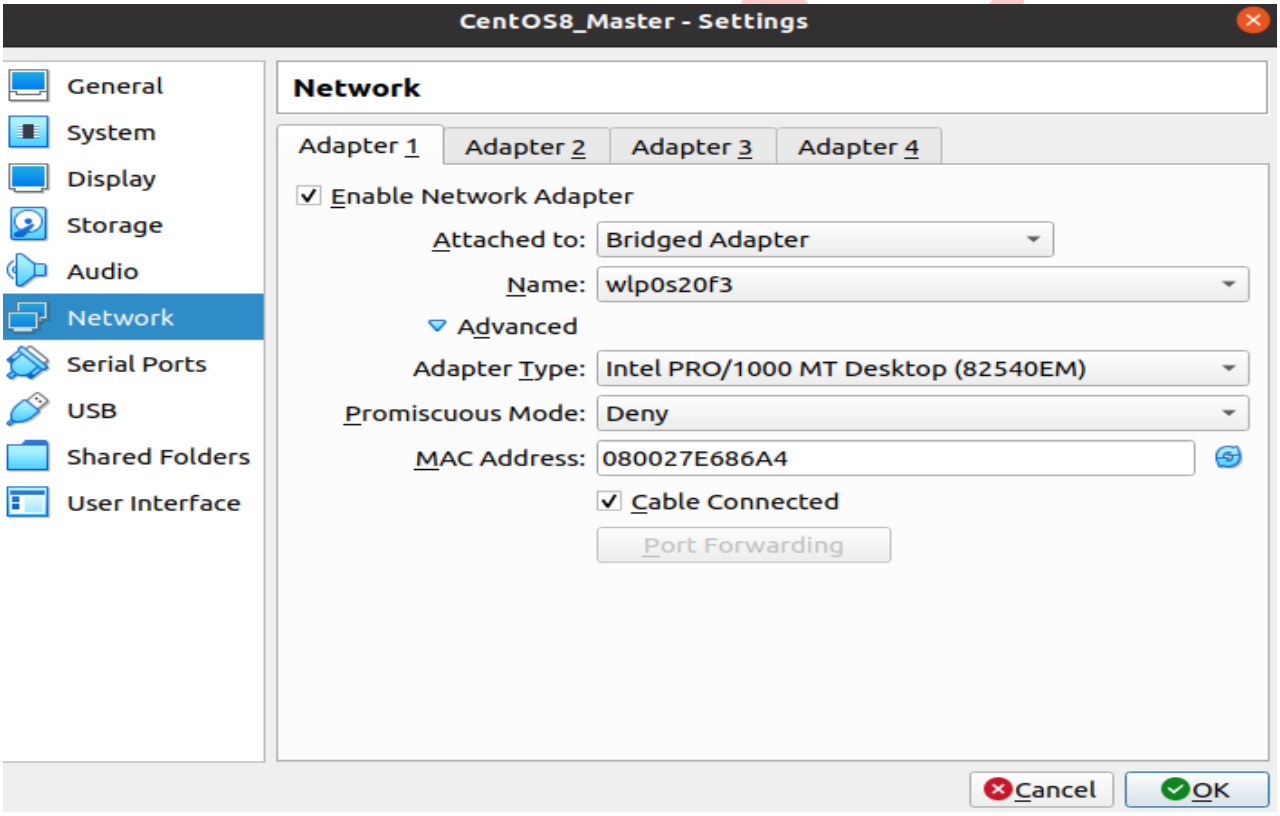
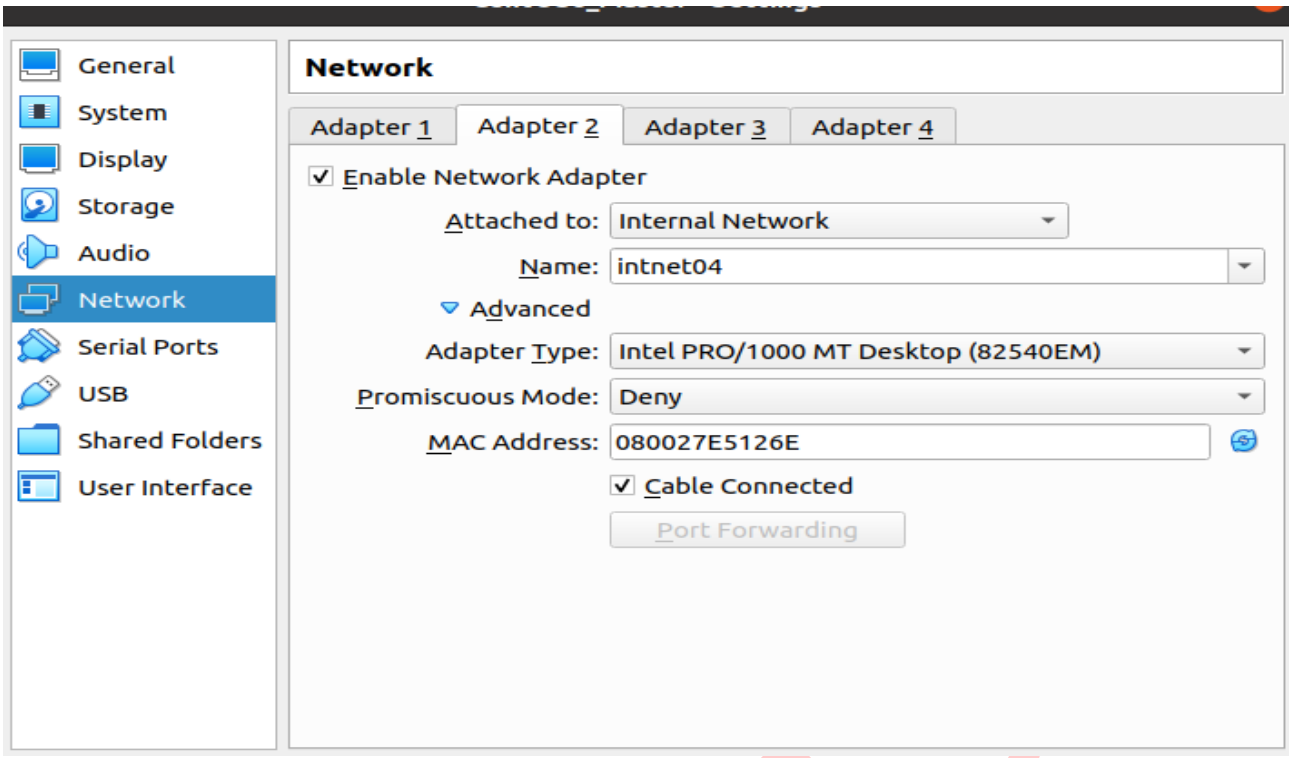
