Build your own HPC cluster

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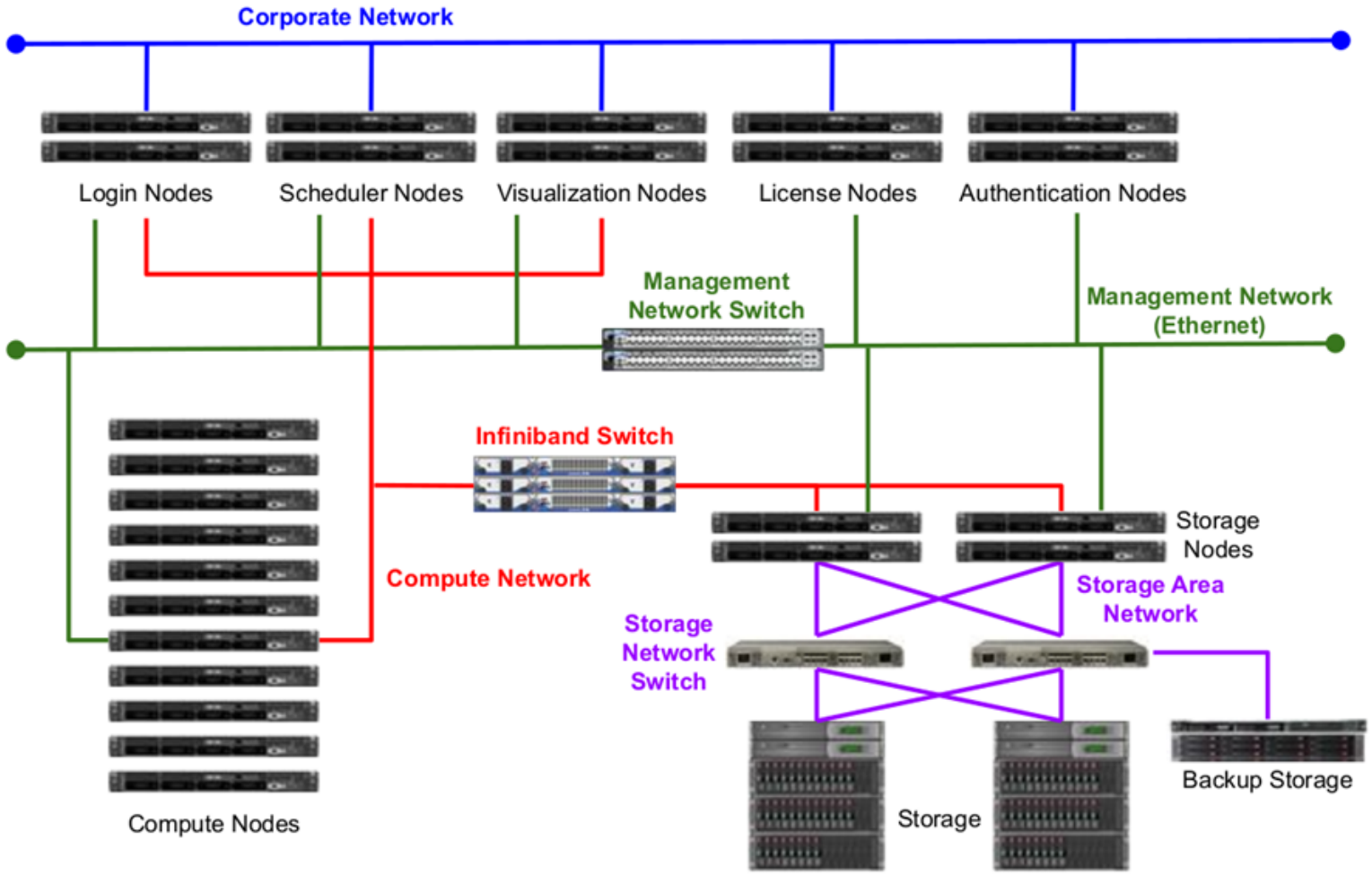
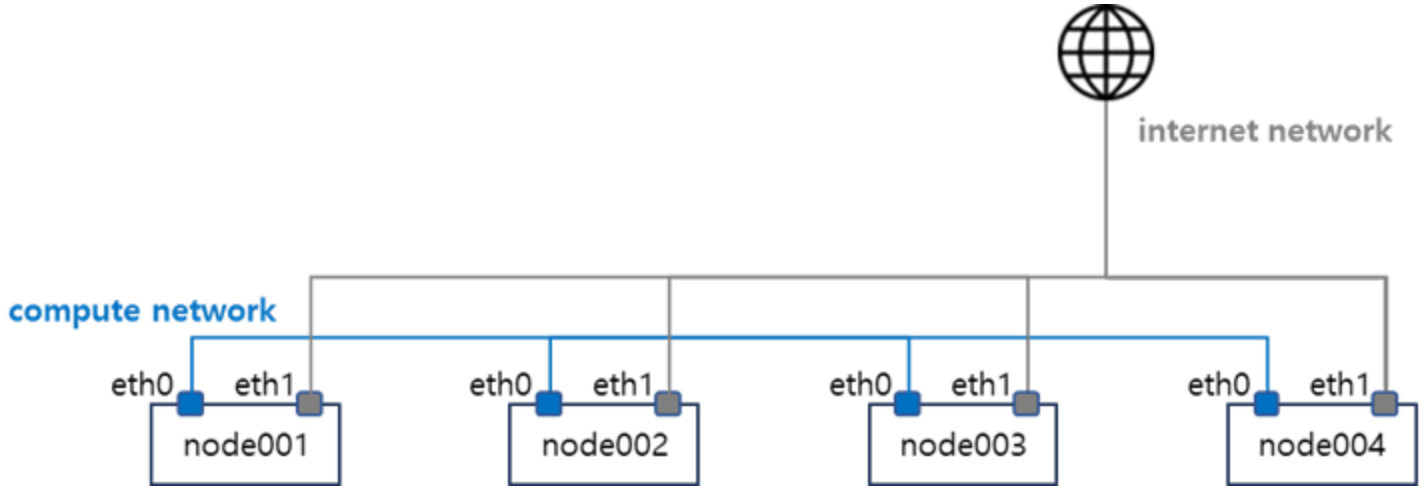
CPO, NEXTFOAM

