Farber HPC Tutorial Series

Farber HPC Basics

Objectives

- Overview: Farber Community Cluster
- Part I: Get your feet wet
- Part II: Jump in

Overview: Farber HPC Basics

Farber Community Cluster

http://docs.hpc.udel.edu/clusters/farber/start

Background

What is the Farber cluster?

- It is the second UD community cluster
- Technical and financial partnership between UD-IT and UD faculty and researchers

Who can use it?

- UD faculty and researchers who purchased compute nodes (stakeholders)
- Researchers sponsored by a stakeholder

Farber Cluster

farber.hpc.udel.edu

Part I: Farber HPC Basics

Getting your feet wet

Getting your feet wet

- Accounts
- Connecting with SSH
- Bash Shell and Working Directory
- File Storage
- Groups and Workgroup(s)
- VALET
- Compiling and Running Jobs
- Help

Accounts

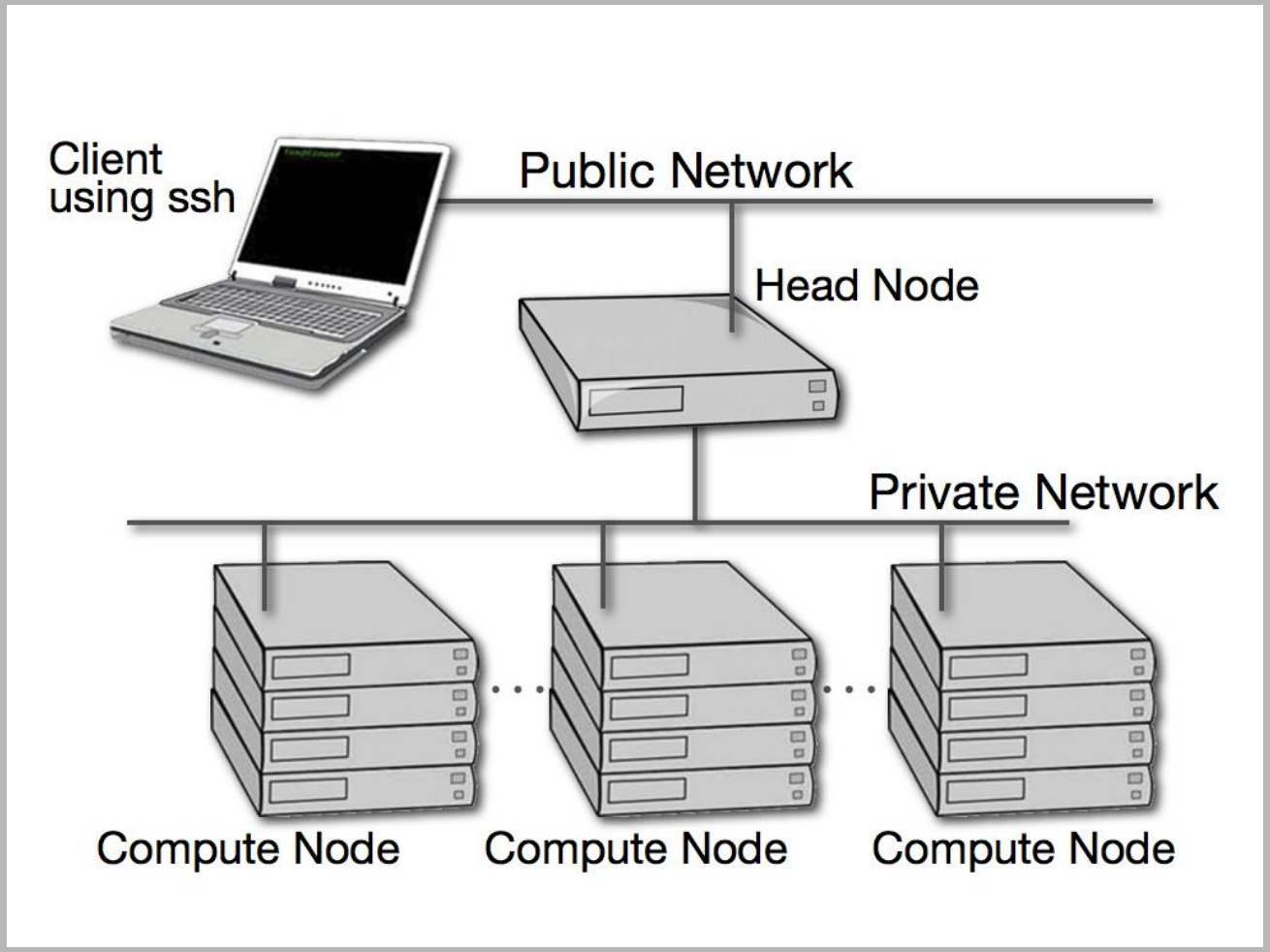
Farber Accounts

Username and Password

- UD = UDelNet ID and password; can only be changed via the on the Network page.
  www.udel.edu/network
- non-UD = `hpcguest<`***uid***`>` and password is generated by IT staff and securely sent via the UD Dropbox; please change it using:
  www.hpc.udel.edu/user?authn=login

