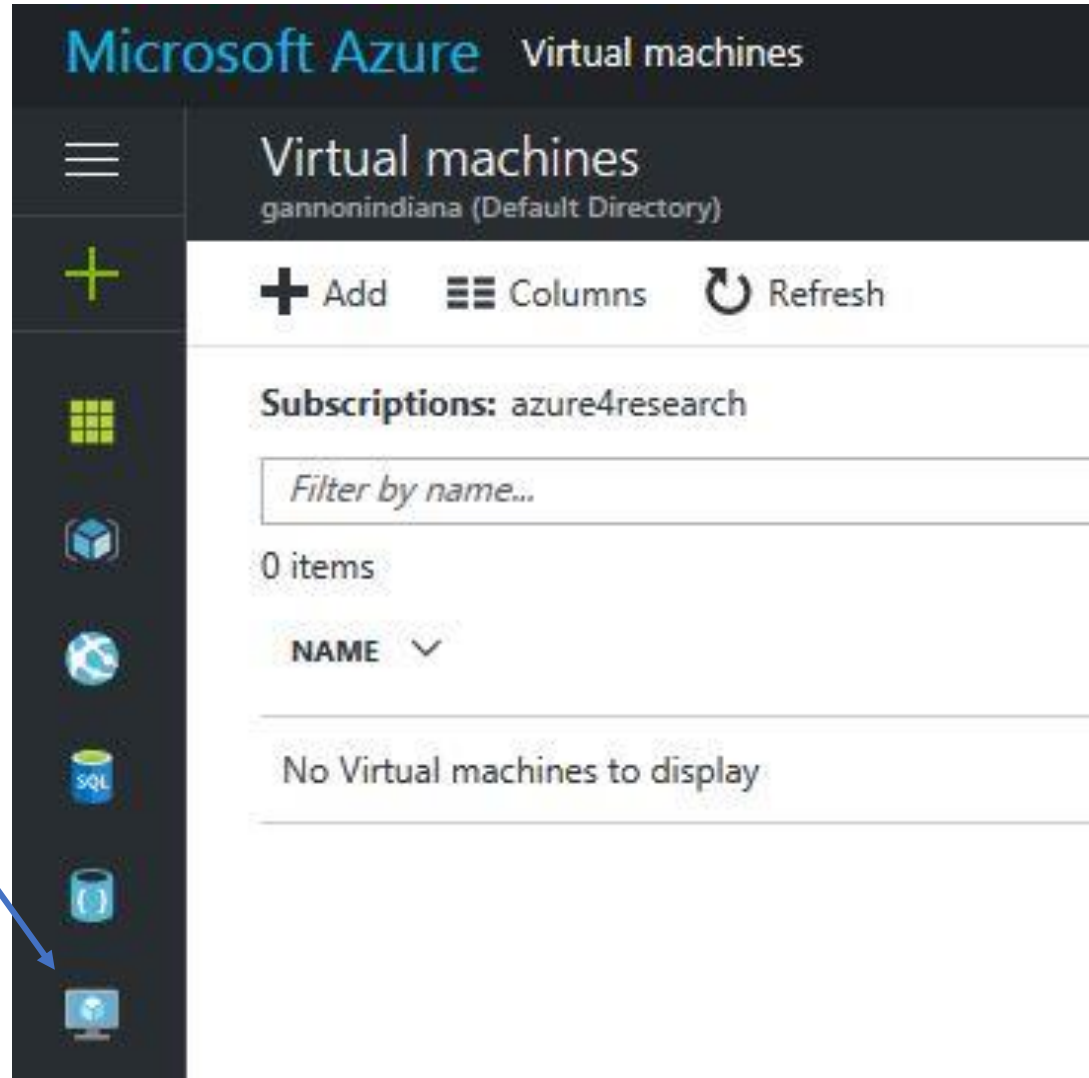


Cloud Computing for Science

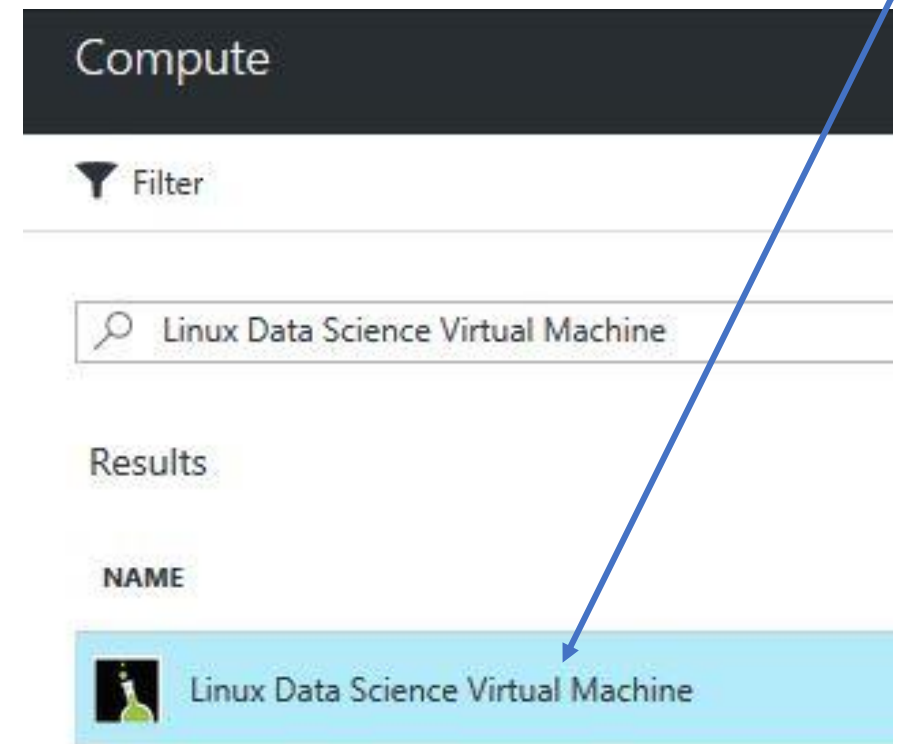
Part 2 Virtual Machines and Containers

Using the Azure portal to create a VM



Click this
To bring up
The VM page
Then click
Add

In the search box enter "data science" and you will see this choice. Pick this one and click here



The Linux Data Science VM

This Linux-based virtual machine contains popular tools for data science and development activities, including Microsoft R Open, Anaconda Python, Azure command line tools, and Jupyter notebooks for Python, R and Julia. It also has machine learning tools and algorithms like mxnet, CNTK, Vowpal Wabbit and xgboost.

What's new

- The Linux data science virtual machine now includes Microsoft R Server 9.0, now with Microsoft R Open 3.3.2 and new options for operationalizing R models
