue and if physical space and someone to look after it is available.
- Virtual machine – Alternative to buying a new server; but the host computer needs to be powerful enough to support multiple running operating systems.
- Docker – Slightly steeper learning curve than the other options, but worth the time invested as an intermediate option between virtual machines and Anaconda.
- Anaconda – Allow users without system administrator's access to create their own environments and install their own software. They can install multiple versions of Python or R (i.e., 4.4.1, 3.6.1, ...) in separate environments to accommodate their code.

MANCHESTER 1824
The University of Manchester

Other advice

Good to periodically re-create Docker containers and Anaconda environments from scratch on another system. Just to check that its external dependencies are all fine. Doing this when we're "free" means we can confront these problems on our own terms.

Lastly, I am not yet convinced if layers of environments is a good approach.

MANCHESTER 1824
The University of Manchester

Conclusion

None of these environments is a good substitute for good documentation.

That is, step-by-step instructions that explains how everything fits together.

MANCHESTER 1824
The University of Manchester

Acknowledgements

We thank

- colleagues in my current and all previous workplaces for their patience while I learned all this,
- reviewers for the helpful suggestions, and
- the organising committee for the opportunity to present our experiences.

Contact details

Raymond Wan and Patrick Yizhi Cai
{raymond.wan,yizhi.cai}@manchester.ac.uk
Manchester Institute of Biotechnology, University of Manchester

LaTeX slides: https://github.com/rwanwork/Conf_RSECon_2024

Homepage of the lab: https://www.cailab.org/

Thank you!

MANCHESTER 1824
The University of Manchester

License

MANCHESTER 1824
The University of Manchester

Additional credits

- LaTeX template from: https://www.overleaf.com/latex/templates/university-of-manchester-presentation-beamer-template/rwcrzjmzcdyn.
- Server clip art from Clipart Library.
- Other figures made using Inkscape version 1.2.2

End of Life

End of Life of software occurs when it is no longer supported by the original developer. No more support is given and no security updates are made available.

In our case, support for Microsoft Windows Server 2012 R2 Datacentre would have ended on 10 October 2023. So, a major update had to occur or else we would lose security updates and, likewise, the ability to connect to our organisation's network.

Back

MANCHESTER 1824
The University of Manchester

Removed packages

When a module, a library, or a package is no longer available, substituting it for a newer version might not be possible if the newer version is not backward compatible.

Also, another module that depends on it in turn might also have to be upgraded, causing a ripple effect.

In the past, solving such problems has taken me hours or days.

MANCHESTER 1824
The University of Manchester

Removed packages

In our case, a web application developed using Ruby on Rails had one of its dependencies (mimemagic) removed from all repositories due to a licensing issue. This occurred after our software had been developed and during its post-development maintenance period.

See this page for an explanation.

Back