

Gromacs 系統安裝步驟

之 VPS(Virtual Private Server，虛擬伺服器)：以 Digital Ocean 廠商示範

1. 先申請一台 VPS 主機。

Droplets

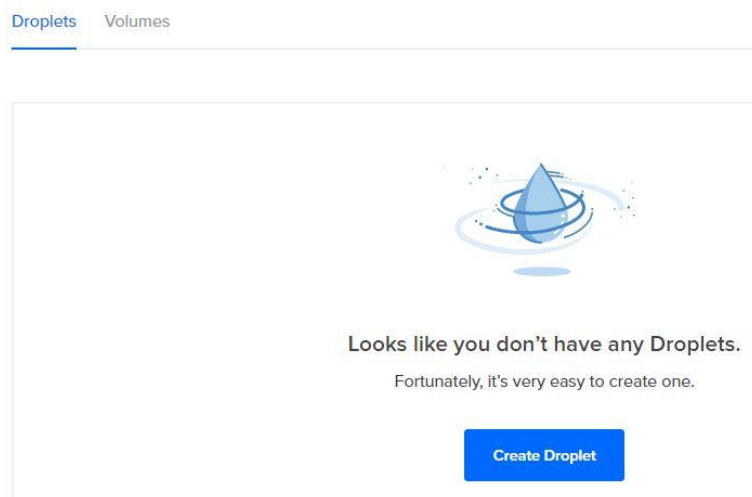


Figure 1

2. VPS 主機請安裝 Ubuntu12.04 LTS(長期支援版)作業系統。

Create Droplets

Choose an image ?

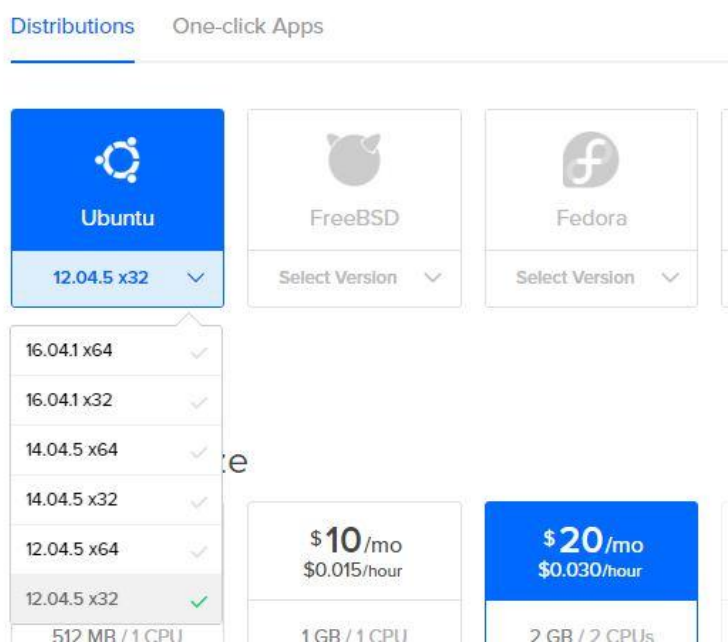


Figure 2

3. 挑選需要的主機規格與區域。

Choose a size

Price	Specs
\$5/mo \$0.007/hour	512 MB / 1 CPU 20 GB SSD Disk 1000 GB Transfer
\$10/mo \$0.015/hour	1 GB / 1 CPU 30 GB SSD Disk 2 TB Transfer
\$20/mo \$0.030/hour	2 GB / 2 CPUs 40 GB SSD Disk 3 TB Transfer

Figure 3

Choose a datacenter region

Region	Grid
New York	1 2 3
San Francisco	1 2
Amsterdam	2 3
Singapore	1

Figure 4

4. 輸入 VPS 主機名稱。

Finalize and create

How many Droplets?
Deploy multiple Droplets with the same configuration.