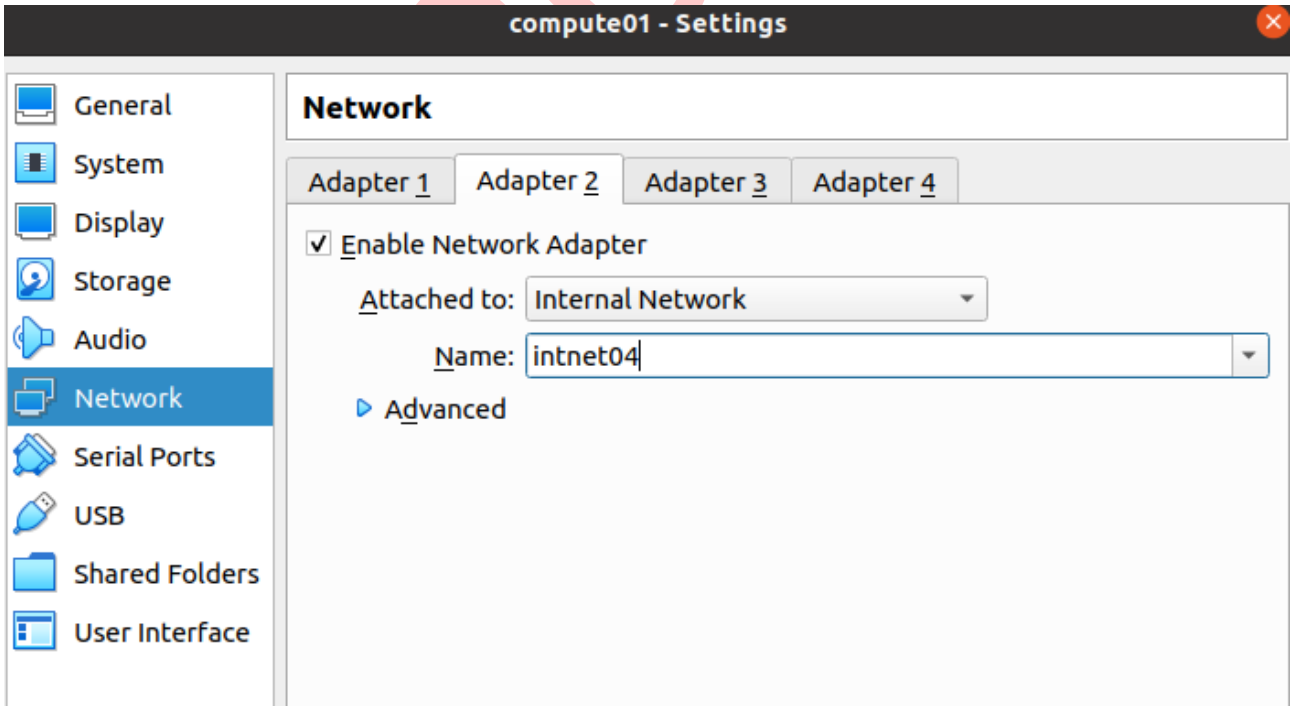
Index -

