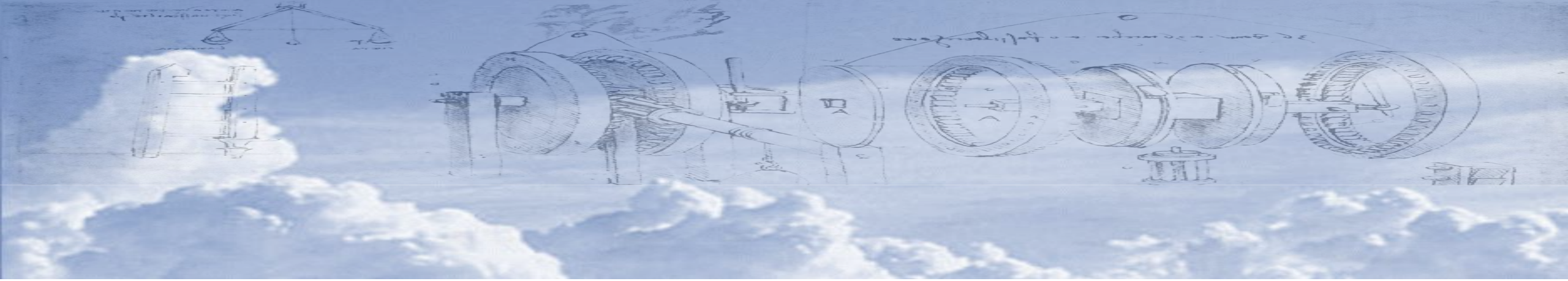
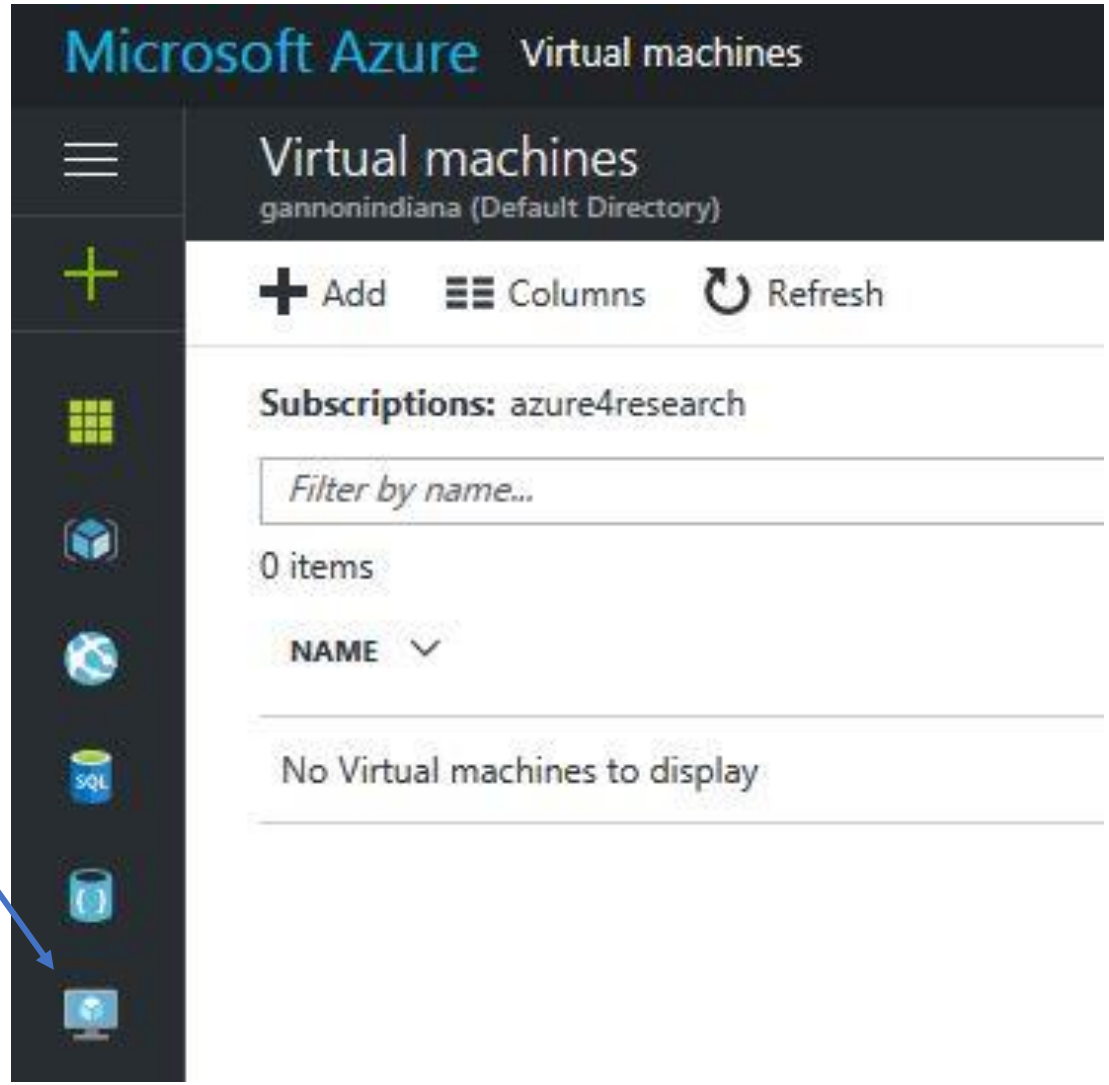