1 Droplet

Choose a hostname
Give your Droplets an identifying name you will remember them by. Your Droplet name can only contain alphanumeric characters, dashes, and periods.

ubuntu-512mb-sgp1-01

Create

Figure 5

5. 等候 VPS 主機建立(通常時間不超過 1 分鐘)。

Droplets

Search By Droplet Name

Droplets Volumes

Name	IP Address	Created
ubuntu-512mb-sgp1-01 512 MB / 20 GB Disk / SGP1 - Ubuntu 12.04.5 x32	128.199. [REDACTED]	1 minute ago

Figure 6

6. 請到信箱收取 VPS 的连接資訊。

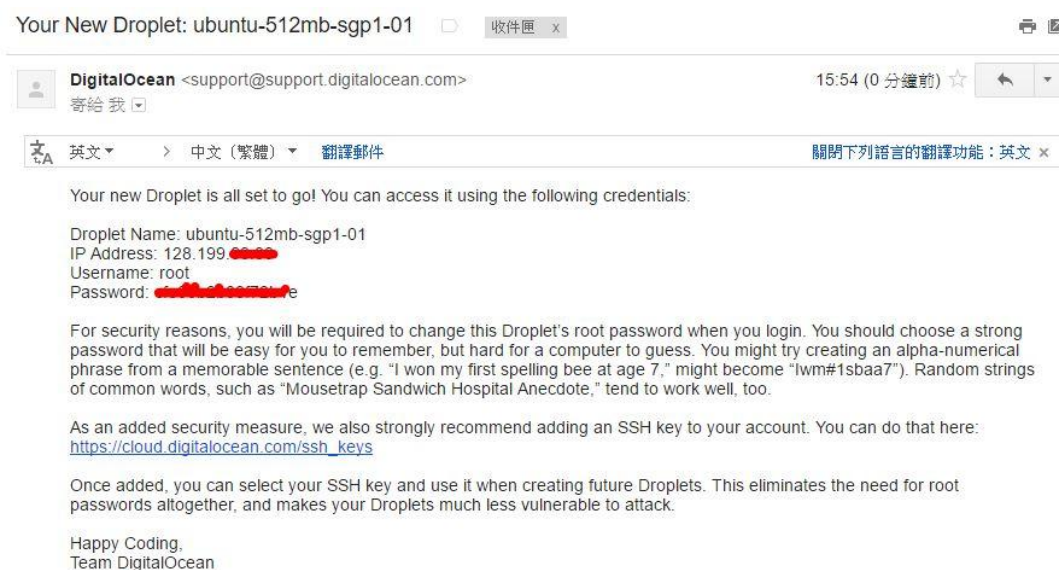


Figure 7

7. VPS 主機建議透過 WinSCP 與 Putty 管理文件與 SSH 終端操作。
WinSCP 可以管理 VPS 檔案，並且可以整合 Putty 開啟 SSH 終端介面。
(載點，Putty <https://tinyurl.com/2r4w>；WinSCP <https://tinyurl.com/h3pceoc>)

