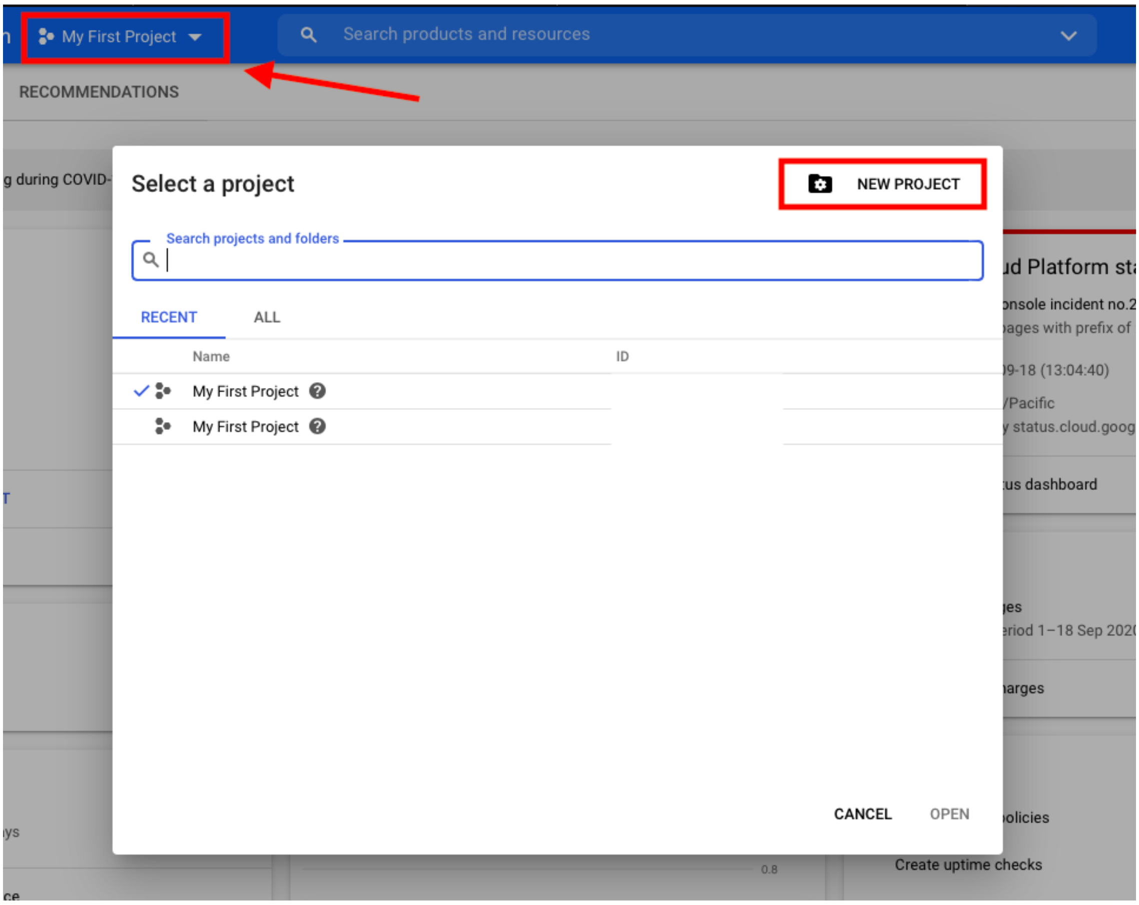
1. **Create a free Google Cloud ([https://cloud.google.com](https://cloud.google.com) ) account with $300 free credit**
2. **Create a new project**