1. Setup -

1 master and 2 compute node wherein master node has 2 network interfaces, Adapter 1 connected to external network having internet connectivity. Compute nodes are connected to master node using internal network (Adapter 2).




General
System
Display
Storage
Audio
Network
Serial Ports
USB
Shared Folders
User Interface
Network
Adapter 1
Adapter 2
Adapter 3
Adapter 4
Enable Network Adapter
Attached to: Internal Network
Name: intnet04
Advanced
Adapter Type: Intel PRO/1000 MT Desktop (82540EM)
Promiscuous Mode: Deny
MAC Address: 080027E5126E
Cable Connected
Port Forwarding


compute01 - Settings
General
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Serial Ports
USB
Shared Folders
User Interface
Network
Adapter 1
Adapter 2
Adapter 3
Adapter 4
Enable Network Adapter
Attached to: Internal Network
Name: intnet04
Advanced

2. Cluster Setup

setup master node hostname
[root@localhost ~]# hostnamectl set-hostname master1.hpccluster
[root@localhost ~]# hostname master1.hpccluster
[root@localhost ~]# reboot

a) Setup local package repository -
[root@master1Packages]# mkdir -p /media/iso
[root@master1 Packages]# mount -t loop CentOS-8.2.2004-x86_64-dvd1.iso /media/iso
[root@master1 Packages]# cp -r /media/iso/BaseOS /media/iso/AppStream /home /puneet
[root@master1 Packages]# cat /etc/yum.repos.d/CentOS-local-Base.repo
[baseos-local]
name=CentOS local baseos
baseurl=file:///home/puneet/BaseOS
gpgcheck=0
enabled=1
[root@master1 Packages]# cat /etc/yum.repos.d/CentOS-local-Appstream.repo
[appstream-local]
name=CentOS local appstream
baseurl=file:///home/puneet/AppStream
gpgcheck=0
enabled=1
[root@master1 Packages]# dnf install httpd
[root@master1 ~]# dnf install createrepo

Now we change the repository setup , we host all packages on http repository as -
[root@master1 ~]# mkdir -p /var/www/html/centosrepos/PowerTools/Packages
[root@master1 ~]# cd /var/www/html/centosrepos/PowerTools/Packages
[root@master1 ~]# dnf --enablerepo=PowerTools install --downloadonly --downloaddir=Packages lua-devel rrdtool-devel munge-devel perl-Switch
[root@master1 ~]# cd ..; createrepo . ; cd /home/puneet
[root@master1 Packages]# mv AppStream/ BaseOS/ /var/www/html/repos/
[root@master1 Packages]# cat /etc/yum.repos.d/CentOS-local-Base.repo
[baseos-local]
name=CentOS local baseos
baseurl=http://10.5.5.1/centosrepos/BaseOS
gpgcheck=0
enabled=1

[root@master1 Packages]# cat /etc/yum.repos.d/CentOS-local-Appstream.repo
[appstream-local]
name=CentOS local appstream
baseurl=http://10.5.5.1/centosrepos/AppStream
gpgcheck=0
enabled=1
[root@master1 ~]# cat /etc/yum.repos.d/CentOS-PowerTools-local.repo
[PowerTools-local]
name=PowerTools-local
baseurl=http://10.5.5.1/centosrepos/PowerTools

gpgcheck=0
enabled=1
[root@master1 ~]# cat /etc/yum.repos.d/CentOS-local-Slurm.repo
[slurm-local]
name=CentOS local slurm
baseurl=http://10.5.5.1/centosrepos/Slurm
gpgcheck=0
enabled=1

b) Assign static IP address to the master node as-

[root@master1 ~]# cat /etc/sysconfig/network-scripts/ifcfg-enp0s8
TYPE=Ethernet
PROXY_METHOD=none
BROWSER_ONLY=no
BOOTPROTO=static
DEFROUTE=yes
IPV4_FAILURE_FATAL=no
#IPV6INIT=yes
#IPV6_AUTOCONF=yes
#IPV6_DEFROUTE=yes
#IPV6_FAILURE_FATAL=no
#IPV6_ADDR_GEN_MODE=stable-privacy
NAME=enp0s8
DEVICE=enp0s8
ONBOOT=no
IPADDR=10.5.5.1
PREFIX=24

[root@master1 Packages]# systemctl start httpd
[root@master1 ~]# dnf clean all
40 files removed
[root@master1 ~]# dnf update
CentOS local appstream
190 MB/s | 5.7 MB   00:00
CentOS local baseos
195 MB/s | 2.2 MB   00:00
Last metadata expiration check: 0:00:01 ago on Sat 07 Nov 2020 03:30:07 AM EST.
Dependencies resolved.
Nothing to do.
Complete!