- [Weka](#) for easy graphical exploration and machine learning
- [Apache Drill](#) for querying non-relational data using SQL
- Spark local 2.0.2 with a PySpark Jupyter kernel
- Single node local Hadoop (HDFS, Yarn)
- Visual Studio Code IDEs, IntelliJ IDEA, PyCharm, Atom
- mxnet for deep learning
- JuliaPro - a curated distribution of Julia Language and tools

Also Jupyter hub running on the ip address:8000

You need a public-private RSA key pair

Linux/Mac

>ssh-keygen

Will create a password protected private key and a public key

When machine is up, login with

>ssh -i privatekey user@ipaddress
(it will ask for the password)

After you log in you need to set your user password

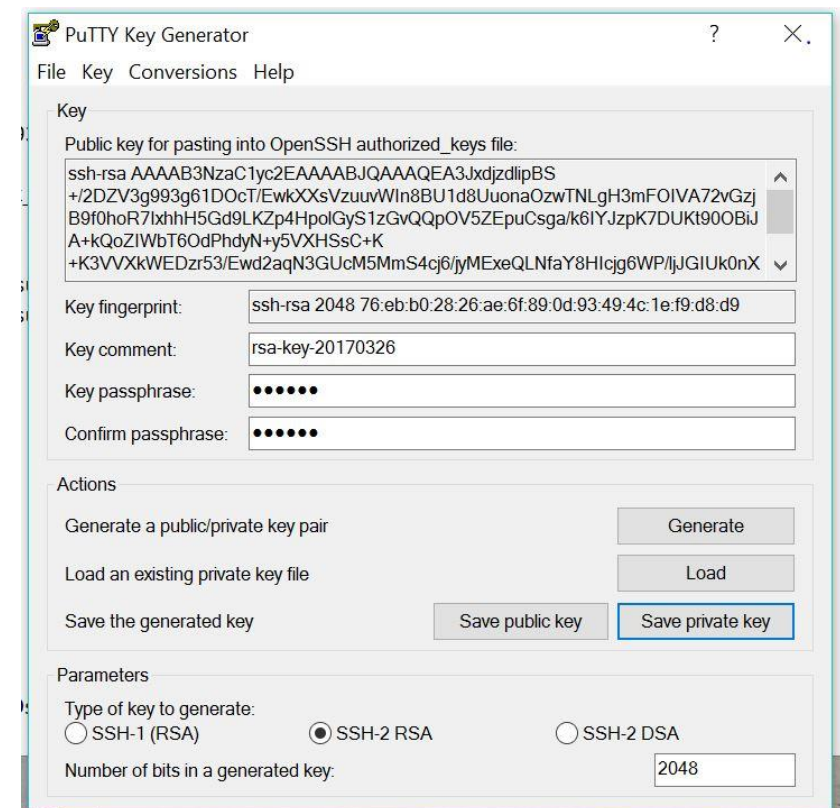
> sudo passwd YourID

>enter your password twice

We will need this later.