Cloud Computing for Science

Part 2 Virtual Machines and Containers

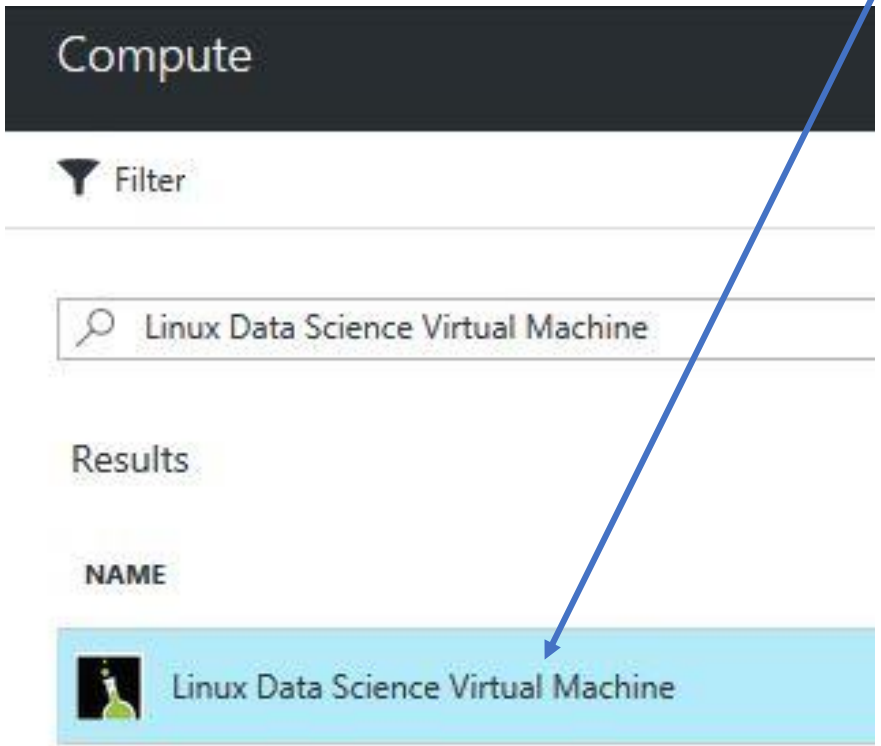
Dennis Gannon

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

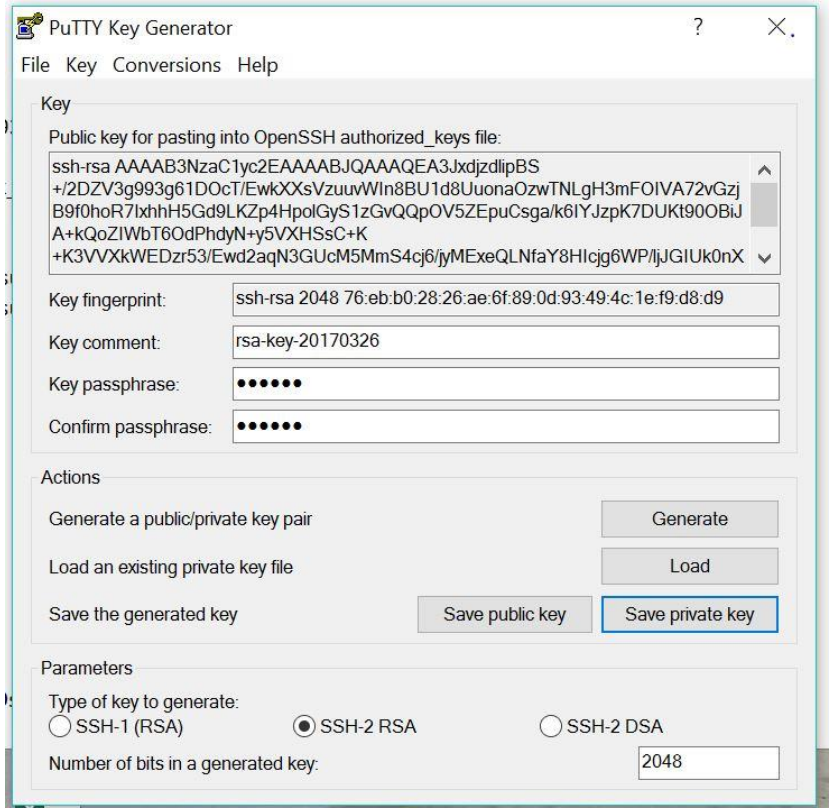
When machine is up, login with

>ssh –i privatekey user@ipaddress

(it will ask for the password)