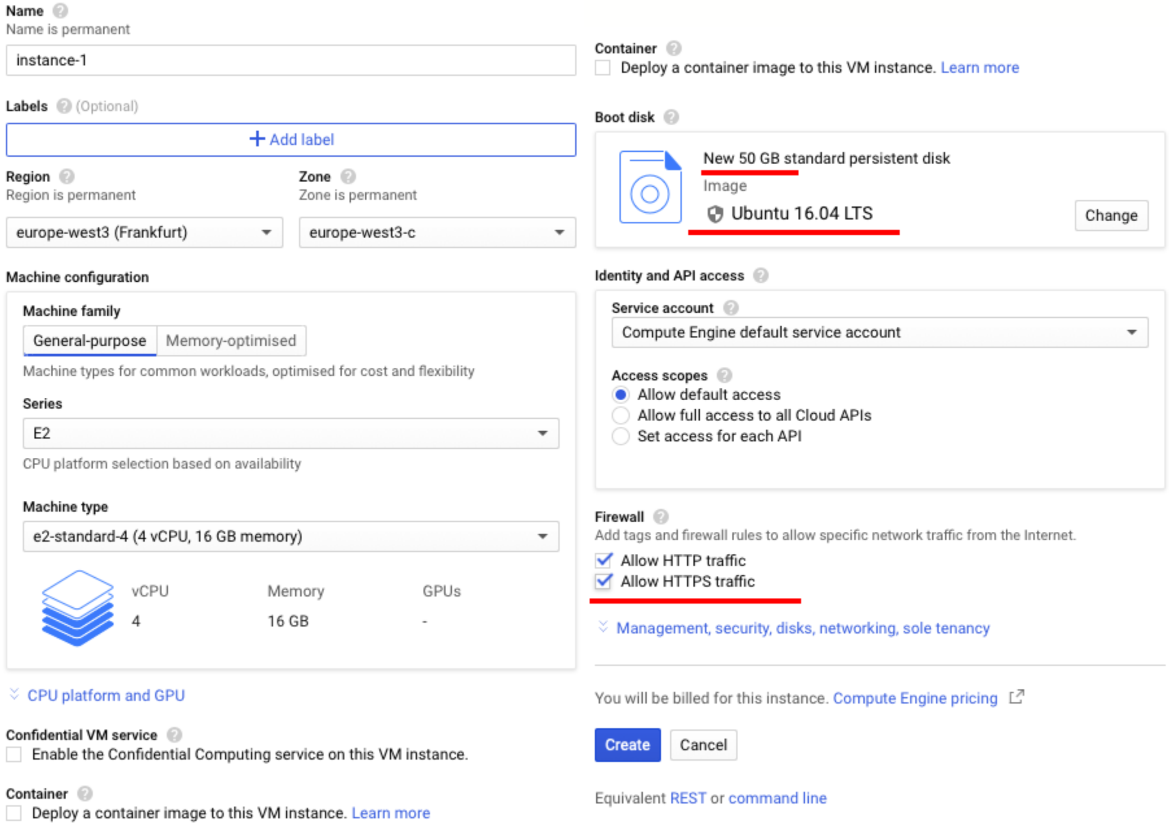


3. **Launch an instance**

- Go to …

  Compute Engine >> VM instances >> create an instance

Add name, select zone and choose your machine type. Do not forget to allow HTTP and HTTPS traffic and edit details as shown in the following screenshots.



Name
Name is permanent
instance-1

Labels (Optional)
+ Add label

Region
Region is permanent
europe-west3 (Frankfurt)

Zone
Zone is permanent
europe-west3-c

Machine configuration

Machine family
General-purpose | Memory-optimised
Machine types for common workloads, optimised for cost and flexibility

Series
E2
CPU platform selection based on availability

Machine type
e2-standard-4 (4 vCPU, 16 GB memory)

| vCPU | Memory | GPUs |
|---|---|---|
| 4 | 16 GB | - |

CPU platform and GPU

Confidential VM service
□ Enable the Confidential Computing service on this VM instance.

Container
□ Deploy a container image to this VM instance. Learn more

Container
□ Deploy a container image to this VM instance. Learn more

Boot disk
New 50 GB standard persistent disk
Image
Ubuntu 16.04 LTS
Change

Identity and API access

Service account
Compute Engine default service account

Access scopes
● Allow default access
○ Allow full access to all Cloud APIs
○ Set access for each API

Firewall
Add tags and firewall rules to allow specific network traffic from the Internet.
☑ Allow HTTP traffic
☑ Allow HTTPS traffic

Management, security, disks, networking, sole tenancy

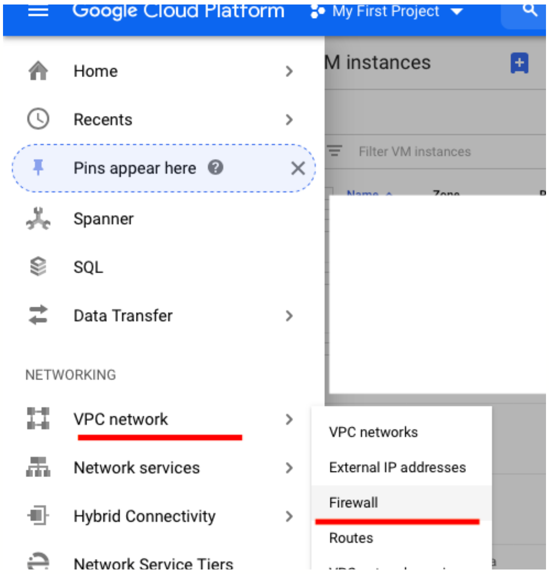
You will be billed for this instance. Compute Engine pricing