[root@master1 ~]# systemctl stop firewalld
[root@master1 ~]# systemctl start httpd

c) Setup a DHCP server for internal network -

[root@master1 ~]# cat /etc/dhcp/dhcpd.conf
option domain-name "hpccluster.org";

default-lease-time 600;
max-lease-time 7200;
log-facility local7;

```
subnet 10.5.5.0 netmask 255.255.255.224 {
  range 10.5.5.3 10.5.5.30;
  option routers 10.5.5.1;
  option broadcast-address 10.5.5.31;
  default-lease-time 600;
  max-lease-time 7200;
}
[root@master1 ~]# systemctl restart dhcpd
```

Setup master node's package repository accesibility for clients -

```
[root@localhost Packages]# scp /etc/yum.repos.d/CentOS-local-Appstream.repo
root@compute01:/etc/yum.repos.d/CentOS-local-Appstream.repo
[root@localhost Packages]# scp /etc/yum.repos.d/CentOS-local-Base.repo
root@compute01:/etc/yum.repos.d/CentOS-local-Base.repo
```

d) Setup NTP server for internal network -

```
[root@master1 ~]# cat /etc/chrony.conf
pool 2.centos.pool.ntp.org iburst
driftfile /var/lib/chrony/drift
makestep 1.0 3
rtcsync
allow 10.5.5.0/24
keyfile /etc/chrony.keys
leapsectz right/UTC
logdir /var/log/chrony

[root@master1 ~]# systemctl start chronyd
[root@master1 ~]# unlink /etc/localtime
[root@master1 ~]# ln  -sf /usr/share/zoneinfo/Asia/Kolkata  /etc/localtime

[root@master1 ~]# ssh 10.5.5.3
root@10.5.5.3's password:
Last login: Sat Nov  7 05:02:07 2020 from 10.5.5.1
[root@compute01 ~]# ln  -sf /usr/share/zoneinfo/Asia/Kolkata  /etc/localtime
[root@compute01 ~]# date
Sat Nov  7 16:09:02 IST 2020
[root@compute01 ~]# timedatectl set-local-rtc true
[root@compute01 ~]# timedatectl set-ntp no
[root@compute01 ~]# timedatectl set-time 15:58:30

 [root@compute01 ~]# cat /etc/chrony.conf
Use public servers from the pool.ntp.org project.
# Please consider joining the pool (http://www.pool.ntp.org/join.html).
#pool 2.centos.pool.ntp.org iburst
pool master1
#server 10.5.5.1
# Record the rate at which the system clock gains/losses time.
driftfile /var/lib/chrony/drift

# Allow the system clock to be stepped in the first three updates
```

```
# if its offset is larger than 1 second.
makestep 1.0 3

# Enable kernel synchronization of the real-time clock (RTC).
rtcsync

# Enable hardware timestamping on all interfaces that support it.
#hwtimestamp *

# Increase the minimum number of selectable sources required to adjust
# the system clock.
#minsources 2

# Allow NTP client access from local network.
#allow 192.168.0.0/16

# Serve time even if not synchronized to a time source.
#local stratum 10

# Specify file containing keys for NTP authentication.
keyfile /etc/chrony.keys

# Get TAI-UTC offset and leap seconds from the system tz database.
leapsectz right/UTC

# Specify directory for log files.
logdir /var/log/chrony

# Select which information is logged.
#log measurements statistics tracking
```

e) Setup name resolution for internal network-

```
[root@master1 ~]# cat /etc/hosts
127.0.0.1   localhost localhost.localdomain localhost4 localhost4.localdomain4
::1         localhost localhost.localdomain localhost6 localhost6.localdomain6
10.5.5.3    compute01 compute01.hpccluster.org
10.5.5.1    master1 master1.hpccluster master.hpccluster.org

[root@compute01 ~]# cat /etc/hosts
127.0.0.1   localhost localhost.localdomain localhost4 localhost4.localdomain4
::1         localhost localhost.localdomain localhost6 localhost6.localdomain6
10.5.5.1    master1 master1.hpccluster master.hpccluster.org
10.5.5.3    compute01 compute01.hpccluster compute01.hpccluster.org
```