Windows

- On Windows10 you can use linux subsystem and follow linux method
- Or Install Putty
- Run PuTTYGen
- Runn Putty to log in.



Configuring and launching

Create virtual machine

Basics

1 Basics
Configure basic settings

2 Size
Choose virtual machine size

3 Settings
Configure optional features

4 Summary
Linux Data Science Virtual Machine

5 Buy

Name

myDataScienceVM

VM disk type

SSD

User name

dbgannon

Authentication type

SSH public key

Password

SSH public key

----- BEGIN SSH2 PUBLIC KEY -----
Comment: "rsa-key-20170210"
AAAAB3NzaC1yc2EAAAABJQAAAQEai+S
oqE+zhRcAt8wsF31YDgpwTQSnVMwQ5c

Subscription

azure4research

Resource group

Create new

Use existing

bookRG

Location

South Central US

OK

2 Size
Choose virtual machine size

3 Settings
Configure optional features

4 Summary
Linux Data Science Virtual Machine

5 Buy

★ Recommended | [View all](#)

DS2_V2	Standard	★	DS3_V2	Standard	★	DS14_V2	Standard	★
2	Cores		4	Cores		16	Cores	
7	GB		14	GB		112	GB	
4	Data disks		8	Data disks		32	Data disks	
6400	Max IOPS		12800	Max IOPS		50000	Max IOPS	
14 GB	Local SSD		28 GB	Local SSD		224 GB	Local SSD	
Load balancing			Load balancing			Load balancing		
Premium disk support			Premium disk support			Premium disk support		
94.49	USD/MONTH (ESTIMATED)		189.72	USD/MONTH (ESTIMATED)		989.52	USD/MONTH (ESTIMATED)	

Purchase

Offer details

Linux Data Science Virtual Machine
by Microsoft

0.0000 USD/hr

⚠

Standard DS14 v2
by Microsoft

1.3300 USD/hr

i

[Terms of use](#) | [privacy policy](#)

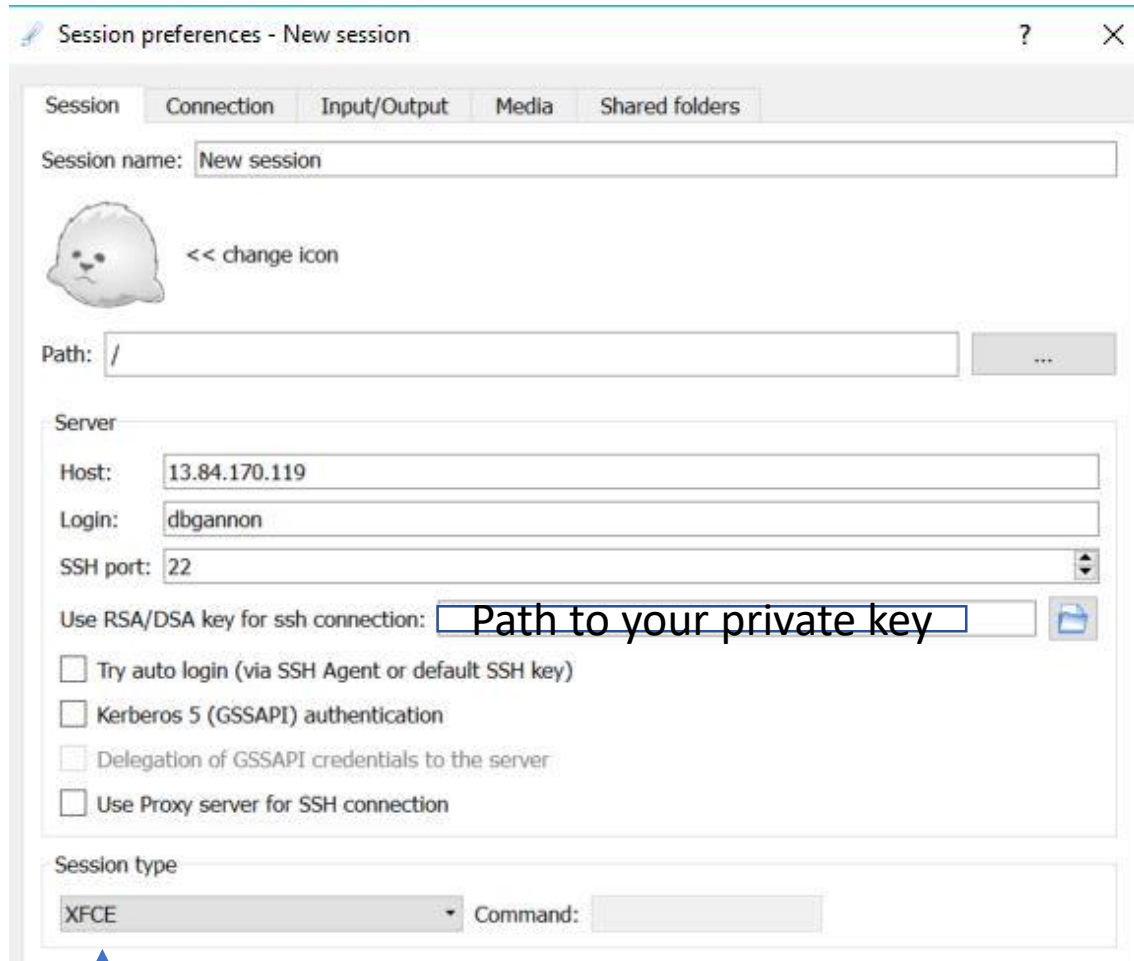
[Pricing for other VM sizes](#)