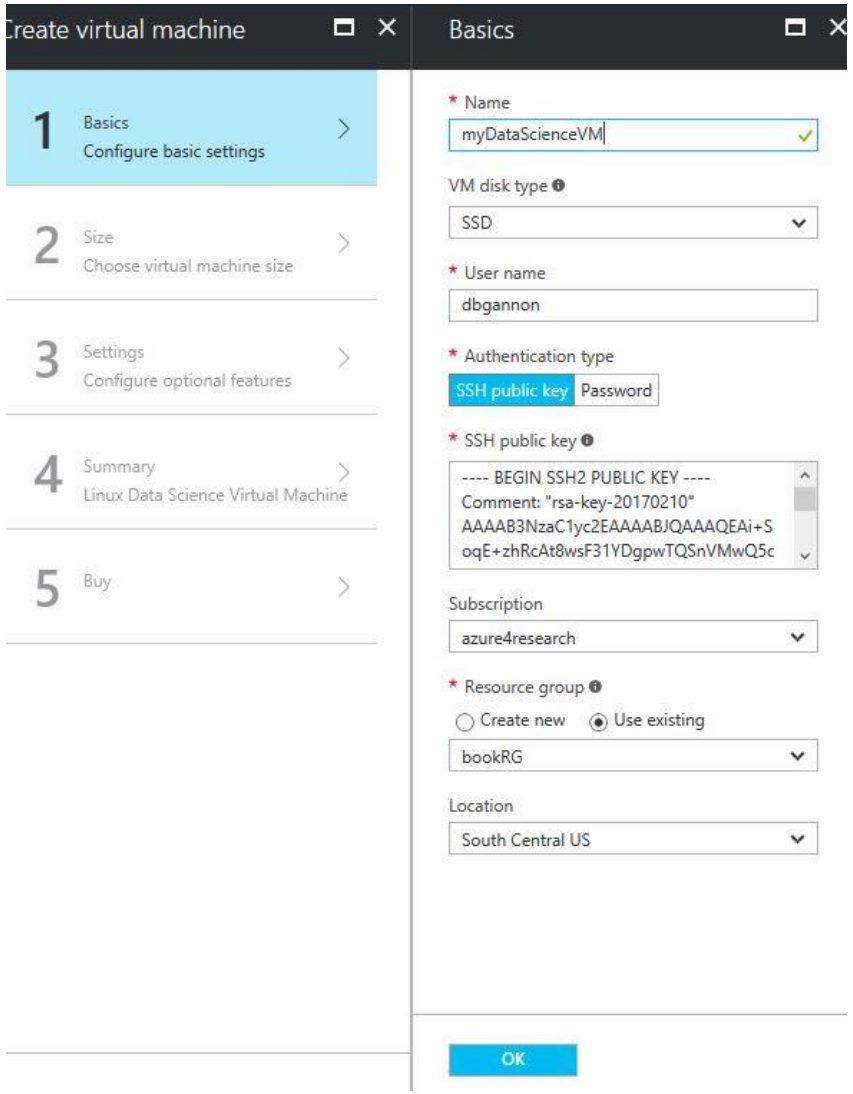
Windows

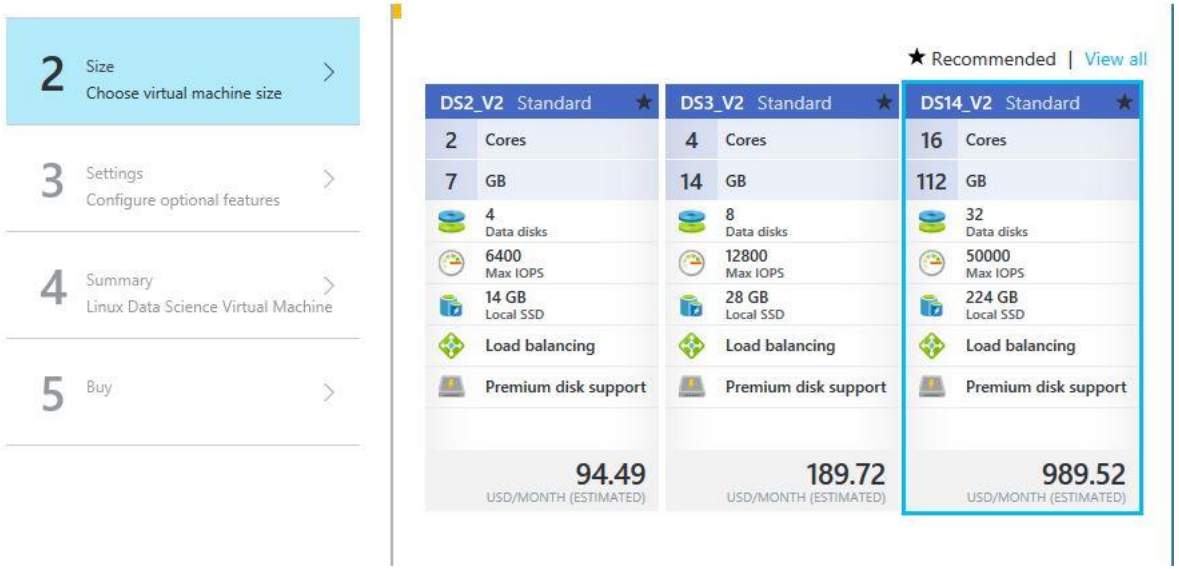
- On Windows10 you can use linux subsystem and follow linux method
- Or Install Putty
- Run PuTTYGen