Connecting with SSH

Overview


Client
using ssh
Public Network
Head Node
Private Network
Compute Node
Compute Node
Compute Node

SSH Client

- SSH is typically used to connect to the cluster's head (login) node.
- Standard Linux and Mac distributions provide an ssh client.
- Windows distributions require installation of an ssh client such as PuTTY.

SSH Public/Private Keys

- Eliminates entering your password for each remote connection - only need to remember a passphrase of your choice
- More convenient and efficient especially with other applications such as scp and sftp

SSH Help

- Follow documentation for Mac and Linux, or Windows configuration to get connected using X11 and SSH with public/private keys.

  http://www.udel.edu/it/research/training/config_laptop/

Connecting to Farber

`ssh -Y` ***username***`@farber.hpc.udel.edu`

```
Using username "traine".

..........................................................

    Farber cluster (farber.hpc.udel.edu)

    This computer system is maintained by University of
    Delaware IT.  Links to documentation and other online
    resources can be found at:

      http://farber.hpc.udel.edu/

    For support, please contact consult@udel.edu

..........................................................
```

Bash Shell and Working Directory

Bash Shell

Bash prompt

- user name = referred to as `$USER`
- cluster name = head (login) node
- `~` = current working directory
- `$` = end of prompt

```
[traine@farber ~]$
```

Working Directory

At login, you start in your home directory (~)

- `/home/<`***uid***`>`
- Referred to as `$HOME`

```
[traine@farber ~]$ pwd
/home/1201
[traine@farber ~]$ echo $HOME
/home/1201
```

File Storage

File Storage on Farber

- Home directory (`/home`)

Other file storage available:

- Lustre (`/lustre/scratch`)
- Node-local scratch (`/scratch`)

Groups and Workgroups

Farber Groups

Group names determine access level to specific system resources

`groups`

- ***Class category*** = everyone, ud-users, hpc-guests, facstaff, students, stakeholders
- ***Investing-entity category*** = represents a unique group name (*workgroup*) for stakeholders and its sponsored users (e.g., `it_css`)

```
[traine@farber ~]$ groups
everyone students ud-users it_css
```

Workgroup(s)

Groups in the ***investing-entity category*** are used to control access to compute nodes, queues and storage.

`workgroup -g <`***investing_entity***`>`

starts a new shell in your workgroup. You must set your workgroup to run a job on the cluster.

```
[traine@farber ~]$ workgroup -q workgroups
 1002  it_css
[traine@farber ~]$ workgroup -g it_css
[(it_css:traine)@farber it_css]$ echo $WORKDIR
/home/work/it_css
```

VALET

VALET

- UD-developed software to help configure your environment for all IT-installed software packages.
- Changes environment such as `PATH`, `LD_LIBRARY_PATH` and `MANPATH`
- Changes software development environment such as `LDFLAGS` and `CPPFLAGS`
- An alternative to the Modules software used at other HPC sites
- Users can also install their own software and create a VALET package for it.

VALET Commands

`vpkg_list`

- a list of all available software packages installed by IT

```
Available packages:
  in /opt/shared/valet/2.0/etc
        acml
        acpype
        apache-ant
        arcgis
        atlas
        blacs
...
...
```

- a web page of all software packages and descriptions derived from VALET
  http://farber.hpc.udel.edu/software.php

VALET Commands

`vpkg_versions <package_id>`

- a list of versions available for <*package_id*>
- default version marked with *

```
[traine@farber ~]$ vpkg_versions intel
Available versions in package (* = default version):

[/opt/shared/valet/2.0/etc/intel.vpkg_json]
intel             Intel Compiler Suite
  2013-sp1.3.174  Version 2013 (SP1.3.174) for x86-64
  2013            alias to intel/2013-sp1.3.174
  2015.0.090      Version 2015 (first release) for x86-64
* 2015            alias to intel/2015.0.090
  14.0.3          alias to intel/2013-sp1.3.174
```