⚠

The highlighted Marketplace purchase(s) are not covered by your Azure credits, and will be billed separately.
You cannot use your Azure monetary commitment funds or subscription credits for these purchases. You will be billed separately for marketplace purchases.

Install X2GO Client

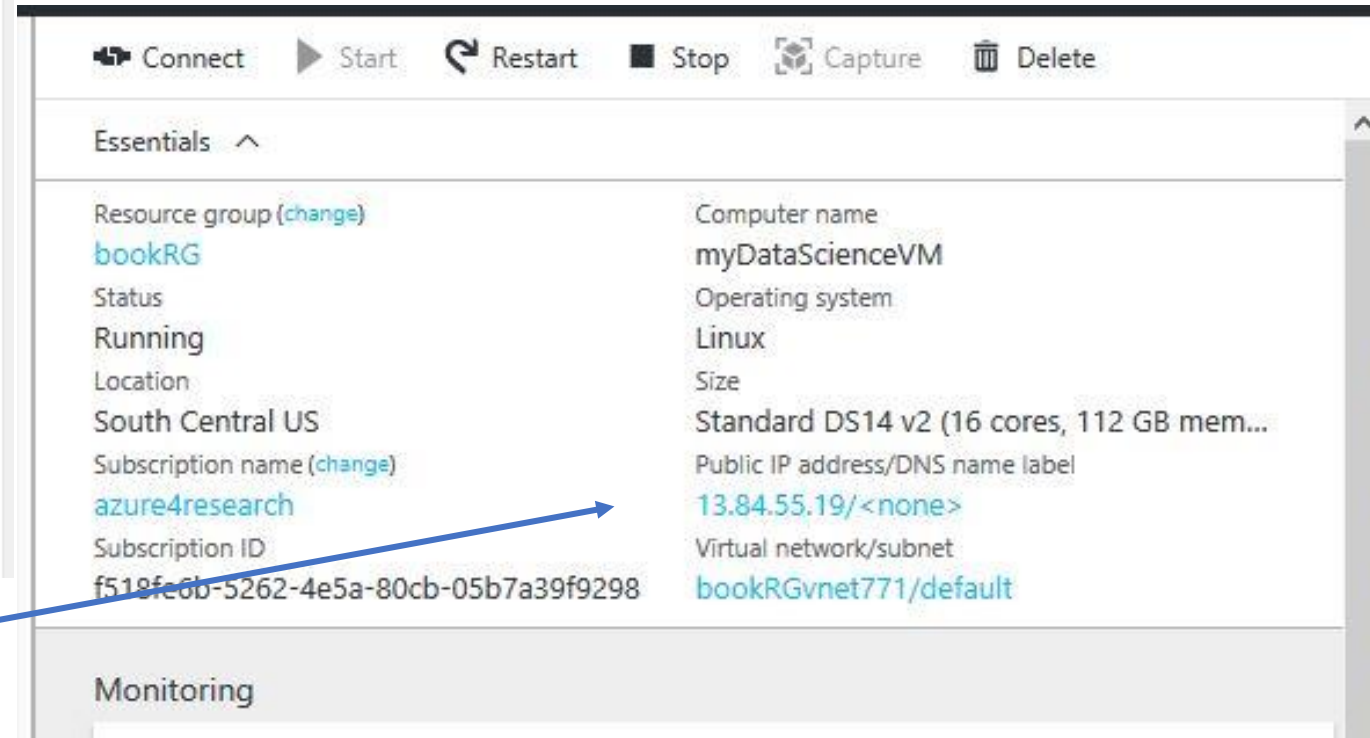
- <http://wiki.x2go.org>
- A client to show the desktop of the Linux Data Science VM
- When VM up Start X2GO client