Typical HPC configuration



1. User / Management Servers
   - Login nodes
     - User login / Job submission
   - Scheduler nodes
     - LSF / PBS / Slurm
   - Visualization nodes
     - NiceDCV / VNC / RD
   - License nodes
   - Authentication nodes
     - LDAP / AD / NIS
2. Compute Nodes
3. Management Network
   - Connects all nodes in the cluster
   - Management / monitoring
4. Compute Network
   - MPI communication & File I/O
5. Mountable Storage System
   - Storage Nodes
     - NFS / Lustre / BeeGFS
   - Storage Area Network
     - Storage system internal network
   - Storage Disk
     - HDD / SSD / FC Disk
6. Backup Storage

Configuration



- All nodes have two NICs (In AWS, one NIC is used)
  - eth0: compute network for MPI and NFS
  - eth1: Internet access for update
- node001 : login, NFS and compute node
- OS : Ubuntu 22.04 server minimal

Launch instances in AWS

- Launch Ubuntu 22.04 instances with public IP address
- Edit inbound rules in the security group
  - Allow ssh access from the internet
  - Allow all inbound traffic between private IP address range
- Record hostnames and IP addresses

hostname	private IP	public IP
node001	-	-
node002	-	-

Headnode setup

Password login for *root*

- Login to headnode using id *ubuntu* and setup *root* password

```
$ sudo passwd
```

- Change account to *root* and enable password login for *root*

```
$ apt-get -y install no vim csh
$ su -

# vi /etc/ssh/sshd_config
PasswordAuthentication yes
PermitRootLogin yes

# systemctl restart sshd
```

- Check that *root* login to headnode using **ssh**

btools for Cluster management

- Install **btools** script in the headnode
  - btools is a series of scripts to automate the execution of commands

```
$ su -
root@node001:~# apt-get -y install git
root@node001:~# cd /root
root@node001:~# git clone https://github.com/zachsnoek/btools
root@node001:~# cd btools
root@node001:~/btools# ./install-btools.sh
root@node001:~/btools# cd /usr/local/sbin
root@node001:/usr/local/sbin# sed -i "s/bin\/sh/bin\/bash/g" *
```

  - In the ubuntu OS, `#!/bin/sh` command in the **btools** files does not work. `#!/bin/sh` to `#!/bin/bash` using **sed** command.

Hostname setup

- Add all hostnames in **/usr/local/sbin/bhosts**

```
root@node001:~# vi /usr/local/sbin/bhosts

node002
node003
...
```

- Append all nodes' ip addresses in **/etc/hosts**

```
root@node001:~# vi /etc/hosts

127.0.0.1 localhost
192.168.200.1 node001
192.168.200.2 node002
```

root login without asking password

- Create a ssh key and copy to all compute nodes for *root* login without password

```
root@node001:~# ssh-keygen -t rsa

root@node001:~# ssh-copy-id root@node002
root@node001:~# ssh-copy-id root@node003
```

- Execute **btools** commands without asking *root* password

```
root@node001:~# bexec hostname

***** node002 *****
node002
***** node003 *****
node003
```