VALET Commands

`vpkg_require <package_id>`
`vpkg_devrequire <package_id>`

- set your environment or development environment for <*package_id*>

```
[(it_css:traine)@farber ~]$ vpkg_require intel
Adding package `intel/2015.0.090` to your environment
[(it_css:traine)@farber ~]$
```

```
[(it_css:traine)@farber ~]$ vpkg_devrequire intel
Adding package `intel/2015.0.090` to your environment
[(it_css:traine)@farber ~]$
```

VALET Commands

`vpkg_rollback all`

- undo all changes to your environment

```
[(it_css:traine)@farber ~]$ vpkg_rollback all
[(it_css:traine)@farber ~]$
```

Compiling and Running Jobs

Compilers

There are three 64-bit compiler suites on Farber:

- gcc (GNU compiler suite)
- Intel Composer SE
- PGI (Portland Group Inc.’s Cluster Development Kit)

We generally recommend that you use the gcc compilers with its rich collection of tools and libraries. If your software/application has a proven Intel/Xeon configuration, then you will get better performance by choosing the intel SE compiler suite. Intel Fortran, `ifort`, is a better implementation of modern Fortran standards than `gfortran`.

Running Applications

In general, applications should be run on the compute nodes, not on the login (head) node.

- Use VALET to set up your runtime environment; should be similar to your compile-time environment.
- Use Grid Engine's `qlogin` or `qsub` to submit an interactive or batch job to run your applications.

C and Fortran Examples

C and Fortran program examples

- `cmatmul` and `fmatmul`

Compile scripts for each compiler

- `compile-gcc` and `compile-intel`

Batch scripts for each compiler

- `serial-gcc.qs` and `serial-intel.qs`

Copy Examples

```
cp -r ~trainf/fhpcI .
cd fhpcI
pwd
ls
```

```
[traine@farber ~]$ cp -r ~trainf/fhpcI .
[traine@farber ~]$ cd fhpcI/
[traine@farber fhpcI]$ pwd
/home/1201/fhpcI
[traine@farber fhpcI]$ ls
cmatmul  fmatmul
```

Compiling Code

Compiling Code: system cc

- Programs can be compiled on the login (head) node or compute nodes.
- Use VALET to set up your compile-time environment

This example uses the system compiler (gcc) to compile a C program to create the executable `tmatmul-gcc`

```
[traine@farber fhpcI]$ cd cmatmul
[traine@farber cmatmul]$ ls *.c
tmatmul.c
[traine@farber cmatmul]$ vpkg_require gcc
Adding package `gcc/system` to your environment
[traine@farber cmatmul]$ make tmatmul
cc     tmatmul.c   -o tmatmul
[traine@farber cmatmul]$ mv tmatmul tmatmul-gcc
[traine@farber cmatmul]$ ls -la tmatmul*
-rw-r--r-- 1 traine everyone  818 Sep 24 17:07 tmatmul.c
-rwxr-xr-x 1 traine everyone 8860 Sep 28 22:26 tmatmul-gcc
```

Compiling Code: intel icc

- Programs can be compiled on the login (head) node or compute nodes.
- Use VALET to set up your compile-time environment

This example uses a script, `compile-intel`, which has the commands to make an Intel version executable `tmatmul-intel`

```
[traine@farber cmatmul]$ . compile-intel
Adding package `intel/2015.0.090` to your environment
icc -Wall -g -debug all   tmatmul.c   -o tmatmul
debug executable in ./tmatmul-intel
[traine@farber cmatmul]$ ls -la tmatmul*
-rw-r--r-- 1 traine everyone  818 Sep 24 17:07 tmatmul.c
-rwxr-xr-x 1 traine everyone 8860 Sep 28 22:26 tmatmul-gcc
-rwxr-xr-x 1 traine everyone 8781 Sep 28 22:28 tmatmul-intel
```

Running Jobs

Running Jobs

- Interactively using `qlogin`

  Grid Engine will submit an interactive job to the queuing system.

- Batch using `qsub` <***job_script***>
  Grid Engine will submit batch job <***job_script***> to the queuing system

Interactive (session) job

`qlogin`

```
[traine@farber cmatmul]$ workgroup -g it_css
[(it_css:traine)@farber cmatmul]$ qlogin
Your job 484 ("QLOGIN") has been submitted
waiting for interactive job to be scheduled ...
Your interactive job 484 has been successfully scheduled.
Establishing /opt/shared/univa/local/qlogin_ssh session to host n038 ...
```