The image shows the 'Session preferences - New session' dialog box. It has tabs for Session, Connection, Input/Output, Media, and Shared folders. The 'Session' tab is active. Fields include: Session name (New session), a default icon (a dog), Path (/), Host (13.84.170.119), Login (dbgannon), SSH port (22), and a field for the RSA/DSA key path labeled 'Path to your private key'. There are checkboxes for 'Try auto login', 'Kerberos 5 authentication', 'Delegation of GSSAPI credentials', and 'Use Proxy server'. At the bottom, 'Session type' is set to 'XFCE' and 'Command' is empty.

↑
Set to this

Azure portal view and IP address

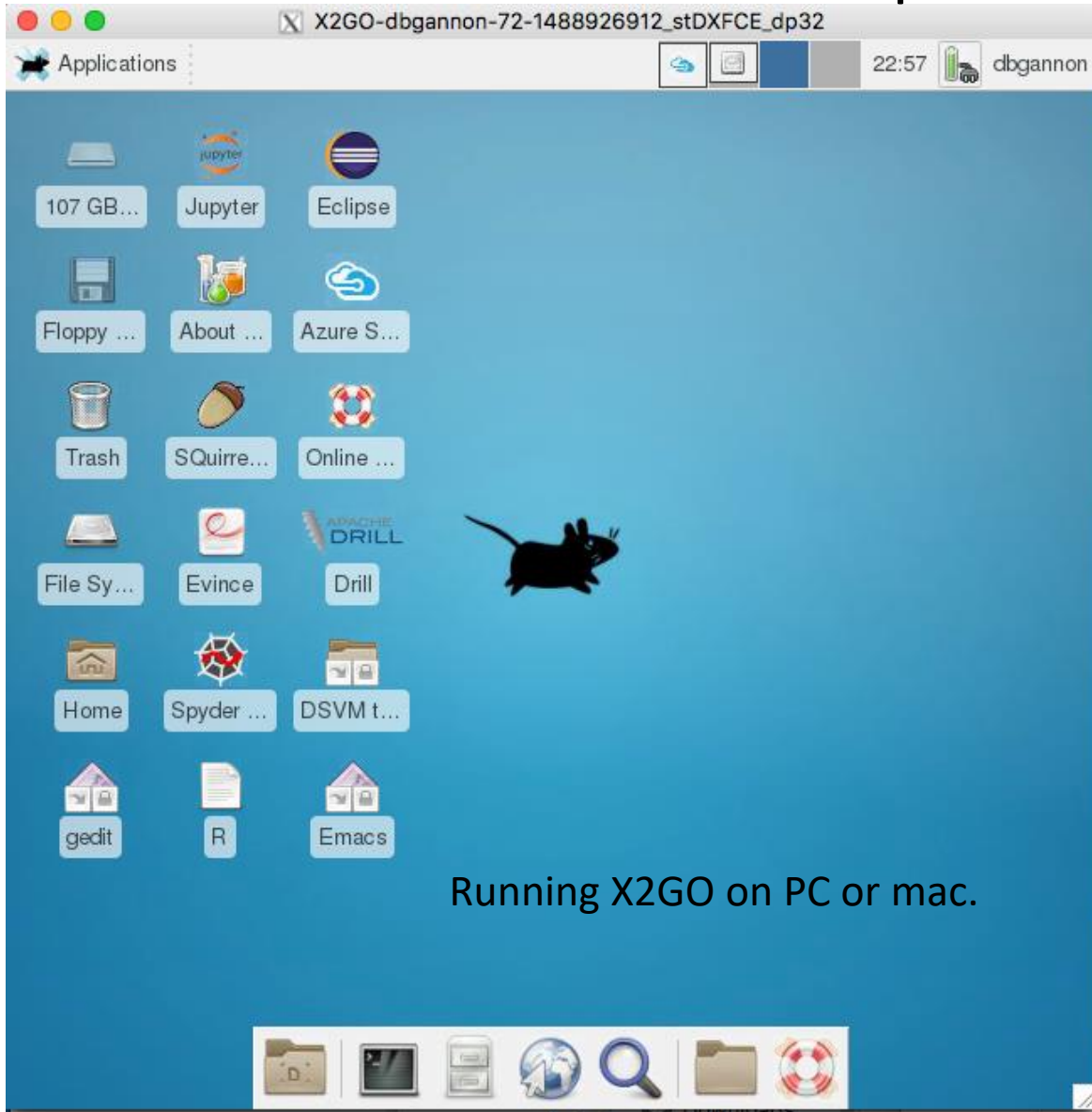


The image shows the Azure portal interface for a virtual machine named 'myDataScienceVM'. The 'Essentials' section displays the following details:

Resource group	Computer name
bookRG	myDataScienceVM
Status	Operating system
Running	Linux
Location	Size
South Central US	Standard DS14 v2 (16 cores, 112 GB mem...
Subscription name	Public IP address/DNS name label
azure4research	13.84.55.19/<none>
Subscription ID	Virtual network/subnet