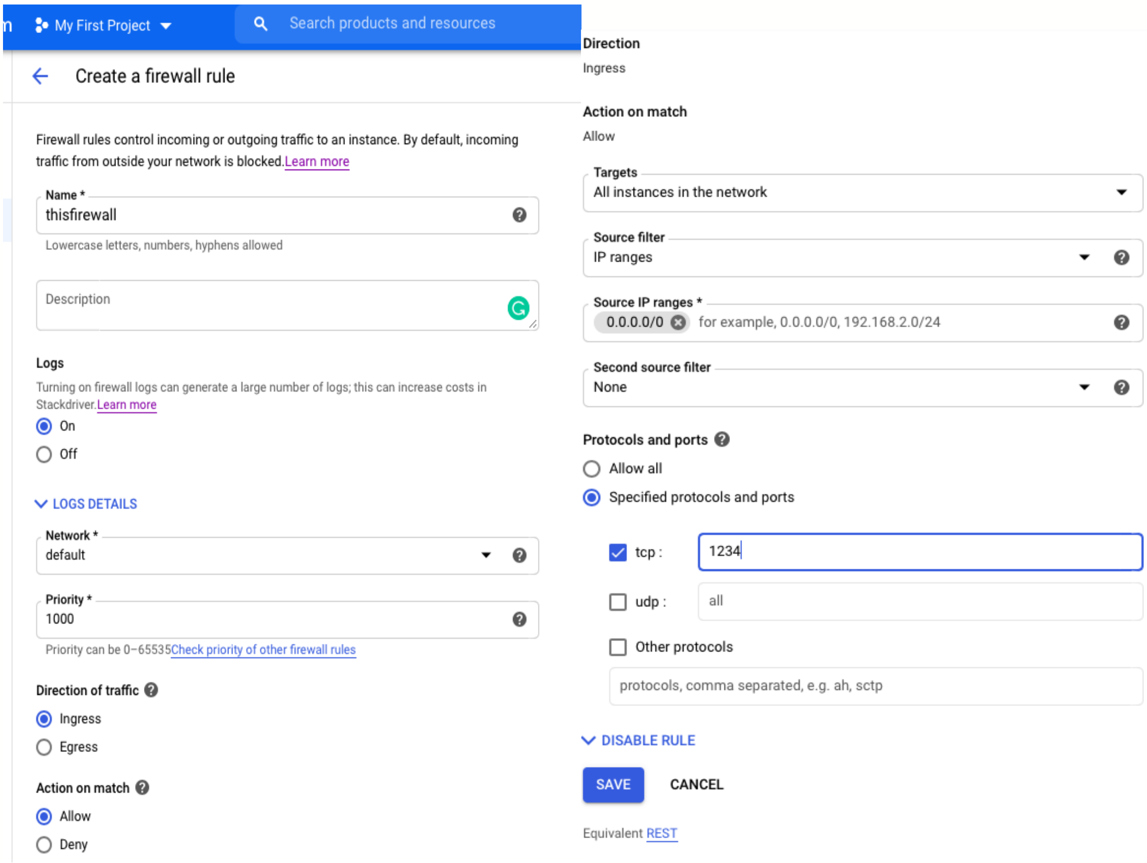
Create | Cancel

Equivalent REST or command line

## 4. Change the Firewall setting

Before starting the server, you need to change the firewall setting by going to the Firewall page and click on “Create firewall”. Add name, set the port number –this can be any number but in this example, I will be using port 1234–, set “Source IP ranges” to 0.0.0.0/0 and edit details as seen in the following screenshots.





Create a firewall rule

Firewall rules control incoming or outgoing traffic to an instance. By default, incoming traffic from outside your network is blocked. Learn more

Name * thisfirewall
Lowercase letters, numbers, hyphens allowed

Description

Logs
Turning on firewall logs can generate a large number of logs; this can increase costs in Stackdriver. Learn more
● On
○ Off

LOGS DETAILS

Network * default

Priority * 1000
Priority can be 0–65535 Check priority of other firewall rules

Direction of traffic
● Ingress
○ Egress

Action on match
● Allow
○ Deny

Direction
Ingress

Action on match
Allow

Targets
All instances in the network

Source filter
IP ranges

Source IP ranges *
0.0.0.0/0 for example, 0.0.0.0/0, 192.168.2.0/24

Second source filter
None

Protocols and ports
○ Allow all
● Specified protocols and ports

☑ tcp : 1234

☐ udp : all

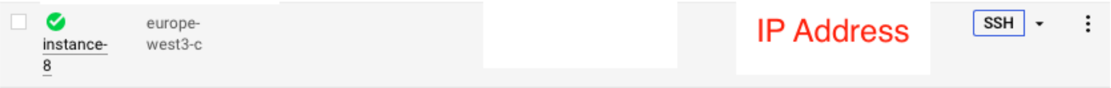
☐ Other protocols

protocols, comma separated, e.g. ah, sctp

Equivalent REST

5. **Start an instance**

Go back to the VM instances page. To start the instance, click SSH. This should navigate you to an SSH terminal.  Note that the external IP address will be used later to access the Jupyter notebook.