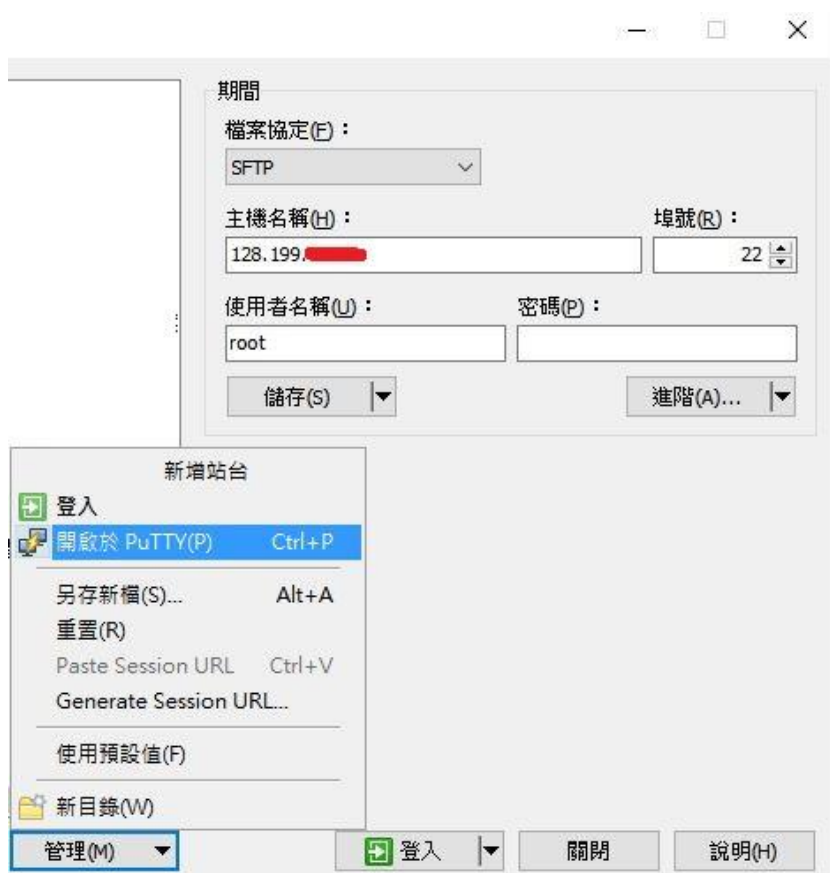


Figure 8

8. 確認金鑰即可執行 SSH 連線。

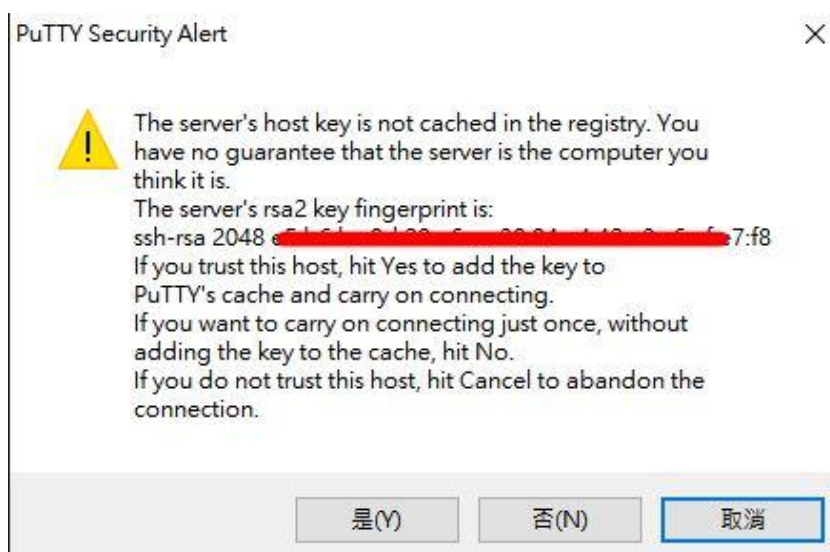


Figure 9

9. 終端機的登入介面輸入用戶名(通常為 root)與密碼即可，部分 VPS 廠商會要求初次登入須更新用戶密碼。



Figure 10

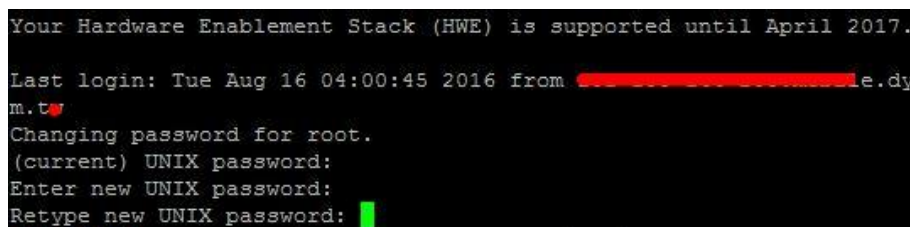


Figure 11

10. 請在終端機輸入

```
sudo apt-get update
```

```
sudo apt-get upgrade
```

更新 Ubuntu 已安裝套件。

```
root@ubuntu-512mb-sgp1-01: ~
```

```
root@ubuntu-512mb-sgp1-01:~# sudo apt-get update
```

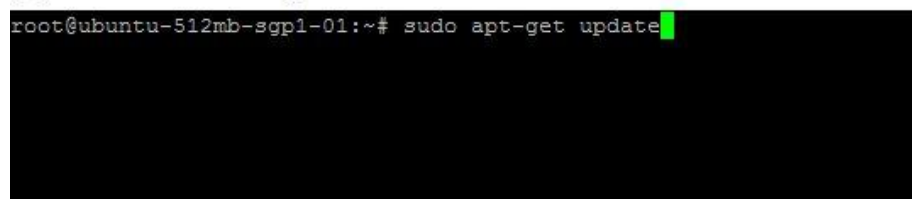


Figure 12

```
root@ubuntu-512mb-sgp1-01: ~
```

```
root@ubuntu-512mb-sgp1-01:~# sudo apt-get upgrade
```