f518fe6b-5262-4e5a-80cb-05b7a39f9298	bookRGvnet771/default

The 'Monitoring' section is partially visible at the bottom.

X2GO XFCE Desktop



Running X2GO on PC or mac.

- To run jupyter use JupyterHub.
 - First you need to set you linux passwd
 - Open the shell tool
 - `>sudo passwd yourID`
 - Add the password twice
 - Go to <https://yourDSVMip:8000>
 - Enter you ID and password
 - Or launch a local Jupyter by clicking on the icon.

Adding a fileshare disk

- This is a disk in blob storage that you can see with AzureExplorer
 - Create a storage account in same location as your DSVM.
 - Create a file share in that account named XXX
 - Grab the storage account key
- Run these commands

```
>sudo yum install samba-client samba-common cifs-utils
```

```
>sudo mkdir /mnt/tutorialshare
```

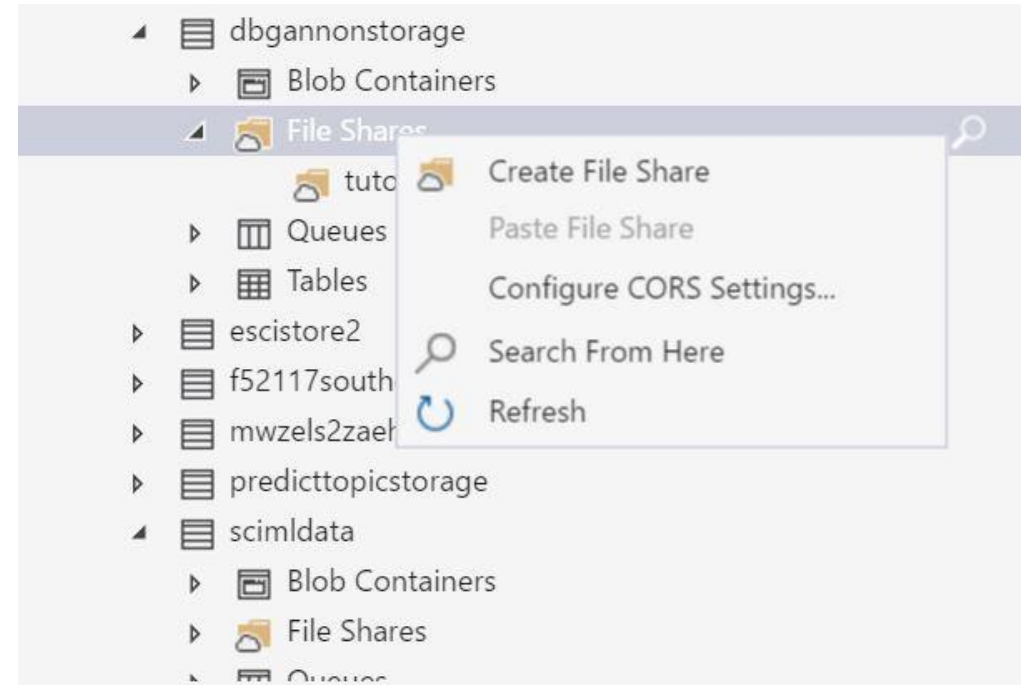
```
>sudo chmod 0777 /mnt/tutorialshare
```

```
>sudo mount -t cifs //yourstorageacct.file.core.windows.net/XXX /mnt/tutorialshare -o  
vers=3.0,user=yourstorageacct,password=you acctpasswd ending in==,dir_mode=0777,file_mode=0777,serverino
```

```
>sudo vi /etc/fstab
```