- Runn Putty to log in.

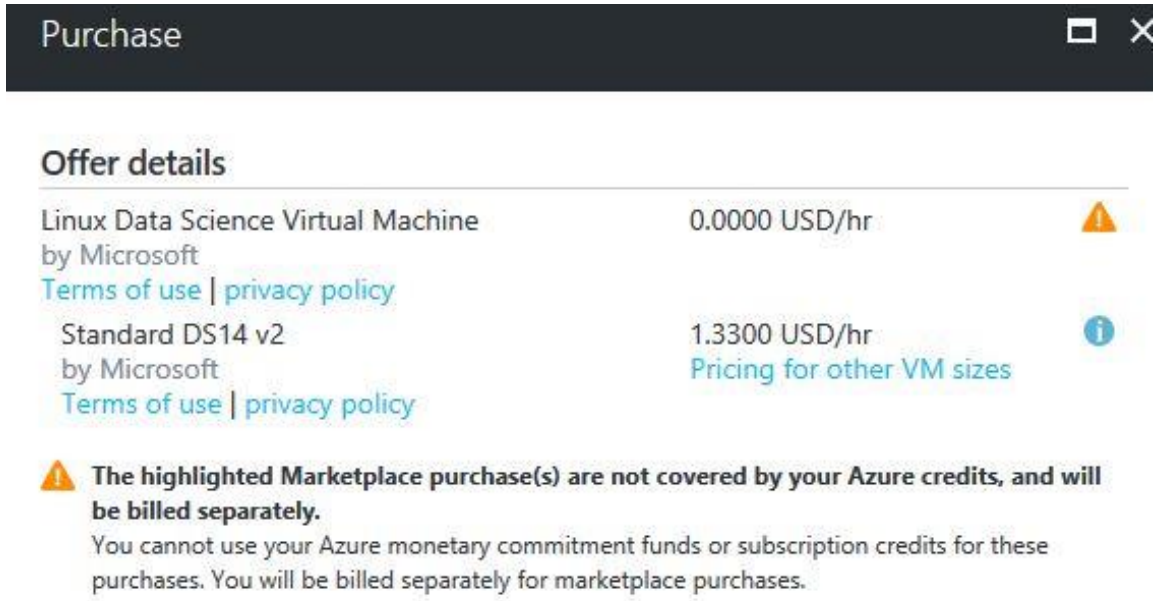


After you log in you need to set your user password
> sudo passwd YourID
>enter your password twice
We will need this later.