f) Setup a shared file system and export to the compute nodes -

```
[root@master1 ~]# dnf install nfs-utils
[root@master1 ~]# systemctl start nfs-server
[root@master1 ~]# exportfs -arv
exporting 10.5.5.0/24:/home

[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "dnf install nfs-utils nfs4-acl-tools -y"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "showmount -e 10.5.5.1"
compute02: Export list for 10.5.5.1:
compute02: /home 10.5.5.0/24
compute01: Export list for 10.5.5.1:
compute01: /home 10.5.5.0/24
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "mount -t nfs  10.5.5.1:/home /home"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "mount |grep nfs"
compute01: sunrpc on /var/lib/nfs/rpc_pipefs type rpc_pipefs (rw,relatime)
compute01: 10.5.5.1:/home on /home type nfs4
(rw,relatime,vers=4.2,rsize=262144,wsize=262144,namlen=255,hard,proto=tcp,timeo=600,retrans=2,sec=sys,cli
entaddr=10.5.5.3,local_lock=none,addr=10.5.5.1)
compute02: sunrpc on /var/lib/nfs/rpc_pipefs type rpc_pipefs (rw,relatime)
compute02: 10.5.5.1:/home on /home type nfs4
(rw,relatime,vers=4.2,rsize=262144,wsize=262144,namlen=255,hard,proto=tcp,timeo=600,retrans=2,sec=sys,cli
entaddr=10.5.5.21,local_lock=none,addr=10.5.5.1)
[root@master1 ~]#
```

g) PDSH installation

wget https://github.com/chaos/pdsh/archive/pdsh-2.34.tar.gz

```
[root@master1 ~]# git clone --recursive --branch pdsh-2.34  https://github.com/chaos/pdsh.git
[root@master1 ~]# cd pdsh
[root@master1 pdsh-pdsh-2.34]# ./bootstrap
[root@master1 pdsh]# ./configure –prefix=/opt/pdsh/2.34
[root@master1 pdsh]# make
[root@master1 pdsh]# make install
[root@master1 pdsh]# export PATH=$PATH:/opt/pdsh/2.34/bin/
[root@master1 ~]# ssh-keygen -t rsa
[root@master1 ~]# ssh-copy-id -i /root/.ssh/id_rsa.pub root@compute01
[root@master1 ~]# ssh-copy-id -i /root/.ssh/id_rsa.pub root@compute02
[root@master1 ~]# scp -r /opt/pdsh/ compute02:/opt
[root@master1 ~]# scp -r /opt/pdsh/ compute01:/opt
```

h) Slurm Setup & installation

```
[root@master1 ~]# cat createusergroup.sh
export MUNGEUSER=1010
groupadd -g $MUNGEUSER munge
useradd  -m -c "MUNGE Uid 'N' Gid Emporium" -d /var/lib/munge -u $MUNGEUSER -g munge  -s
/sbin/nologin munge
export SLURMUSER=1012
groupadd -g $SLURMUSER slurm
useradd  -m -c "SLURM workload manager" -d /var/lib/slurm -u $SLURMUSER -g slurm  -s /bin/bash slurm
[root@master1 ~]# pdcp -Rssh -w compute01,compute02 createusergroup.sh /root/
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "chmod +x ./create.sh"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "/root/create.sh"
[root@master1 ~]# um install munge munge-libs munge-devel -y
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "yum install munge munge-libs munge-devel -y"
[root@master1 ~]# /usr/sbin/create-munge-key
[root@master1 ~]# pdcp -Rssh -w compute01,compute02  /etc/munge/munge.key /etc/munge/
[root@master1 ~]#  cat setpermission.sh
#!/bin/bash
mkdir -p /etc/munge/ /var/log/munge/ /var/lib/munge/ /run/munge/
chown -R munge: /etc/munge/ /var/log/munge/ /var/lib/munge/ /run/munge/
chmod 0700 /etc/munge/ /var/log/munge/ /var/lib/munge/
chmod 0711 /run/munge/
[root@master1 ~]# chmod +x setpermission.sh
[root@master1 ~]# ./setpermission.sh
[root@master1 ~]# pdcp -Rssh -w compute01,compute02 setpermission.sh /root/
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "chmod +x /root/setpermission.sh"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "/root/setpermission.sh"
[root@master1 ~]# systemctl start munge
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "systemctl start munge"
[root@master1 ~]# munge -n | unmunge
[root@master1 ~]#  munge -n | ssh compute02 unmunge
[root@master1 ~]# yum install mariadb-server -y
[root@master1 ~]# cat /etc/my.cnf.d/innodb.cnf
[mysqld]
 innodb_buffer_pool_size=500M
 innodb_log_file_size=32M
 innodb_lock_wait_timeout=1000
[root@master1 ~]# systemctl start mariadb
[root@master1 ~]# mysql_secure_installation
Set root password? [Y/n] Y
New password:
Re-enter new password:
Password updated successfully!
Reloading privilege tables..  ... Success!
Remove anonymous users? [Y/n] Y
Disallow root login remotely? [Y/n] Y
Remove test database and access to it? [Y/n] Y
Reload privilege tables now? [Y/n] Y
[root@master1 ~]# systemctl restart mariadb
[root@master1 ~]# dnf install openssl openssl-devel pam-devel numactl numactl-devel hwloc hwloc-libs hwloc-
devel lua lua-devel lua-libs readline-devel rrdtool ncurses-devel libibmad libibumad python3
```

