Introduction to PDC's environment



PDC Center for High Performance Computing Izhar ul Hassan

izhaar@pdc.kth.se

PDC

KTH, Sweden

HPC Summer School 2012

Izhar ul Hassan, PDC [1/26]

Outline

- Ferlin
- How to login
- KTH vetenskap och konst de
- PDC Center for High Performance Computing

- Where to store files
- How to compile and run a program

Clusters at PDC

- Ekman
- Ferlin
- Povel
- Ellen
- PDC Center for High Performance Computing
- Lindgren
- See http://www.pdc.kth.se/ resources/computers

Izhar ul Hassan, PDC [3/26]

Cluster Nodes

- Login nodes don't run jobs here!
- Interactive nodes for test runs; alone or shared among users
- Dedicated nodes (compute nodes) for running final programs



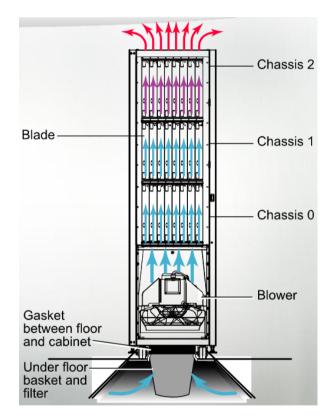


PDC Center for High Performance Computing

Izhar ul Hassan, PDC [4/26]

Lindgren Cabinet

- 3 chassis per cabinet
- 8 blades per chassis
- 4 nodes per blade
- 24 cores per node
- 16 Cabinets, 1516 compute nodes, 36,384 cores





PDC Center for High Performance Computing

Izhar ul Hassan, PDC [5/26]

Ferlin

- 672 Compute nodes
- 8 nodes for login, scheduling and management
- 8 cores, 16 GB of RAM per node
- 40gb of local storage (/scratch) on each node



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [6/26]

Kerberos





PDC Center for High Performance Computing Now this Cerberus had three heads of dogs, the tail of a dragon, and on his back the heads of all sorts of snakes.

- PDC uses ssh together with kerberos for login.
- Kerberos system for authenticating users and services on a network.
- Kerberos server, trusted by users and services.
- A Kerberos principal (*username@NADA.KTH.SE*) is a user's or service's username for a certain Kerberos realm (*NADA.KTH.SE*).

Login from any computer

- You can reach PDC from any computer and network!
- The **Kerberos implementation Heimdal** can be installed on most operating systems (Mac, Windows, Linux)
- An SSH command that knows GSSAPI key-exchange can forward Kerberos tickets
- Names of the commands depend on your operating system!
- Follow the instructions for your operating system: http://www.pdc. kth.se/resources/software/login-1



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [8/26]

Login Set up on Mac

- You can reach PDC from any computer and network!
- The Kerberos implementation Heimdal is already installed on Mac
- ssh already knows how to forward kerberos tickets
- Copy ssh config file and krb5.conf files according to instructions at:
- Follow the instructions for your operating system: http://www.pdc. kth.se/resources/software/login-1/macintosh



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [9/26]

Login Set up on Linux

- You can reach PDC from any computer and network!
- Install Kerberos implementation Heimdal for your version of Linux
- Install ssh that can forward kerberos tickets
- Copy ssh config file and krb5.conf files according to instructions at:
- http://www.pdc.kth.se/resources/software/login-1/ linux/copy_of_index_html



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [10/26]

Login Set up on Windows

- You can reach PDC from any computer and network!
- Install Open source Cygwin or SecureCRT
- Trial version of secureCRT can be downloaded from: http://www. vandyke.com/download/securecrt/download.html
- Follow the instructions at:
- http://www.pdc.kth.se/resources/software/login-1/
 windows/



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [11/26]

Common Kerberos Commands

- kinit proves your identity
- klist list your Kerberos tickets
- kdestroy destroy your Kerberos ticket file
- kpasswd change your Kerberos password

kinit -f -l 7d username@NADA.KTH.SE

klist -Tf

PDC Center for High Performance Computing

Credentials cache : FILE:/tmp/krb5cc 500 Principal: username@NADA.KTH.SE Expires Flags Principal Issued Mar 25 09:45 Mar 25 19:45 FI krbtgt/NADA.KTH.SE@NADA.KTH.SE Mar 25 09:45 Mar 25 19:45 afs/pdc.kth.se@NADA.KTH.SE



Izhar ul Hassan, PDC [12/26]

Login using Kerberos tickets

• Get a forwardable Kerberos ticket on your local system:

kinit -f -l 7d username@NADA.KTH.SE

• Forward your ticket via ssh:



PDC Center for High Performance Computing

- ssh -l username ferlin.pdc.kth.se
- The prompt changes when logged in. Check your tickets on the remote system:

klist -Tf

You have reached the login node

File Systems

- scratch node local, temporary
- AFS home directories accessible from anywhere, with backup



AFS

- Your **Home Directory** Your home directory is located in AFS.
- When you login you arrive in your AFS home directory.
- The path to your PDC AFS home directory is /afs/pdc.kth.se/home/u/user
- Some pre-existing files and folders to keep: .bashrc .forward Public
 Private . . .
- Oldfiles contain your home directory, as it was yesterday, i.e. a backup.



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [15/26]

Modules

 Modification of the user's environment; handles PATH, MANPATH ... module avail - show available modules module show modulename - Display information about modulename module load modulename module list - Show loaded modules

• Common PDC modules are: easy, afsws and heimdal.



How to run

- Interactive Jobs
- Batch Jobs



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [17/26]

Login to Interactive Nodes

- Login to Ferlin as shown in previous slide
- Find out which are interactive nodes on Ferlin: module add easy spusage | grep interactive
- You will get a list of interactive nodes.
- Open a new terminal and login to one of the nodes from the list e.g.:
 - ssh -l yourUsername k09n40.pdc.kth.se
- You can login to other interactive nodes



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [18/26]

Running a Serial Job on an Interactive Node

- Get a Kerberos ticket on your local computer kinit -f -1 7d username@NADA.KTH.SE
- Login on one of the *interactive* node on Ferlin as shown on previous slide
- Go to the directory where your programs reside
- Compile:

```
gfortran hello_serial.f90 -o hello_serial_f90
gcc hello_serial.c -o hello_serial_c
```

- Run:
 - ./hello_serial_f90
 - ./hello_serial_c



Running an MPI job on Interactive Node

- Get Kerberos tickets on your local computer (using kinit)
- Login to Ferlin (using ssh command)
- Find which are interactive nodes
- Login to one of the interactive nodes
- Go to the directory where your programs reside mpif90 hello_mpi.f90 -o hello_mpi_f90 mpicc hello mpi.c -o hello mpi c
- Run:

mpirun -np 8 -machinefile \$SP_HOSTFILE hello_mpi_f90
mpirun -np 8 -machinefile \$SP_HOSTFILE hello_mpi_c

• For more information on how to run your jobs, please visit:

http://www.pdc.kth.se/resources/computers/ferlin/
how-to



Job script

```
#!/bin/bash
module add mpi
processes_per_node=8
total_processes=`expr $processes_per_node \* $SP_PROCS`
PRG="$1"
shift
ARGS="$*"
mpirun -np $total_processes -machinefile $SP_HOSTFILE $PRG $ARGS
```

PDC Center for High Performance Computing

- Submit the job on 4 dedicated nodes by using the command!
- esubmit -n 4 ./helloWorldScript

Izhar ul Hassan, PDC [21/26]

When does my job start on Dedicated Nodes

- Many users continuously submit jobs to Ferlin
- Each job needs a certain time and a number of nodes/cores to run
- The queue system (scheduler) keeps track of the submitted jobs and when, and where, each job can run on the cluster
- Every user belongs to at least one time allocation on a cluster. You belong to the time allocation edu13.SG2224
- A time allocation states how many node hours per month you have on a specific cluster.



PDC Center for High Performance Computing

Izhar ul Hassan, PDC [22/26]

Common Mistakes

- Please do not run your jobs on the Login Node.
- Make sure your tickets are long enough to run your job and copy your output.
- Do not forget to add the required module when you login.



Finding Information

- man, -help, -h, apropos ...
- http://www.pdc.kth.se/education/tutorials/summerschool



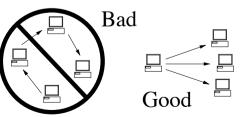
- Flash News
- Mailinglists
- Course assistants
- support@pdc.kth.se

Important!

REMEMBER! You are NOT allowed to write your password on any computer that you are remotely connected to!!!. If you expose your password you endanger not only your own work, you are putting all other cluster users at risk.



- Once you have your local Kerberos ticket you never need to type your password again!
- Get forwardable Kerberos tickets (pass the -f flag to kinit).
- Kerberos enabled software knows to forward/use local Kerberos tickets for remote authentication.
- Forward your forwardable tickets when opening a remote connection.



Thank you for listening!



PDC Center for High Performance Computing

HPC Summer School 2012

Izhar ul Hassan, PDC [26/26]