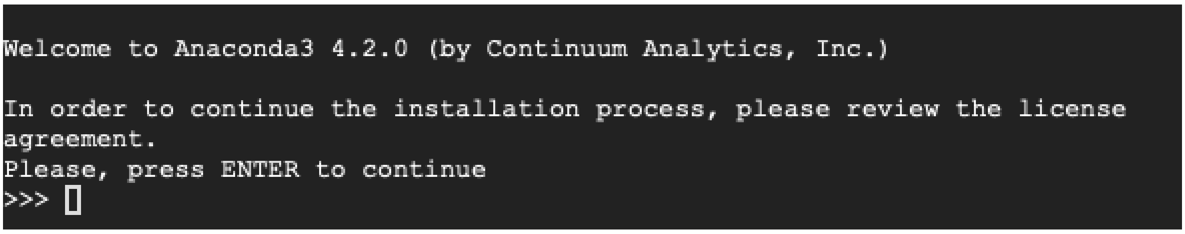


6. **In your SSH terminal, enter the codes (without “$”) as followed to prepare the environment and launch a Jupyter notebook.**

**To install Anaconda**

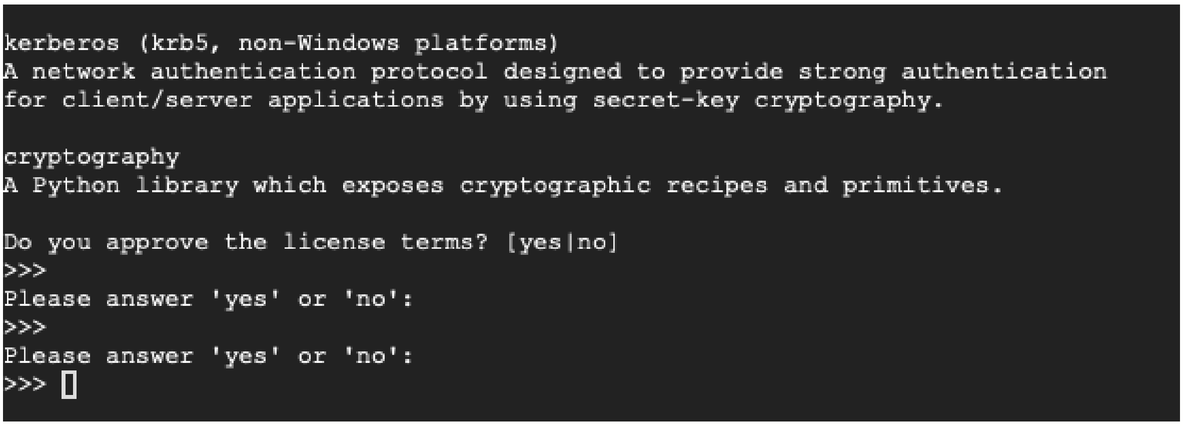
$ wget https://repo.continuum.io/archive/Anaconda3-4.2.0-Linux-x86_64.sh

$ bash Anaconda3-4.2.0-Linux-x86_64.sh



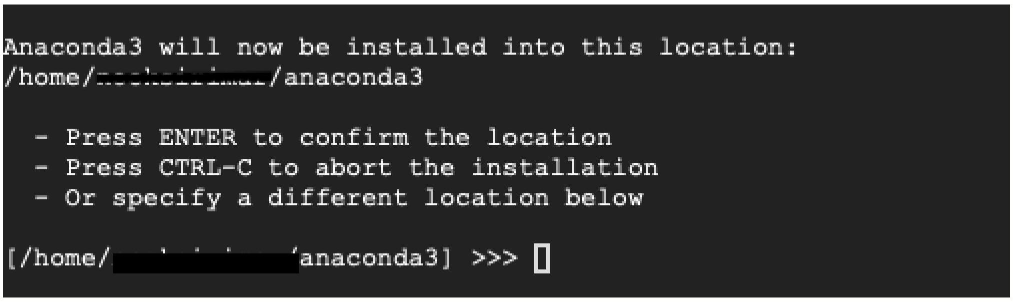
```
Welcome to Anaconda3 4.2.0 (by Continuum Analytics, Inc.)

In order to continue the installation process, please review the license
agreement.
Please, press ENTER to continue
>>> 
```