h) Install dependencies for slurm compilation -

```
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "dnf install openssl openssl-devel pam-devel numactl numactl-devel hwloc hwloc-libs lua lua-libs readline-devel rrdtool ncurses-devel libibmad libibumad python3 bzip2-devel mysql-devel perl-ExtUtils-MakeMaker perl-DBI -y"

[root@master1 ~]# wget https://download.schedmd.com/slurm/slurm-20.02.5.tar.bz2
[root@master1 ~]# rpmbuild -tb slurm-20.02.5.tar.bz2
[root@master1 ~]# mkdir -p /var/www/html/centosrepos/Slurm/Packages
[root@master1 ~]# mv /root/rpmbuild/RPMS/x86_64/*  /var/www/html/centosrepos/Slurm/Packages
[root@master1 ~]#  cd /var/www/html/centosrepos/Slurm/
[root@master1 ~]#  createrepo .
[root@master1 Slurm]# cat /etc/yum.repos.d/CentOS-local-Slurm.repo
[slurm-local]
name=CentOS local slurm
baseurl=http://10.5.5.1/centosrepos/Slurm
gpgcheck=0
enabled=1
[root@master1 Slurm]# pdcp -Rssh -w compute01,compute02 /etc/yum.repos.d/CentOS-local-Slurm.repo /etc/yum.repos.d/
[root@master1 Slurm]# dnf install slurm* perl-Switch*
[root@master1 Slurm]# pdsh -Rssh -w compute01,compute02  "dnf install perl-Switch*  slurm slurm-contribs slurm-devel  slurm-libpmi slurm-openlava slurm-pam_slurm slurm-perlapi slurm-slurmctld slurm-slurmd slurm-slurmdbd slurm-torque slurm-example-configs  cryptsetup-y"
```

setup slurm database daemon service -

```
[root@master1 ~]# mysql -u root -p
 mysql> grant all on slurm_acct_db.* TO 'slurm'@'localhost' identified by 'some_pass' with grant option;
 mysql> create database slurm_acct_db;

[root@master1 ~]# cat /etc/slurm/slurmdbd.conf
 AuthType=auth/munge
  DbdAddr=10.5.5.1
  DbdHost=master1
  SlurmUser=slurm
  DebugLevel=4
  LogFile=/var/log/slurm/slurmdbd.log
  PidFile=/var/run/slurmdbd.pid
  StorageType=accounting_storage/mysql
  StorageHost=master1
  StoragePass=pp
  StorageUser=slurm
  StorageLoc=slurm_acct_db

[root@master1 ~]# systemctl start slurmdbd
[root@master1 ~]# systemctl enable slurmdbd
[root@master1 ~]# systemctl status slurmdbd
```

define cluster configuration -

```
[root@master1 ~]# cat /etc/slurm/slurm.conf
 ClusterName=hpccluster
 ControlMachine=master1
 ControlAddr=10.5.5.1
 SlurmUser=slurm
 AuthType=auth/munge
 ProctrackType=proctrack/linuxproc
 StateSaveLocation=/var/spool/slurmd
 SlurmdSpoolDir=/var/spool/slurmd
 SlurmctldLogFile=/var/log/slurm/slurmctld.log
 SlurmdDebug=3
 SlurmdLogFile=/var/log/slurm/slurmd.log
 AccountingStorageHost=master1
 AccountingStoragePass=pp
 AccountingStorageUser=slurm
 NodeName=compute01 CPUs=1 Sockets=1 RealMemory=320 CoresPerSocket=1 ThreadsPerCore=1
State=UNKNOWN
 PartitionName=INTEL Nodes=compute01 Default=YES MaxTime=INFINITE State=UP

[root@master1 ~]# pdcp -Rssh -w compute01,compute02 /etc/slurm/slurm.conf   /etc/slurm/
[root@master1 ~]# pdcp -Rssh -w compute01,compute02  /etc/slurm/slurmdbd.conf  /etc/slurm/
[root@master1 ~]# cat createlogfiles.sh
#!/bin/bash
mkdir -p /var/spool/slurmctld
mkdir -p /var/spool/slurmd
chown slurm:slurm /var/spool/slurmctld
chown slurm: /var/spool/slurmd
chmod 755 /var/spool/slurmctld
mkdir -p /var/log/slurm
touch /var/log/slurm/slurmctld.log
touch /var/log/slurm/slurm_jobacct.log /var/log/slurm/slurm_jobcomp.log
chown -R slurm:slurm /var/log/slurm/
[root@master1 ~]# ./createlogfiles.sh

[root@master1 ~]# cat createlogfiles_compute.sh
mkdir /var/spool/slurmd
chown slurm: /var/spool/slurmd
chmod 755 /var/spool/slurmd
mkdir /var/log/slurm/
touch /var/log/slurm/slurmd.log
chown -R slurm:slurm /var/log/slurm/slurmd.log
[root@master1 ~]# pdcp -Rssh -w compute01,compute02 /root/createlogfiles_compute.sh  /root/
[root@master1 ~]# pdsh -Rssh -w compute01,compute02  "chmod +x /root/createlogfiles_compute.sh "
[root@master1 ~]# pdsh -Rssh -w compute01,compute02  "/root/createlogfiles_compute.sh "
[root@master1 ~]# slurmd -C
NodeName=master1 CPUs=2 Boards=1 SocketsPerBoard=1 CoresPerSocket=2 ThreadsPerCore=1
RealMemory=1826
[root@master1 ~]# pdsh -Rssh -w compute01,compute02  "systemctl start slurmd"
[root@master1 ~]# systemctl start slurmctld
[root@master1 ~]# sinfo
```

```
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
INTEL*       up   infinite      1   down compute01
INTEL*       up   infinite      1   down compute02
[root@master1 ~]# scontrol update NodeName=compute01 State=RESUME
[root@master1 ~]# scontrol update NodeName=compute02 State=RESUME
[root@master1 ~]# sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
INTEL*       up   infinite      2   idle compute[01-02]
[root@master1 ~]# su - puneet


[puneet@master1 ~]$ srun -p INTEL -n1 --pty /bin/bash
[puneet@compute01 ~]$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
INTEL*       up   infinite      1  alloc compute01
INTEL*       up   infinite      1   idle compute02
[puneet@compute01 ~]$ exit
```