Configuring and launching

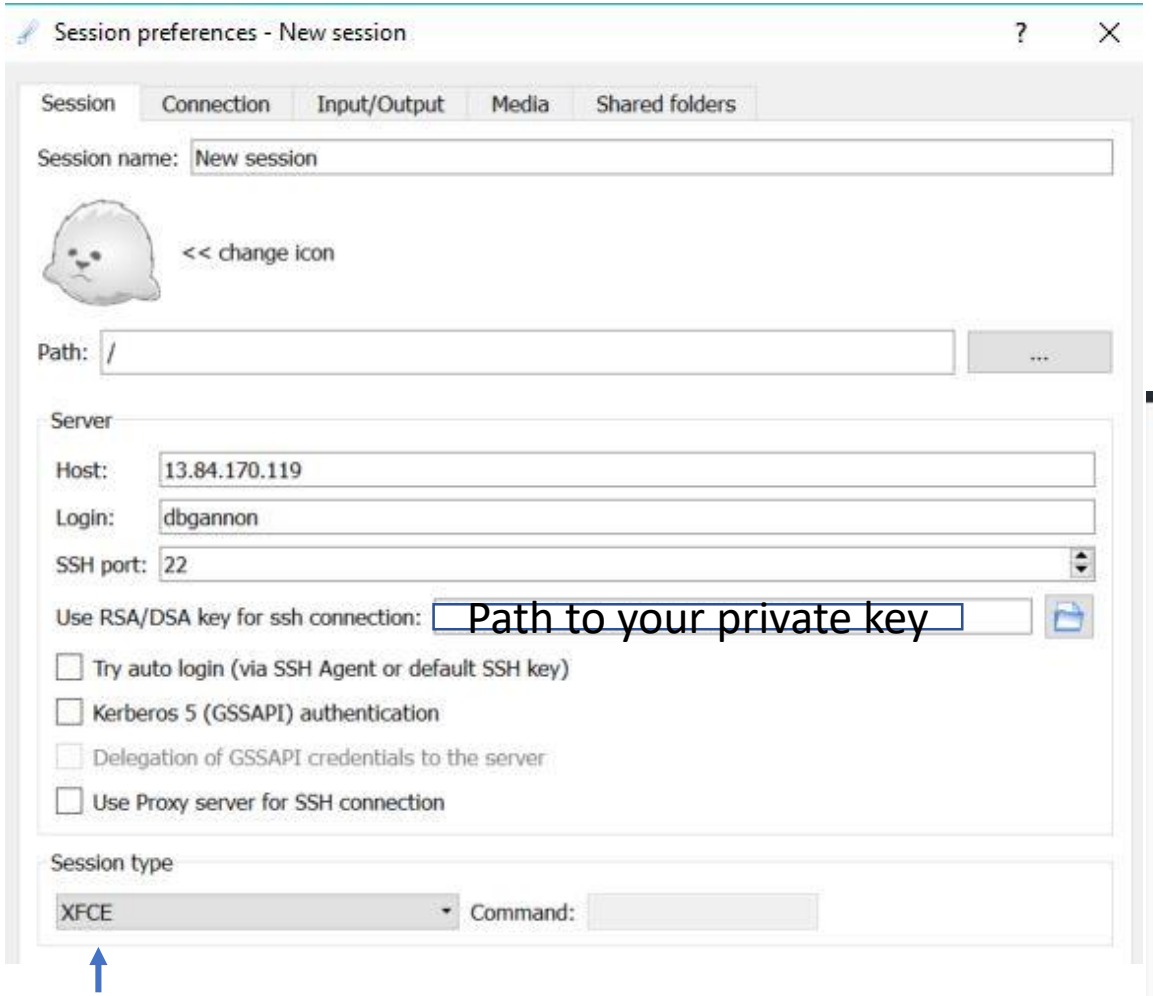




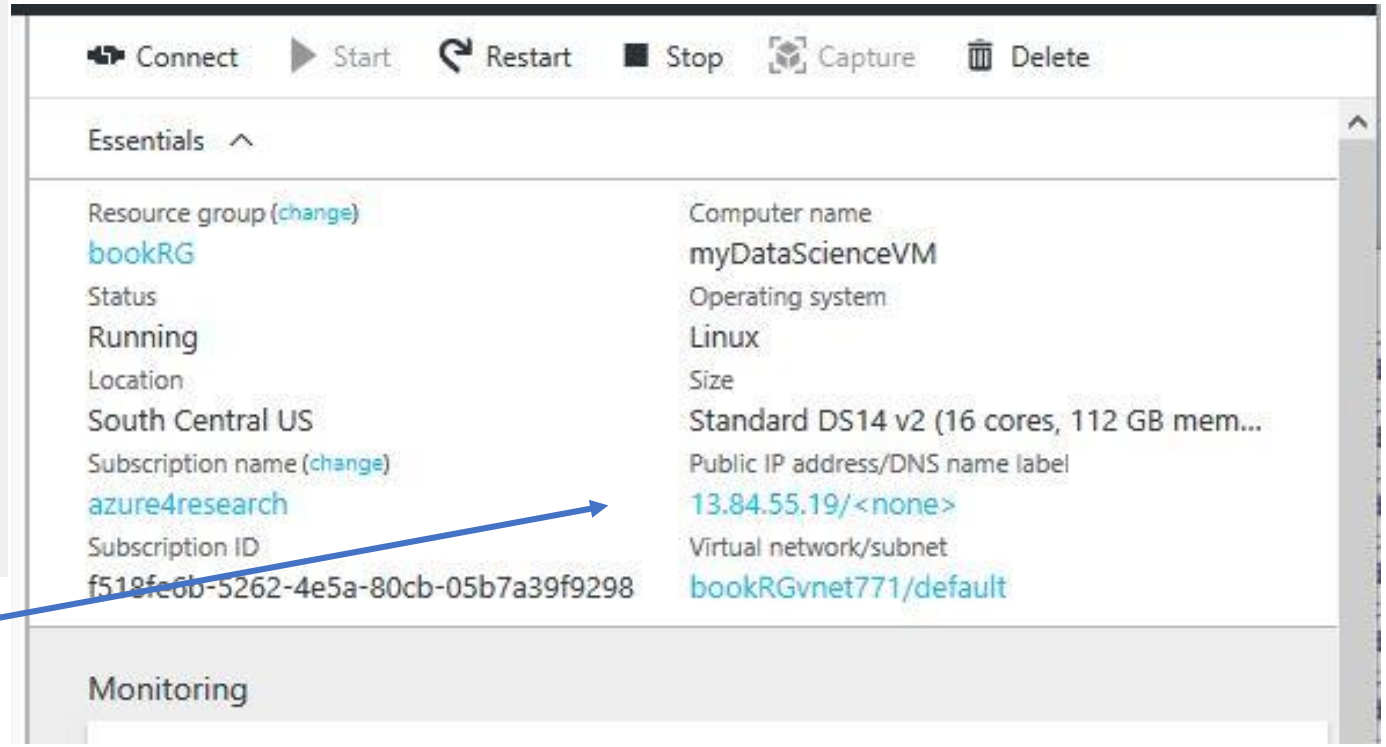


Install X2GO Client

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

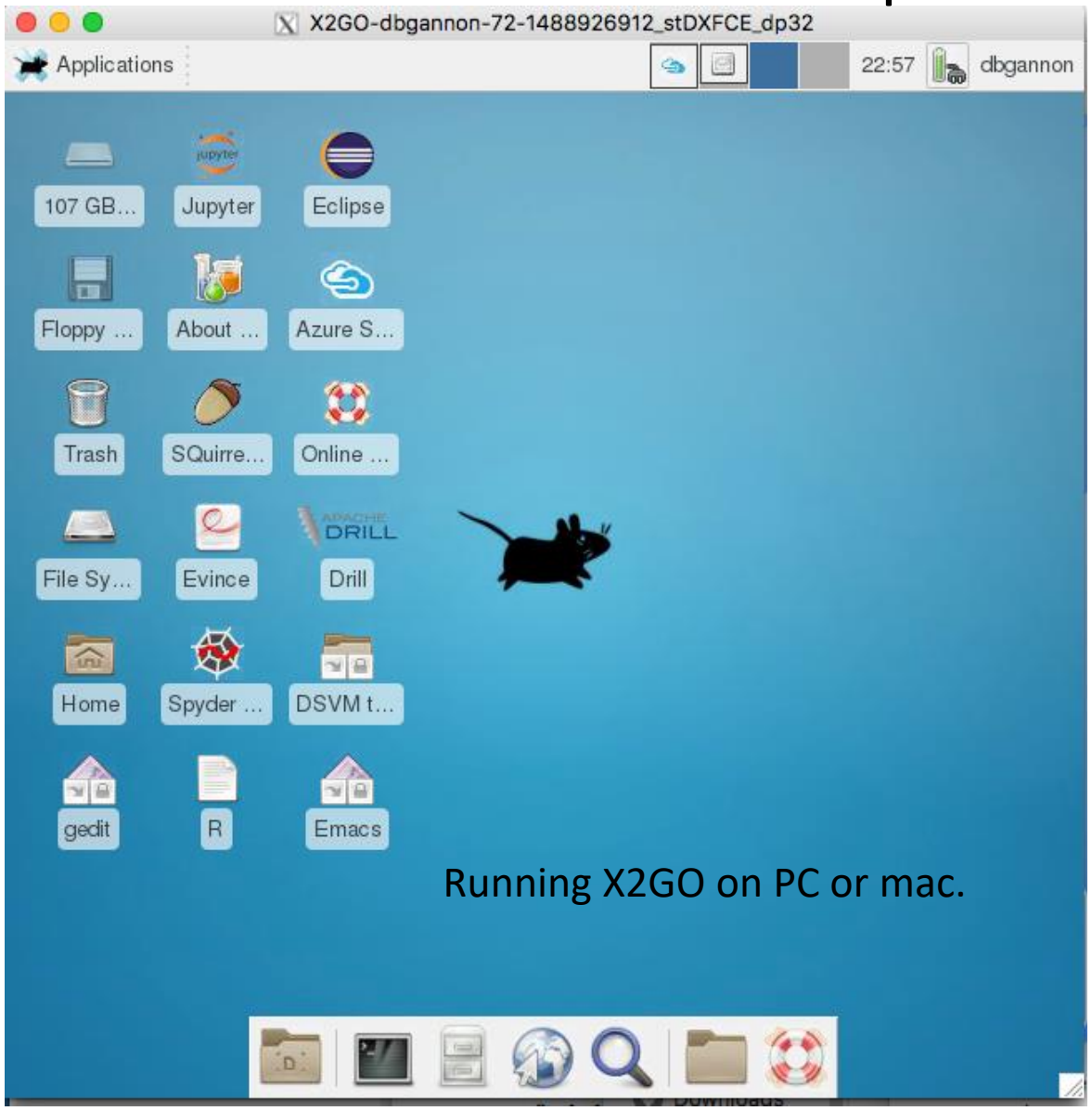


Set to this



Azure portal view and IP address

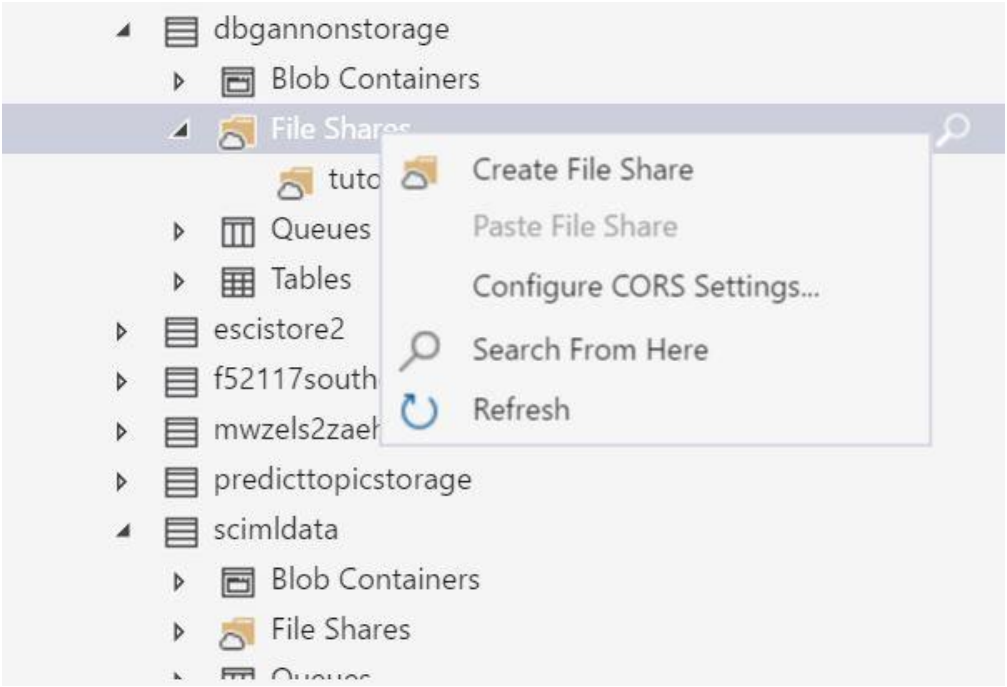
X2GO XFCE Desktop