## Press Enter.



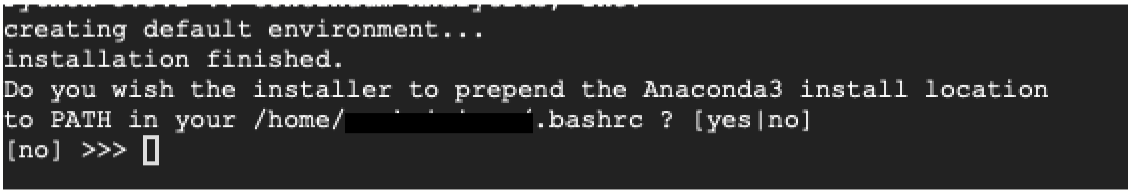
```
kerberos (krb5, non-Windows platforms)
A network authentication protocol designed to provide strong authentication
for client/server applications by using secret-key cryptography.

cryptography
A Python library which exposes cryptographic recipes and primitives.

Do you approve the license terms? [yes|no]
>>>
Please answer 'yes' or 'no':
>>>
Please answer 'yes' or 'no':
>>> 
```

## Enter “yes”.



```
Anaconda3 will now be installed into this location:
/home/[redacted]/anaconda3

  - Press ENTER to confirm the location
  - Press CTRL-C to abort the installation
  - Or specify a different location below

[/home/[redacted]anaconda3] >>>
```

## Press Enter.



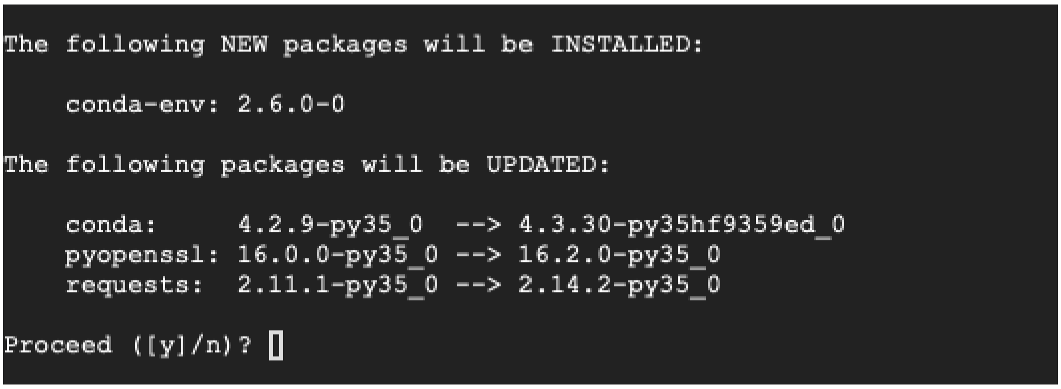
```
creating default environment...
installation finished.
Do you wish the installer to prepend the Anaconda3 install location
to PATH in your /home/[redacted].bashrc ? [yes|no]
[no] >>>
```

## Enter “yes”.

$ source ~/.bashrc

**To install python3.6 and tensorflow2 (these steps can take a few minutes)**

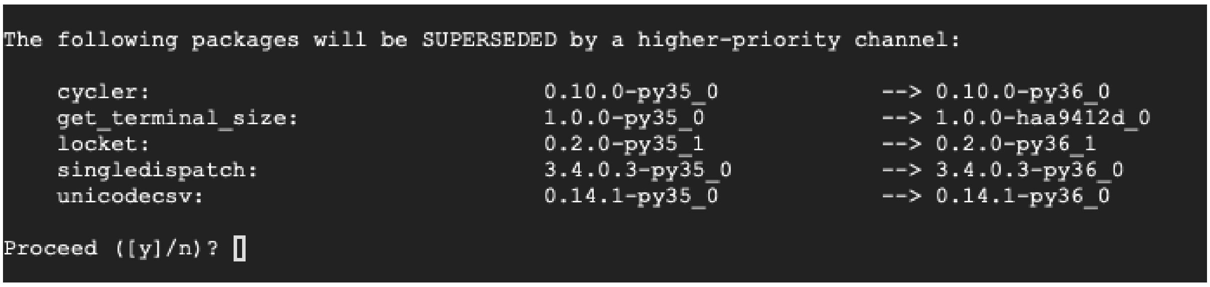
$ conda update conda



```
The following NEW packages will be INSTALLED:

    conda-env: 2.6.0-0

The following packages will be UPDATED:

    conda:     4.2.9-py35_0  --> 4.3.30-py35hf9359ed_0
    pyopenssl: 16.0.0-py35_0 --> 16.2.0-py35_0
    requests:  2.11.1-py35_0 --> 2.14.2-py35_0

Proceed ([y]/n)?
```

##Enter “y”.