3) setup singularity dependencies on master & compute nodes-

```
[root@master1 ~]# wget https://golang.org/dl/go1.15.4.linux-amd64.tar.gz
[root@master1 ~]# tar -xf go1.15.4.linux-amd64.tar.gz
[root@master1 ~]#  mv go /usr/local/
[root@master1 ~]# export PATH=$PATH:/usr/local/go/bin
[root@master1 ~]# which go
/usr/local/go/bin/go
[root@master1 ~]# pdcp -Rssh -w compute01,compute02 go1.15.4.linux-amd64.tar.gz /root/
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "tar -xf go1.15.4.linux-amd64.tar.gz"
[root@master1 ~]# pdsh -Rssh  -w compute01,compute02 "mv go /usr/local/"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo export PATH=\$PATH:/usr/local/go/bin >>
~/.bashrc'
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo export PATH=\$PATH:/usr/local/go/bin >>
/home/puneet/.bashrc'
[root@master1 ~]# echo 'export PATH=$PATH:/usr/local/go/bin' >> /home/puneet/.bashrc
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo export GOPATH=/usr/local/go >> ~/.bashrc'
[root@master1 ~]# echo 'export GOPATH=/usr/local/go' >> /home/puneet/.bashrc
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo export GOPATH=/usr/local/go >>
/home/puneet/.bashrc'
[root@master1 ~]# echo 'export PATH=/usr/local/go/bin:${PATH}:${GOPATH}/bin' >> ~/.bashrc
[root@master1 ~]#  source ~/.bashrc
```

Setup singularity on master node -

```
[root@master1 ~]# wget https://github.com/hpcng/singularity/archive/v3.6.4.tar.gz
[root@master1 ~]# tar -xf v3.6.4.tar.gz
[root@master1 ~]# cd singularity-3.6.4/
[root@master1 ~]#  dnf groupinstall 'Development Tools'
[root@master1 ~]# git clone https://github.com/sylabs/singularity.git
[root@master1 ~]# cd singularity
[root@master1 ~]# git checkout v3.6.4
[root@master1 ~]# ./mconfig –prefix=/opt/singularity
[root@master1 ~]# make -C ./builddir
[root@master1 ~]# make -C ./builddir install
[root@master1 ~]# pdcp  -r -Rssh -w compute01,compute02  singularity /root/
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "cd  singularity ; ./mconfig --prefix=/opt/singularity"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "cd  singularity ;make C ./builddir clean"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "cd  singularity ;make -C ./builddir"
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 "cd  singularity ;make -C ./builddir install"
[root@master1 ~]# pdcp -r -Rssh -w compute01,compute02 /opt/singularity /opt
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo export PATH=\$PATH:/opt/singularity/bin/ >>
~/.bashrc'
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo export PATH=\$PATH:/opt/singularity/bin/ >>
/home/puneet/.bashrc'
[root@master1 ~]# echo 'export PATH=$PATH:/opt/singularity/bin/' >> /home/puneet/.bashrc
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo source
/opt/singularity/etc/bash_completion.d/singularity >> ~/.bashrc'
[root@master1 ~]# pdsh -Rssh -w compute01,compute02 'echo source
/opt/singularity/etc/bash_completion.d/singularity >> /home/puneet/.bashrc'
```

Testing singularity setup on master node -
[root@master1 ~]# su - puneet
[puneet@master1 ~]$ singularity run library://godlovedc/funny/lolcow

[puneet@master1 ~]$ singularity pull docker://godlovedc/lolcow
INFO: Converting OCI blobs to SIF format
INFO: Starting build...
Getting image source signatures
Copying blob 9fb6c798fa41 done
Copying blob 3b61febd4aef done
Copying blob 9d99b9777eb0 done
Copying blob d010c8cf75d7 done
Copying blob 7fac07fb303e done
Copying blob 8e860504ff1e done
Copying config 73d5b1025f done
Writing manifest to image destination
Storing signatures
INFO: Creating SIF file...

