Containers: Vagrant, Docker, Singularity

Dorota Jarecka: djarecka@mit.edu

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    - operating system
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    - software dependencies: Python/MATLAB/R + libraries
  - We try to avoid
    - *the computer I used was shut down a year ago, can't rerun the results from my publication...*
    - *the analysis were run by my student, have no idea where and how...*
    - etc.

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  - Sharing your code or using a repository might not be enough
  - We try to avoid
    - *well, I forgot to mention that you have to use Clang, gcc never worked for me...*
    - *don't see any reason why it shouldn't work on Windows... (I actually have no idea about Windows, but won't say it...)*
    - **it works on my computer...**
    - etc.

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    - *I just want to Undo the last five hours of my life...*

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    - runc
    - lxc/lxd
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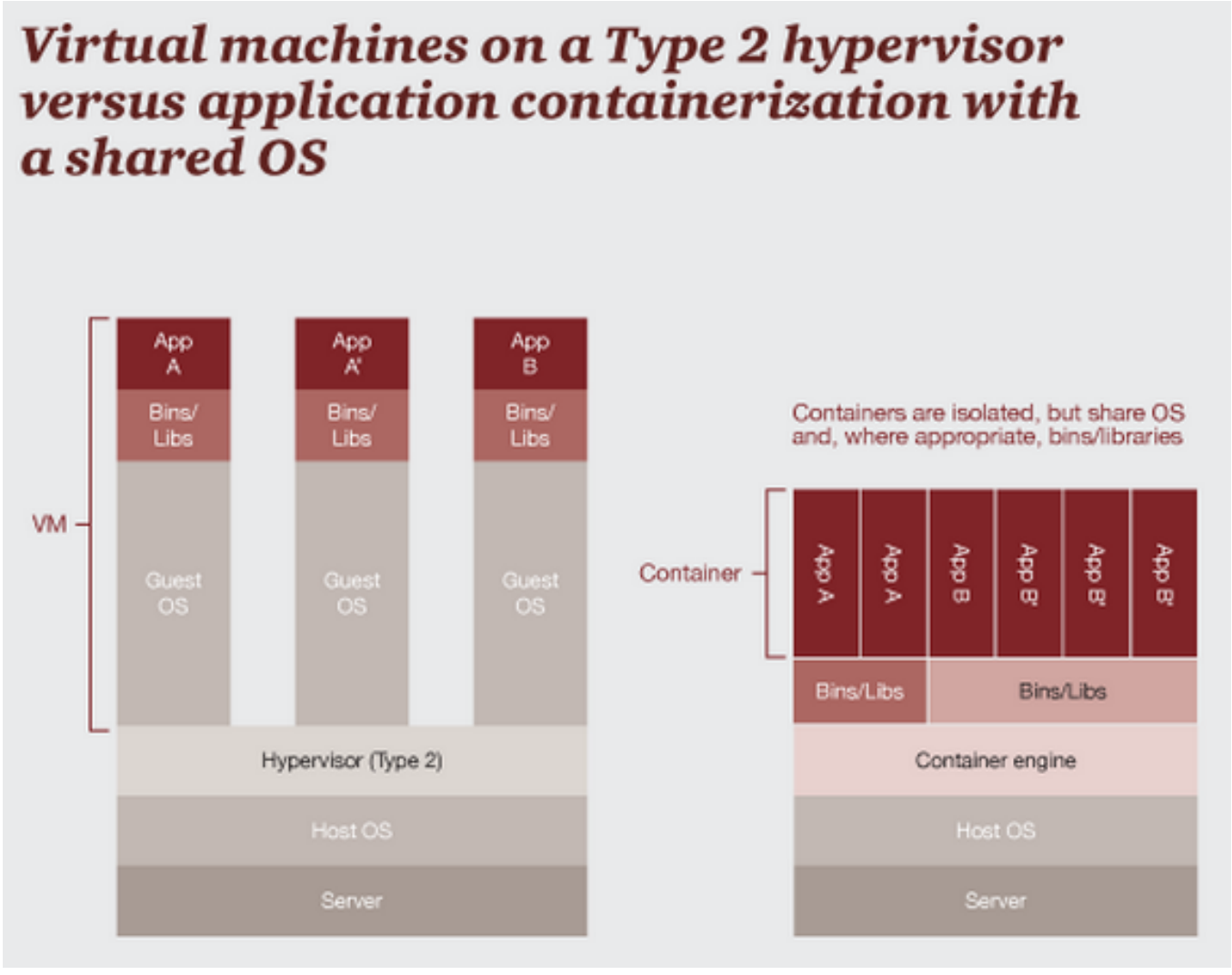
    - runc
    - lxc/lxd
    - Singularity
- The details differ (and matter depending on application)

Virtual Machines vs Container



Vagrant

- is a command line utility for managing virtual machines
- provides easy to configure, reproducible, and portable work environments
- on top of VirtualBox, VMware, AWS, or any other provider (VirtualBox is the default machine)

Vagrant: Creating a computing environments using

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```
$ mkdir vm
$ cd vm
$ vagrant init ubuntu/trusty64
$ vagrant up    # the same as vagrant up –provider virtualbox
$ vagrant ssh    # or vagrant ssh -c /bin/sh
```

Vagrant: installing new software

- installing Emacs

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  within the VM:

```
$ sudo apt-get update
$ sudo apt-get install emacs
$ emacs
$ exit
```

- installing FSL
  - follow the instruction from NeuroDebian (once it's fixed)

Docker

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- an open-source project
- bundle libraries and required settings only (not a full operating system)
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- testing your Docker installation:

```
$ docker run hello-world
```

Docker

- Using existing images

```
$ docker pull busybox
$ docker images
$ docker run busybox
$ docker run busybox echo “hello from busybox”
$ docker run -it busybox sh
$ docker ps
$ docker rm
$ docker run -it --rm busybox
$ docker run -it --rm -v YourDirectory:/src busybox
```

Docker: Installing software with Dockerfile

- Dockerfile content

```
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- Building a new container

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- Running your new container

```
$ docker run -ti --rm fslR
```

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$ docker images
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$ docker pull nipype/nipype
$ docker images
$ docker run -it --rm nipype/nipype
```

  - within the nipype container

```
$ cd /src/nipype/nipype/pipeline/engine/
$ py.test
```

Docker: Docker Hub

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- Anaconda - a python distribution
- Miniconda - a package manager

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- can run existing Docker containers
- Satra's presentation – Singularity on Openmind