$ conda install python=3.6

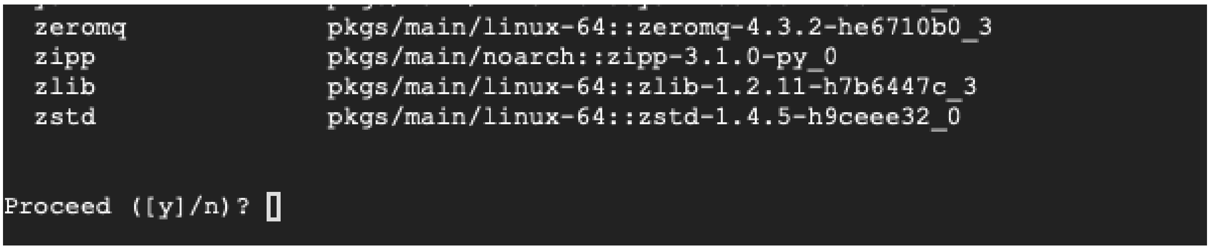


```
The following packages will be SUPERSEDED by a higher-priority channel:

    cycler:                          0.10.0-py35_0          --> 0.10.0-py36_0
    get_terminal_size:               1.0.0-py35_0           --> 1.0.0-haa9412d_0
    locket:                          0.2.0-py35_1           --> 0.2.0-py36_1
    singledispatch:                  3.4.0.3-py35_0         --> 3.4.0.3-py36_0
    unicodecsv:                      0.14.1-py35_0          --> 0.14.1-py36_0

Proceed ([y]/n)?
```

##Enter “y”.

**To create ImaGene environment**

$ conda create -n ImaGene python=3.6 tensorflow=2 keras numpy scipy scikit-image scikit-learn matplotlib pydot pymc3 ipython jupyter

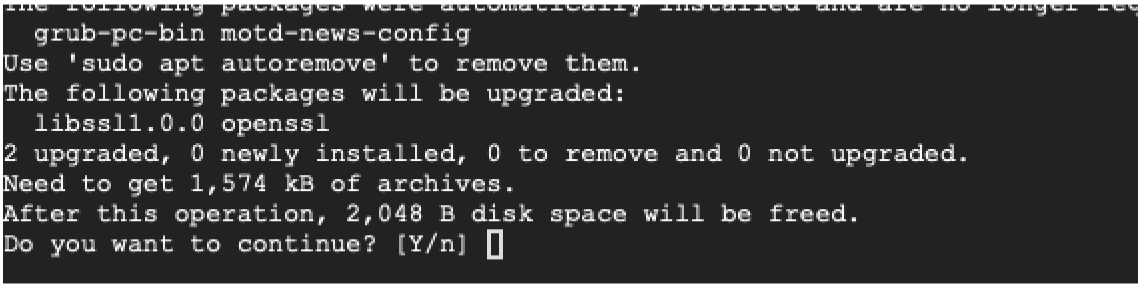


```
  zeromq              pkgs/main/linux-64::zeromq-4.3.2-he6710b0_3
  zipp                pkgs/main/noarch::zipp-3.1.0-py_0
  zlib                pkgs/main/linux-64::zlib-1.2.11-h7b6447c_3
  zstd                pkgs/main/linux-64::zstd-1.4.5-h9ceee32_0


Proceed ([y]/n)? 
```

##Enter “y”.

**To install Java**

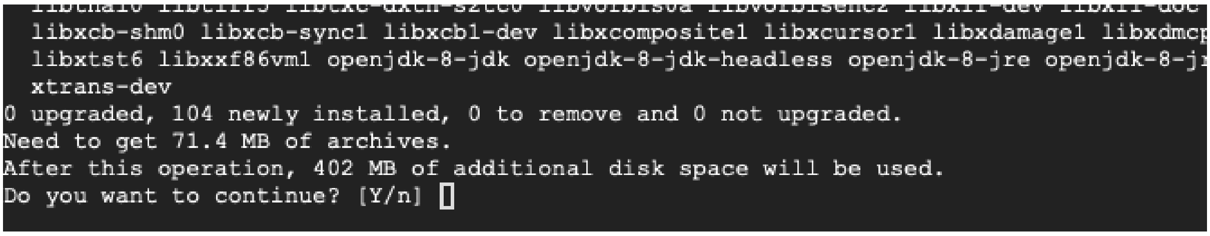
$ sudo apt-get update && sudo apt-get upgrade



```
The following packages were automatically installed and are no longer req
  grub-pc-bin motd-news-config
Use 'sudo apt autoremove' to remove them.
The following packages will be upgraded:
  libssl1.0.0 openssl
2 upgraded, 0 newly installed, 0 to remove and 0 not upgraded.
Need to get 1,574 kB of archives.
After this operation, 2,048 B disk space will be freed.
Do you want to continue? [Y/n] 
```

##Enter “y”.