NFS server setup

- Head node **/home** is shared to all compute nodes by NFS
- Install NFS server package and start NFS service in headnode

```
root@node001:~# apt install -y nfs-kernel-server nfs-common
root@node001:~# systemctl enable nfs-server
root@node001:~# systemctl start nfs-server
root@node001:~# systemctl status nfs-server
● nfs-server.service - NFS server and services
```

- Export **/home** to all compute nodes

```
root@node001:~# vi /etc/exports
/home 192.168.200.0/24(rw,no_root_squash)
root@node001:~# exportfs -a
```

192.168.200.0/24 is the ip address range of NFS network. Change your IP range

Compute nodes setup

Sync headnode file to compute nodes

- **bpush** command copies headnode file to all compute nodes

```
bpush <headnode file> <destiation directory>
```

- Copy headnode **/etc/hosts** file to all compute node using **bpush** command

```
root@node001:~# bpush /etc/hosts /etc/
***** node002 *****
***** node003 *****
***** node004 *****
```

- Check **/etc/hosts** file is sync to all compute nodes using **bexec** command

```
root@node001:~# bexec "cat /etc/hosts"
```

NFS client setup

- Install NFS client package in all compute nodes using **bexec**

```
root@node001:~# bexec "apt-get install -y nfs-common"
```

- Check the NFS setup by mount **/home** of headnode

```
root@node001:~# bexec "mount -t nfs node001:/home /home"
root@node001:~# bexec "df | grep home"
***** node002 *****
node001:/home  3844551680        0 3649184768   0% /home
***** node003 *****
node001:/home  3844551680        0 3649184768   0% /home
```

- Edit **/etc/fstab** of all compute nodes to mount at boot time using **bexec**

```
root@node001:~# bexec "sed -i -e '$a node001:\/home \/nome nfs defaults 0 0' /etc/fstab"
```

Additional works

- **/etc/bash.bashrc** of Ubuntu disables non-interactive shell commands by default
  - **mpirun** can not be run in compute nodes
  - **[-z "$PS1"] && return** of **/etc/bash.bashrc** should be commented out
  - Edit **/etc/bash.bashrc** to enable remote command to be executed

```
root@node001:~# sed -i '/&& return/s/^/#/' /etc/bash.bashrc
root@node001:~# bexec "sed -i '/&& return/s/^/#/' /etc/bash.bashrc"
```

- Disable **StrictHostKeyChecking** in all compute nodes

```
root@node001:~# vi /etc/ssh/ssh_config
StrictHostKeyChecking no
root@node001:~# bpush /etc/ssh/ssh_config /etc/ssh/
```

Final work

- Update and install packages in all nodes

```
root@node001:~# apt-get -y update
root@node001:~# apt-get -y install net-tools iputils-ping wget git vim build-essential flex libz-dev csh rsync
root@node001:~# bexec "apt-get update"
root@node001:~# bexec "apt-get -y install net-tools iputils-ping wget git vim build-essential flex libz-dev csh rsync"
```

- Install Intel OneAPI for compilers and MPI for all nodes

```
# wget -O- https://apt.repos.intel.com/intel-gpg-keys/GPG-PUB-KEY-INTEL-SW-PRODUCTS.PUB
| gpg --dearmor | sudo tee /usr/share/keyrings/oneapi-archive-keyring.gpg > /dev/null
# echo "deb [signed-by=/usr/share/keyrings/oneapi-archive-keyring.gpg]
https://apt.repos.intel.com/oneapi all main" | sudo tee /etc/apt/sources.list.d/oneAPI.list
# apt update
# apt install -y intel-basekit intel-hpckit
```

    - Execute above commands using **bexec** for all nodes

User Creation

- Create a user account in head node and assign initial password

```
root@node001:~# adduser nextfoam
```

- Sync the account information to all compute nodes using **bsync**

```
root@node001:~# bsync
```

- Create a MPI hostfile and copy to user's home directory

```
# vi /root/mpihosts
node001:32
node002:32
# cp /root/mpihosts /home/nextfoam
# chown -R nextfoam.nextfoam /home/nextfoam/mpihosts
```

- Send account information and initial password to user by e-mail etc.

What users need to do

- Change password after login

```
nextfoam@node001:~$ passwd
Changing password for nextfoam.
Current password:
New password:
Retype new password:
passwd: password updated successfully
```

- Create a ssh key to access compute nodes

```
nextfoam@node001:~$ ssh-keygen -t rsa
```

- Copy public key **id_rsa.pub** to **authorized_keys** for not password asking

```
nextfoam@node001:~$ cp ~/.ssh/id_rsa.pub ~/.ssh/authorized_keys
```

Questions?