4) Setup a singularity container with netlib HPL & run it on compute node -

[puneet@master1 HH]$ wget https://download.open-mpi.org/release/open-mpi/v4.0/openmpi-4.0.5.tar.gz
[puneet@master1 HH]$ tar -xf openmpi-4.0.5.tar.gz
[puneet@master1 HH]$ cd openmpi-4.0.5/
[puneet@master1 openmpi-4.0.5]$ ./configure --prefix=/home/puneet/MySoftwares/OMPI/4.0.5
[puneet@master1 openmpi-4.0.5]$ make
[puneet@master1 openmpi-4.0.5]$ make install

[puneet@master1 openmpi-4.0.5]$ wget https://github.com/mpitutorial/mpitutorial/tree/gh-pages/tutorials/mpi-hello-world/code/mpi_hello_world.c

singularity pull docker://centos:7.8.2003
[puneet@master1 JJ]$ singularity build centos-base.simg docker://centos:7.8.2003

```
[puneet@master1 ~]$ sudo /opt/singularity/bin/singularity build MyCentos.simg hpl.def
[puneet@master1 ~]$ cat submit.slrm
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks=2
#SBATCH --ntasks-per-node=1
#SBATCH --partition=INTEL
export PATH=$PATH:/home/puneet/MySoftwares/OMPI/4.0.5/bin/
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/puneet/MySoftwares/OMPI/4.0.5/bin/
date
mpirun -np 2 -npernode 1 /opt/singularity/bin/singularity exec /home/puneet/MyCentos.simg
/opt/MyBenchmarks/HPL/2.3/src/hpl-2.3/bin/LinuxGNU/xhpl

[puneet@master1 ~]$ sbatch submit.slrm
[puneet@master1 ~]$ cat slurm-31.out
Thu Nov 19 20:52:45 IST 2020
compute01.hpccluster.org
compute02.hpccluster.org
================================================================================
HPLinpack 2.3  --  High-Performance Linpack benchmark  --   December 2, 2018
Written by A. Petitet and R. Clint Whaley,  Innovative Computing Laboratory, UTK
Modified by Piotr Luszczek, Innovative Computing Laboratory, UTK
Modified by Julien Langou, University of Colorado Denver
================================================================================

An explanation of the input/output parameters follows:
T/V    : Wall time / encoded variant.
N      : The order of the coefficient matrix A.
NB     : The partitioning blocking factor.
P      : The number of process rows.
Q      : The number of process columns.
Time   : Time in seconds to solve the linear system.
Gflops : Rate of execution for solving the linear system.

The following parameter values will be used:

N      :   16000
NB     :     384
PMAP   : Row-major process mapping
P      :       1
Q      :       2
PFACT  :    Left
NBMIN  :       2
NDIV   :       2
RFACT  :    Left
BCAST  :   1ring
DEPTH  :       0
SWAP   : Mix (threshold = 64)
L1     : transposed form
U      : transposed form
EQUIL  : yes
ALIGN  : 8 double precision words

--------------------------------------------------------------------------------

- The matrix A is randomly generated for each test.
- The following scaled residual check will be computed:
      ||Ax-b||_oo / ( eps * ( || x ||_oo * || A ||_oo + || b ||_oo ) * N )
- The relative machine precision (eps) is taken to be               1.110223e-16
- Computational tests pass if scaled residuals are less than                16.0

================================================================================
T/V                N    NB     P     Q               Time                 Gflops
--------------------------------------------------------------------------------
```

```
WR00L2L2       16000   384     1     2             41.59             6.5664e+01
HPL_pdgesv() start time Thu Nov 19 20:54:02

HPL_pdgesv() end time   Thu Nov 19 20:54:43

--------------------------------------------------------------------------------
||Ax-b||_oo/(eps*(||A||_oo*||x||_oo+||b||_oo)*N)=             PASSED
================================================================================

Finished      1 tests with the following results:
              1 tests completed and passed residual checks,
              0 tests completed and failed residual checks,
              0 tests skipped because of illegal input values.
--------------------------------------------------------------------------------

End of Tests.
================================================================================
[puneet@master1 ~]$
```