$ sudo apt-get install default-jdk



```
  libthai0 libtiff5 libtxc-dxtn-s2tc0 libvorbis0a libvorbisenc2 libx11-dev libx11-doc
  libxcb-shm0 libxcb-sync1 libxcb1-dev libxcomposite1 libxcursor1 libxdamage1 libxdmcp
  libxtst6 libxxf86vm1 openjdk-8-jdk openjdk-8-jdk-headless openjdk-8-jre openjdk-8-jr
  xtrans-dev
0 upgraded, 104 newly installed, 0 to remove and 0 not upgraded.
Need to get 71.4 MB of archives.
After this operation, 402 MB of additional disk space will be used.
Do you want to continue? [Y/n] 
```

##Enter “y”.

**To download MSMS files and unzip the files**

$ git clone https://github.com/mfumagalli/ImaGene

$ wget https://www.mabs.at/ewing/msms/msms3.2rc-b163.zip

$ sudo apt-get install unzip

$ unzip msms3.2rc-b163.zip

### To install a bc package for creating simulations

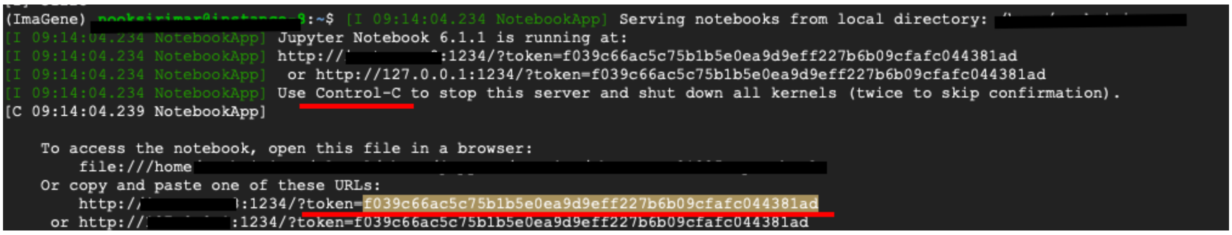
```
$ sudo apt install bc
```

### To activate ImaGene environment

```
$ source activate ImaGene
```

### To generate a config file and launch a Jupyter notebook

```
$ jupyter notebook --generate-config
$ jupyter notebook --ip=0.0.0.0 --port=1234 --no-browser &
```

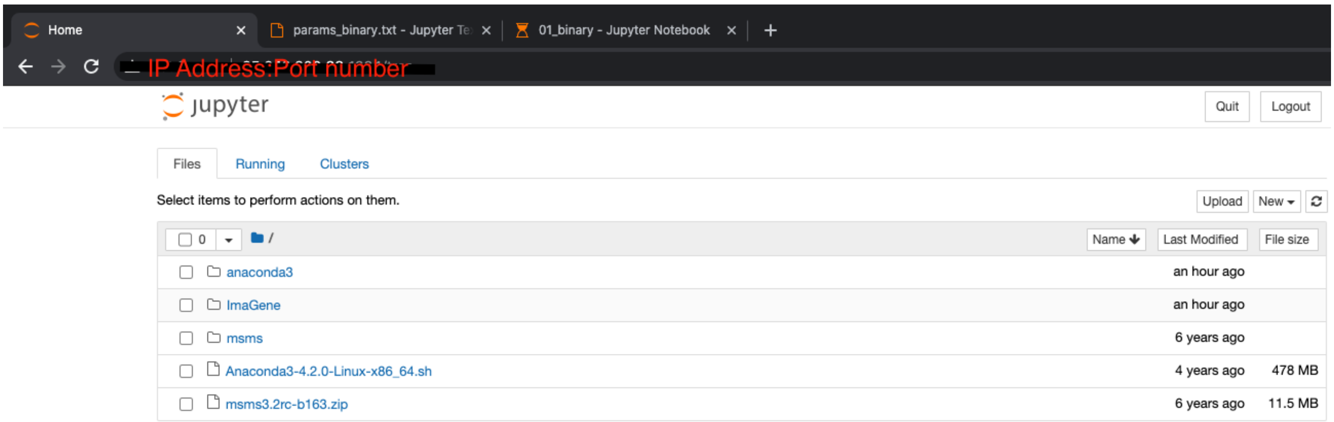


```
(ImaGene) [redacted]:~$ [I 09:14:04.234 NotebookApp] Serving notebooks from local directory: [redacted]
[I 09:14:04.234 NotebookApp] Jupyter Notebook 6.1.1 is running at:
[I 09:14:04.234 NotebookApp] http://[redacted]:1234/?token=f039c66ac5c75b1b5e0ea9d9eff227b6b09cfafc044381ad
[I 09:14:04.234 NotebookApp]  or http://127.0.0.1:1234/?token=f039c66ac5c75b1b5e0ea9d9eff227b6b09cfafc044381ad
[I 09:14:04.234 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 09:14:04.239 NotebookApp]

    To access the notebook, open this file in a browser:
        file:///home[redacted]
    Or copy and paste one of these URLs:
        http://[redacted]:1234/?token=f039c66ac5c75b1b5e0ea9d9eff227b6b09cfafc044381ad
     or http://[redacted]:1234/?token=f039c66ac5c75b1b5e0ea9d9eff227b6b09cfafc044381ad
```