Interactive Run

Run `tmatmul-gcc` on a compute node and exit

```
[(it_css:traine)@n038 cmatmul]$  vpkg_require gcc
Adding package `gcc/system` to your environment
[(it_css:traine)@n038 cmatmul]$ ./tmatmul-gcc
B:
        1.00000         1.00000         1.00000
        1.00000         1.50000         2.25000
        1.00000         2.00000         4.00000
        1.00000         3.00000         9.00000
C:
        1.00000         0.00000
        0.00000         1.00000
        0.50000         0.50000
B*C with loops:
        1.50000         1.50000
        2.12500         2.62500
        3.00000         4.00000
        5.50000         7.50000
[(it_css:traine)@n038 cmatmul]$ exit
exit
Connection to n038 closed.
/opt/shared/univa/local/qlogin_ssh exited with exit code 0
```

Batch Job

`qsub` <***job_script***>

- Sample <***job_script***> was copied from `/opt/templates/gridengine/serial.qs` and modified as `serial-gcc.qs`

```
[(it_css:traine)@farber cmatmul]$ qsub serial-gcc.qs
Your job 410 ("serial-gcc.qs") has been submitted
```

Batch job output

```
[(it_css:traine)@farber cmatmul]$ cat *.o410

[CGROUPS] UD Grid Engine cgroup setup commencing
[CGROUPS] Setting 1073741824 bytes (vmem 1073741824 bytes) on n036 (master)
[CGROUPS]   with 1 core = 0
[CGROUPS] done.

Adding package `gcc/system` to your environment
B:
        1.00000         1.00000         1.00000
        1.00000         1.50000         2.25000
        1.00000         2.00000         4.00000
        1.00000         3.00000         9.00000
C:
        1.00000         0.00000
        0.00000         1.00000
        0.50000         0.50000
B*C with loops:
        1.50000         1.50000
        2.12500         2.62500
        3.00000         4.00000
        5.50000         7.50000
```

Batch Job template

`qsub <`***job_script***`>`

- Sample <***job_script***> was copied from `/opt/templates/gridengine/serial.qs` and modified as `serial-intel.qs`

```
#$ -m eas
#$ -M <your email address>
vpkg_require intel/2015
./tmatmul-intel
```

```
[(it_css:traine)@farber cmatmul]$ qsub serial-intel.qs
Your job 485 ("serial-intel.qs") has been submitted
```

Batch Job Script

serial-intel.qs

```
[(it_css:traine)@farber cmatmul]$ more serial-intel.qs
#
# Template:  Basic Serial Job
# Revision:  $Id: serial.qs 523 2014-09-16 14:29:54Z frey $
#
# Change the following to #$ and set the amount of memory you need
# per-slot if you're getting out-of-memory errors using the
# default:
# -l m_mem_free=2G
#
# If you want an email message to be sent to you when your job ultimately
# finishes, edit the -M line to have your email address and change the
# next two lines to start with #$ instead of just #
# -m eas
# -M my_address@mail.server.com
#

# Add vpkg_require commands after this line:
vpkg_require intel/2015

# Now append all of your shell commands necessary to run your program
# after this line:
./tmatmul-intel
[(it_css:traine)@farber cmatmul]$
```

Batch Run Output

Output in <*job_script*>.o<*job_id*>

```
[(it_css:traine)@farber cmatmul]$ more serial-intel.qs.o485

[CGROUPS] UD Grid Engine cgroup setup commencing
[CGROUPS] Setting 1073741824 bytes (vmem 1073741824 bytes) on n038 (master)
[CGROUPS]   with 1 core = 0
[CGROUPS] done.

Adding package `intel/2015.0.090` to your environment
B:
        1.00000         1.00000         1.00000
        1.00000         1.50000         2.25000
        1.00000         2.00000         4.00000
        1.00000         3.00000         9.00000

 <Same C: as above>

B*C with loops:
        1.50000         1.50000
        2.12500         2.62500
        3.00000         4.00000
        5.50000         7.50000
```

Exercise

Exercise

- Pick a compiler: gcc or intel
- Compile and batch run the Fortran example in `fmatmul` using
  `compile-<`***compiler***`>` to compile
  `serial-<`***compiler***`>.qs` to batch run

Example using Fortran program to create the executable `tmatmul-gcc` using the system gfortran (gcc) compiler

```
[(it_css:traine)@farber cmatmul]$ cd ~/fhpcI/fmatmul
[(it_css:traine)@farber fmatmul]$ pwd
/home/1201/fhpc/fmatmul
[(it_css:traine)@farber fmatmul]$
```

Compile Code

- create `tmatmul-gcc` fortran executable

`source compile-gcc`

```
[(it_css:traine)@farber fmatmul]$ more compile-gcc
vpkg_rollback all
vpkg_devrequire gcc
export FC=gfortran
export FFLAGS='-ffree-form -Wall -g'
make tmatmul &&  mv tmatmul tmatmul-gcc
test -x tmatmul-gcc && echo "debug version in ./tmatmul-gcc"
```