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 //yourstorageaccnt.file.core.windows.net/XXX /mnt/tutorialshare -o vers=3.0,user=yourstorageaccnt,password=you accntpasswrd ending in==,dir_mode=0777,file_mode=0777,serverino

>sudo vi /etc/fstab

Add this line at the end

//yourstorageaccnt.file.core.windows.net/XXX /mnt/tutorialshare vers=3.0,user=yourstorageaccnt,password=you accntpasswrd 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 linix in a container. -it give you the i/o for the shell.

Containers as a way to share science

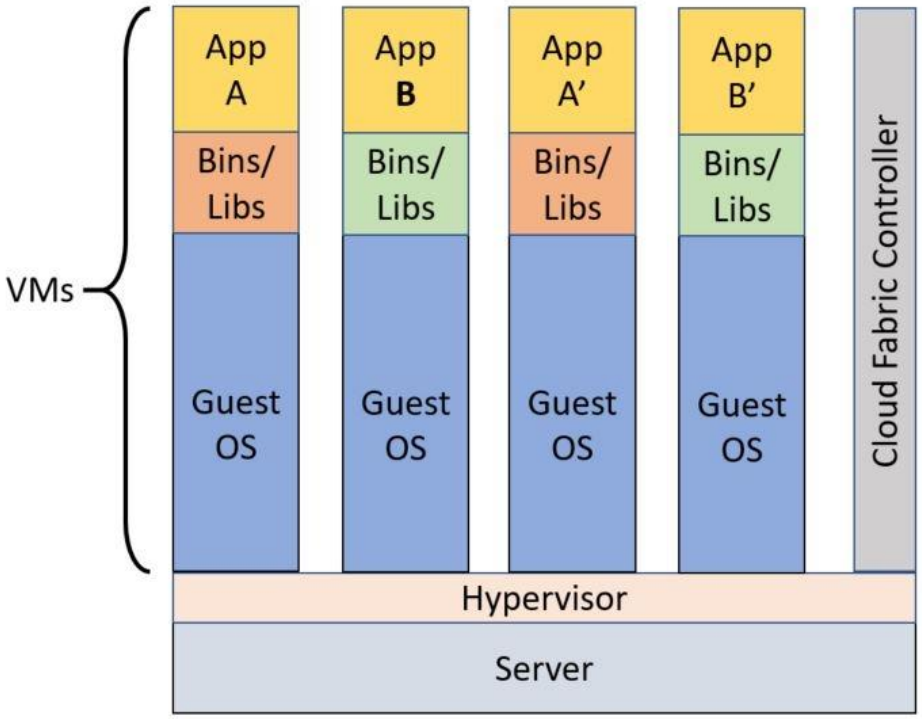
- Lots of our sample jupyter notebooks
- For this tutorial we have a container