You can access the notebook by clicking on one of the three links as seen in the screenshot. An alternative way of accessing the notebook is to type in the URL search box …

http:// (external IP Address of the instance):Port number

You may be asked for a token to log in to the notebook. The token is highlighted in the previous screenshot. This will navigate you to the Jupyter welcoming page. The ImaGene folder should already be there. You can access and run the codes using the Jupyter interface. All data will be saved to the server.

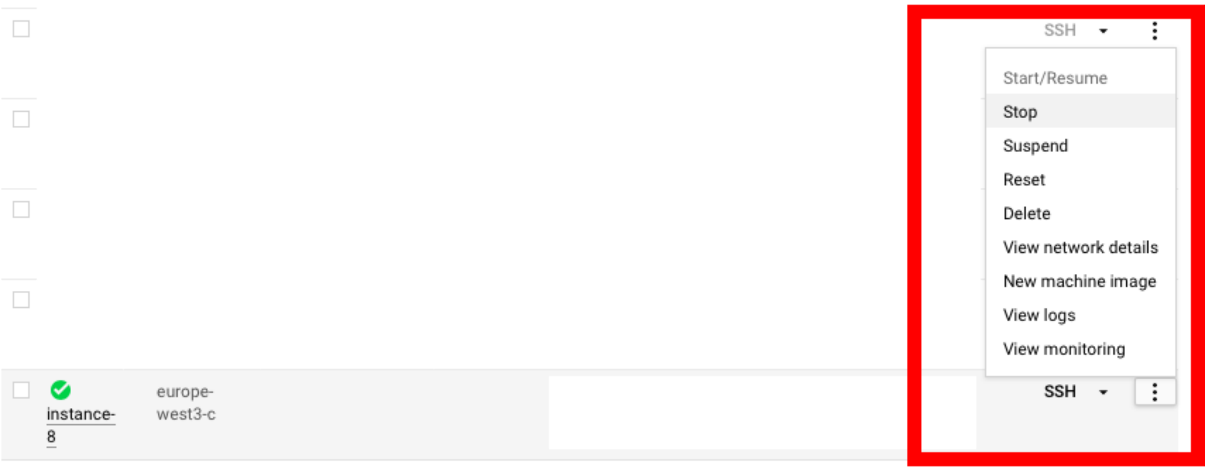

Home
params_binary.txt - Jupyter Te
01_binary - Jupyter Notebook
[redacted] IP Address:Port number
jupyter
Quit
Logout
Files
Running
Clusters
Upload
New
0
/

Select items to perform actions on them.

| Name | Last Modified | File size |
|---|---|---|
| anaconda3 | an hour ago | |
| ImaGene | an hour ago | |
| msms | 6 years ago | |
| Anaconda3-4.2.0-Linux-x86_64.sh | 4 years ago | 478 MB |
| msms3.2rc-b163.zip | 6 years ago | 11.5 MB |

## 7. Stop the instance

Do not forget to stop the server when you are done to avoid any extra charge.



## 8. Restart the instance

To restart the server and re-access the notebook, you just have to re-activate the ImaGene environment and re-launch a Jupyter notebook by entering …

```
$ source activate ImaGene
$ jupyter notebook --ip=0.0.0.0 --port=1234 --no-browser &
```