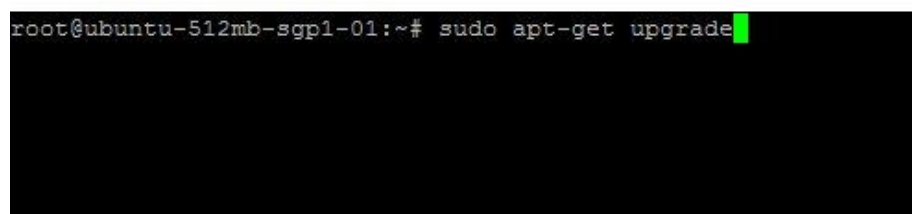


Figure 13

```
root@ubuntu-512mb-sgp1-01: ~
```

```
root@ubuntu-512mb-sgp1-01:~# sudo apt-get upgrade
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following packages have been kept back:
  linux-headers-generic-lts-trusty linux-image-generic-lts-trusty
The following packages will be upgraded:
  curl libcurl3 libcurl3-gnutls openssh-client openssh-server
5 upgraded, 0 newly installed, 0 to remove and 2 not upgraded.
Need to get 1,914 kB of archives.
After this operation, 0 B of additional disk space will be used.
Do you want to continue [Y/n]? y
```

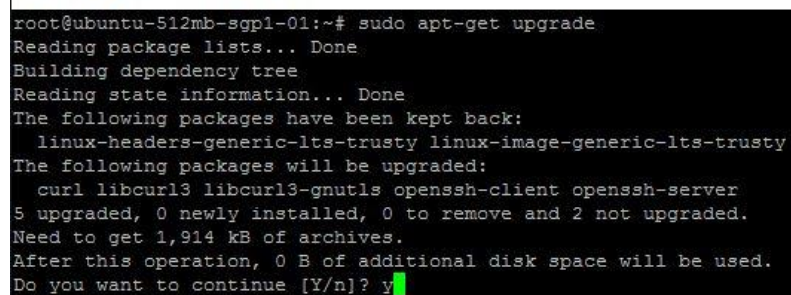
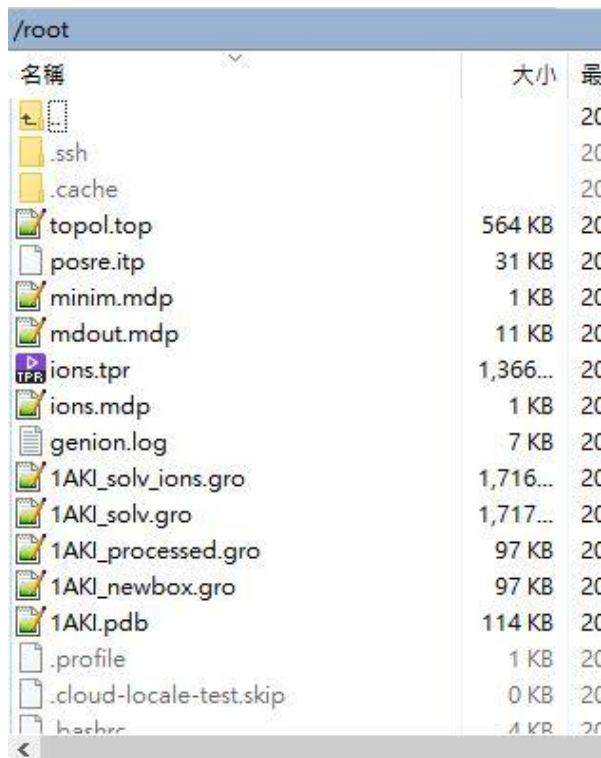


Figure 14

11. 接下來可以開始安裝 Gromacs4.5 到 VPS 主機，請在終端分別輸入
sudo apt-get install gromacs 下方的套件可選擇安裝(自訂)
sudo apt-get install gromacs-dev
sudo apt-get install gromacs-mpich
sudo apt-get install gromacs-openmpi
輸入使用者密碼完成安裝即可。
12. 透過 WinSCP 將欲處理的檔案上傳到 VPS 的使用者家目錄(通常是/root)。