Add this line at the end

```
//yourstorageacct.file.core.windows.net/XXX /mnt/tutorialshare vers=3.0,user=yourstorageacct,password=you  
acctpasswd ending in==,dir_mode=0777,file_mode=0777,serverino
```



Containers

An alternative to virtual machines for encapsulating software

Using Docker to manage containers

- Download Docker for your pc or mac
 - <https://docs.docker.com/engine/installation/>
- Or login to your Azure data science linux vm
- Type
 `sudo docker ps`
- Type
 `sudo docker run -it ubuntu`
- You are now running Ubuntu linux in a container. -it give you the i/o for the shell.

Containers as a way to share science

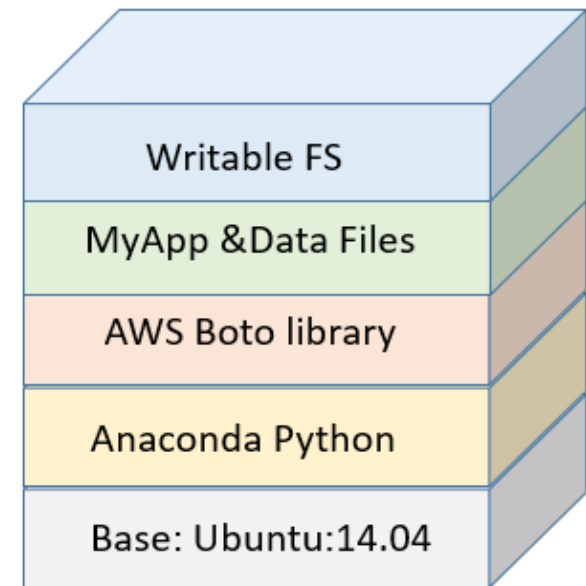
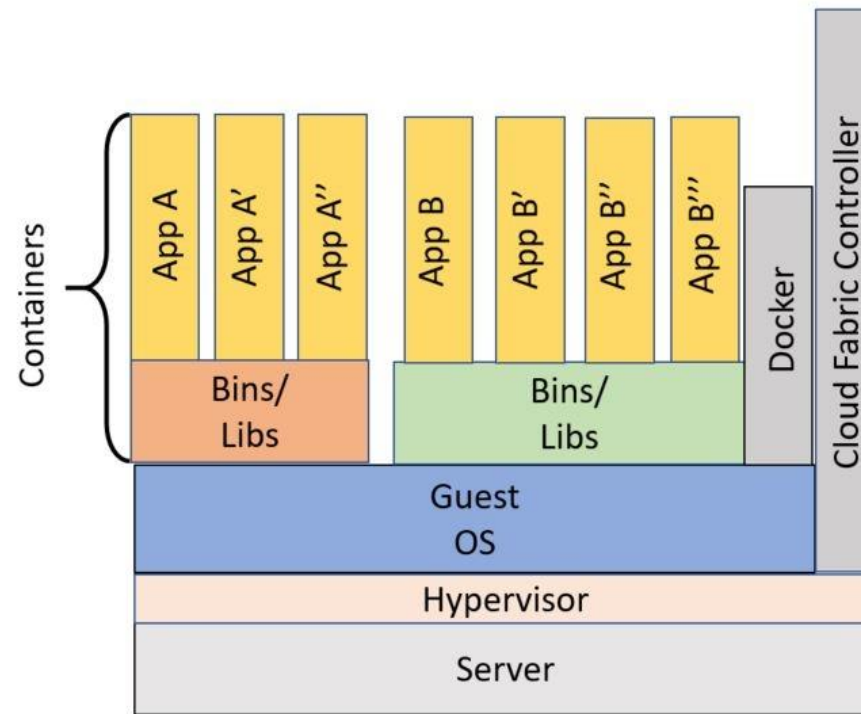
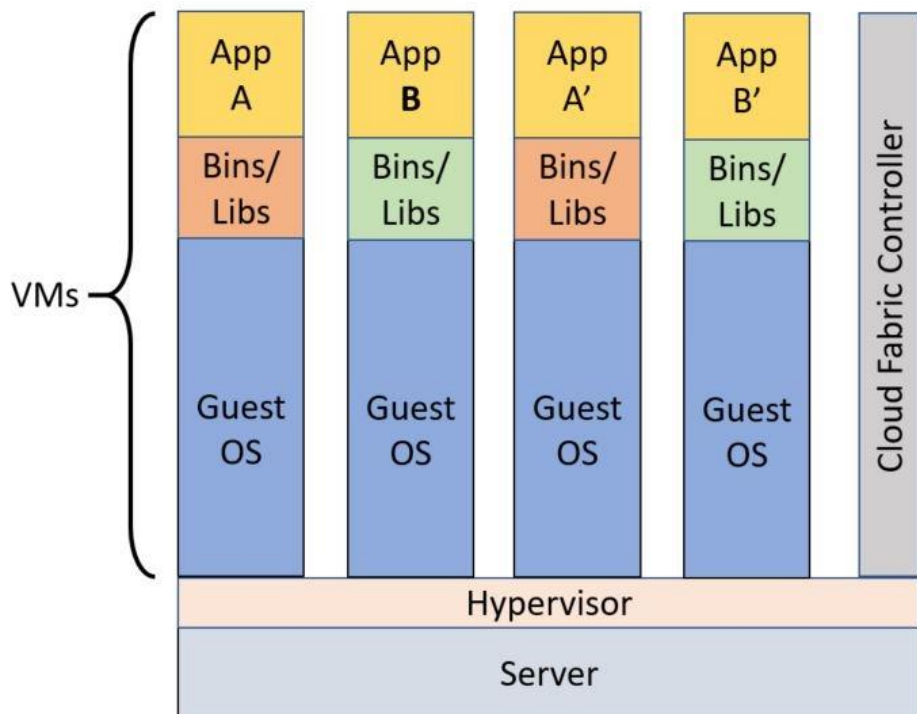
- Lots of our sample jupyter notebooks
- For this tutorial we have a container

```
>docker run -it -p 8888:8888 dbgannon/tutorial
```