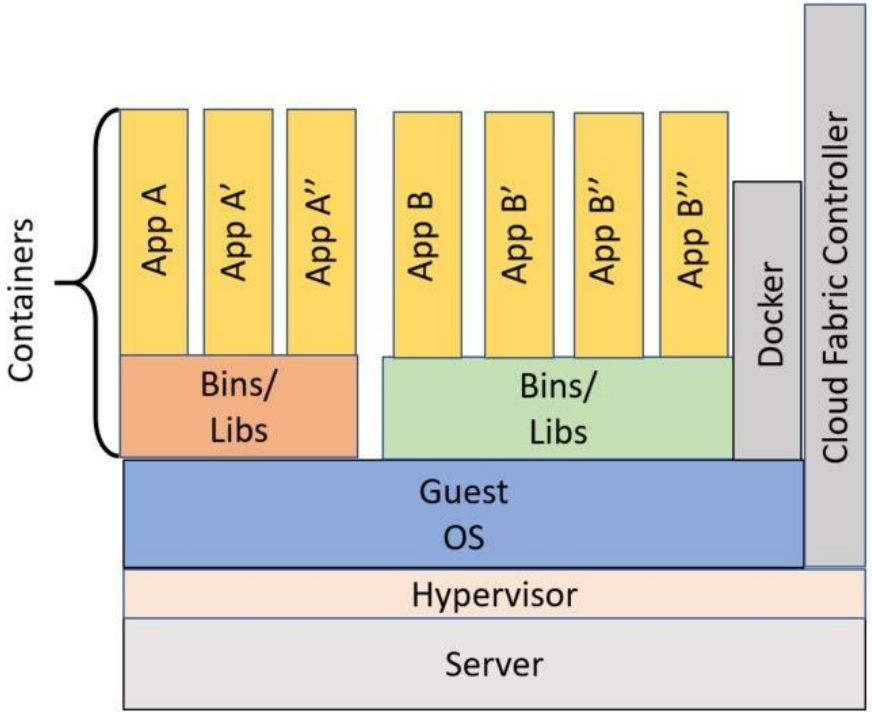
  >docker run –it –p 8888:8888 dbgannon/tutorial

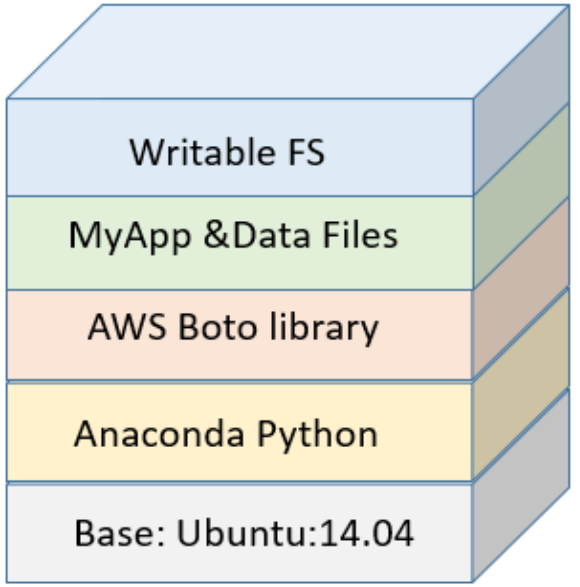
  password = tutorial
  - contains lots of our sample jupyter notebooks
- Many other Science containers:
  - Bio - Galaxy and Hamburg genome toolkit
  - Geosciences – geoserver
  - Astronomy – LOFAR, PyImager, MegTree
  - Engineering – Ubercloud project (theubercloud.com)
  - Math – Matlab, Axiom

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” .

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"]
```

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'
```

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 archeticture
  - Containers vs VMs
  - Building a container
- NEXT – swarms of containers in the cloud