名稱	大小	最
.		20
.ssh		20
.cache		20
topol.top	564 KB	20
posre.itp	31 KB	20
minim.mdp	1 KB	20
mdout.mdp	11 KB	20
ions.tpr	1,366...	20
ions.mdp	1 KB	20
genion.log	7 KB	20
1AKI_solv_ions.gro	1,716...	20
1AKI_solv.gro	1,717...	20
1AKI_processed.gro	97 KB	20
1AKI_newbox.gro	97 KB	20
1AKI.pdb	114 KB	20
.profile	1 KB	20
.cloud-locale-test.skip	0 KB	20
hachrc	4 KB	20

Figure 15

- 由於 VPS 的 SSH 終端無法長時間連線，偶爾會發生中斷的情形導致工作中止，可以透過 Screen 套件保存工作階段，恢復終端連線即可恢復工作階段，請在終端介面輸入

```
sudo apt-get install screen
```

輸入使用者密碼後完成安裝。

- 啟動 Screen 功能，請在終端輸入

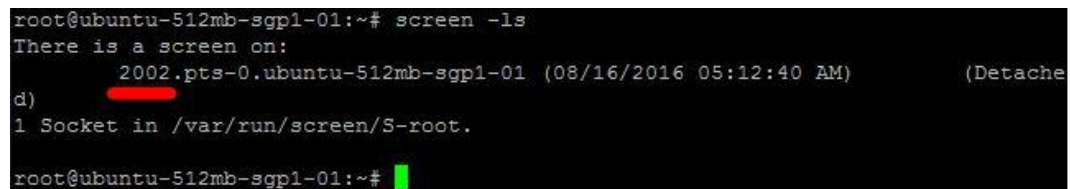
```
screen
```

看到一串 Screen 的使用許可訊息即可。

- 當 SSH 終端介面中斷後，重新連線時可以在終端介面輸入

```
screen -ls
```

查看已保存的 Screen 工作資訊與工作編號。



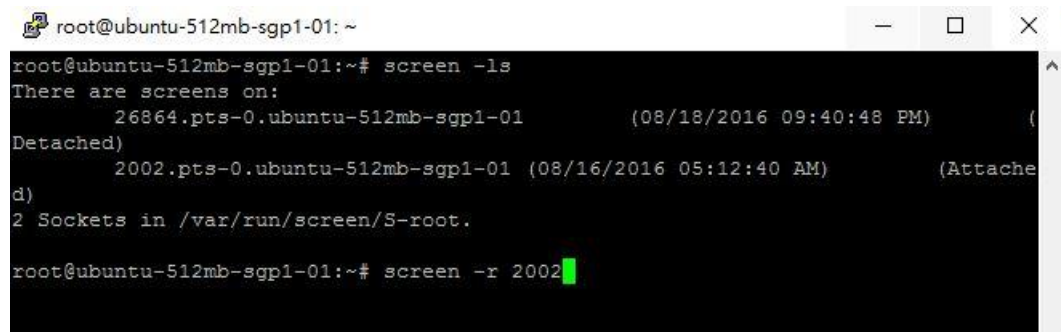
```
root@ubuntu-512mb-sgp1-01:~# screen -ls
There is a screen on:
  2002.pts-0.ubuntu-512mb-sgp1-01 (08/16/2016 05:12:40 AM) (Detache
d)
1 Socket in /var/run/screen/S-root.
root@ubuntu-512mb-sgp1-01:~#
```

Figure 16

- 欲恢復斷線後的工作進程，可以在終端輸入

```
screen -r #工作編號#
```

(例如，`screen -r 2002`，即可恢復先前的工作狀態)



```
root@ubuntu-512mb-sgp1-01:~# screen -ls
There are screens on:
  26864.pts-0.ubuntu-512mb-sgp1-01 (08/18/2016 09:40:48 PM) (
Detached)
  2002.pts-0.ubuntu-512mb-sgp1-01 (08/16/2016 05:12:40 AM) (Attache
d)
2 Sockets in /var/run/screen/S-root.
root@ubuntu-512mb-sgp1-01:~# screen -r 2002
```

Figure 17