 - password = tutorial
 - contains lots of our sample jupyter notebooks
- Many other Science containers:
 - Bio - Galaxy and Hamburg genome toolkit
 - Geosciences – geoserver
 - Astronomy – LOFAR, PyImager, MegTree
 - Engineering – Ubercloud project (theubercloud.com)
 - Math – Matlab, Axiom

What are VMs? containers?

- Virtual machines use a “hypervisor” to provide a complete virtualization of the hosts hardware. A VM is an instance of a complete operating system and file system running on the virtualized hardware.
- Containers share components of the hosts OS and file system and are more similar to a process.



Advantages

Virtual machines	Containers
Heavyweight	Lightweight
Fully isolated and hence more secure	Process-level isolation; hence less secure
No automation for configuration	Script-driven configuration
Slow deployment	Rapid deployment
Easy port and IP address mapping	More abstract port and IP mappings
Custom images not portable across clouds	Completely portable

Creating a container from other containers

- A directory with
 - A “Dockerfile”
 - Things you want in the container
 - A script
 - A directory of data file: datadir
 - A directory of the notebook examples
 - An openssl certificate and key file
- A secure hash of a password “tutorial” as a ‘sha1:....’ string
- To build the container I ran

`docker build -t="dbgannon/tutorial" .`

Script file is

```
mkdir /home/jovyan/work/notebooks
cp /tutorial_notebooks/* /home/jovyan/work/notebooks
start-notebook.sh --certfile=/mycert.pem --keyfile=/mycert.key \
--NotebookApp.password='sha1:c02ed938ef17:0934044bb76008a364781d85db149a65fe9bb480'
```

Docker file for tutorial

```
# Version: 0.1.0
FROM jupyter/all-spark-notebook
MAINTAINER your name "dennis gannon"
RUN pip install azure-storage ==0.32.0
RUN pip install boto3
RUN easy_install pika
RUN easy_install bottle
COPY book-notebooks /tutorial_notebooks
COPY datadir /datadir
COPY script /
COPY mycert.pem /
COPY mycert.key /
CMD ["bash", "/script"]
```

Much more about containers

- You can mount your own directory in the container so data generated in the container can persist.
 - Docker run -v your_director:container_director -it -p
 - Containers can share mounted directories
- Docker compose – allows for container composition
- Singularity – a container system for supercomputer applications.

Section Summary

- Brief look at Virtual Machines
 - Installed Linux Data Science VM on Azure
- Containers
 - Some examples
 - An introduction to Container architecture
 - Containers vs VMs
 - Building a container
- NEXT – swarms of containers in the cloud