Batch Job Run

- Submit a job to run the fortran executable `tmatmul-gcc`

```
qsub serial-gcc.qs
```

```
[(it_css:traine)@farber fmatmul]$ qsub serial-gcc.qs
Your job 612 ("serial-gcc.qs") has been submitted
[(it_css:traine)@farber fmatmul]$
```

Batch Job Output

```
[(it_css:traine)@farber fmatmul]$ more serial-gcc.qs.o612

[CGROUPS] UD Grid Engine cgroup setup commencing
[CGROUPS] Setting 1073741824 bytes (vmem 1073741824 bytes) on n038 (master)
[CGROUPS]   with 1 core = 0
[CGROUPS] done.

Adding package `gcc/system` to your environment
 B:
        1.0000          1.0000          1.0000
        1.0000          1.5000          2.2500
        1.0000          2.0000          4.0000
        1.0000          3.0000          9.0000
 C:
        1.0000          0.0000
        0.0000          1.0000
        0.50000         0.50000
 B*C with intrinsic matmul
        1.5000          1.5000
        2.1250          2.6250
        3.0000          4.0000
        5.5000          7.5000
 B*C  with loops
        1.5000          1.5000
        2.1250          2.6250
        3.0000          4.0000
        5.5000          7.5000
```

Need Help?

- **Submit** a Research Computing Help Request form; *High Performance Computing*; *Farber Cluster*
- **Phone**: (302) 831-6000
- **Text**: (302) 722-6820

Part II: Farber HPC Basics

Jumping in

Jumping in

- File Storage and recovery options
- Bash startup files
- Compiling, Running and Monitoring Jobs
- Local (non-standard) Commands

File Storage

File Storage on Farber

- Home directory 72 TB of usable space
  - Personal directory: 20GB (`/home/<`***uid***`>`)
    `df -h $HOME`
  - Workgroup directory: 1TB+
    (`/home/work/<`***investing-entity***`>`)
    `df -h $WORKDIR`
- Lustre ~288 TB of usable space
  - Public scratch directory (`/lustre/scratch`)
  - IT staff will run regular cleanup procedures to purge aged files or directories
- Node-local scratch (`/scratch`)

Recovery Options

Recovering files /home

`/home` filesystem is a larger permanent storage with snapshots.

- Use read-only `$HOME/.zfs/snapshot` to recover files

```
[traine@farber cmatmul]$ ls -al tmatmul.c
-rw-r--r-- 1 traine everyone 818 Sep 24 17:07 tmatmul.c
[traine@farber cmatmul]$ rm tmatmul.c
[traine@farber cmatmul]$ $ echo 'oops !!' && ls -al tmatmul.c
oops !!
ls: cannot access tmatmul.c: No such file or directory
[traine@farber cmatmul]$ pwd
/home/1201/fhpcI/cmatmul
[(it_css:traine)@farber fmatmul]$ ls ~/.zfs/snapshot
12  18  Fri  Mon  now  prev  prev-1  Sat  Sun  Thu  Tue  Wed
[traine@farber cmatmul]$ cp -p ~/.zfs/snapshot/now/fhpcI/cmatmul/tmatmul.c .
[traine@farber cmatmul]$ ls -al tmatmul.c
-rw-r--r-- 1 traine everyone 818 Sep 24 17:07 tmatmul.c
```

Recovering workgroup files

Workgroup files have their own read-only snapshots, which also span a week in `$WORKDIR/.zfs/snapshot`

```
[traine@farber cmatmul]$ workgroup -g it_css
[(it_css:traine)@farber cmatmul]$ ls $WORKDIR/.zfs/snapshot/
12  18  Fri  Mon  now  prev  prev-1  Sat  Sun  Thu  Tue  Wed
```

Bash Startup Files

Keep startup files clean

- Make sure you understand what your startup files are doing.
- Environments are different for the login (head) node versus the compute nodes.
- If you make changes, test by starting a new login, don't logout.
- You can always restore your startup files to the system versions.

Startup files

- `.bash_profile`
- `.bashrc`
- `.bash_udit`
- `.bash_logout`

.bash_profile

- Executed once at login
- `.bashrc` in your home directory is sourced
- Add lines to set your environment and start programs after the comment line in red

```
[traine@farber ~]$ more .bash_profile
# .bash_profile

# Get the aliases and functions
if [ -f ~/.bashrc ]; then
        . ~/.bashrc
fi

# User specific environment and startup programs

PATH=$PATH:$HOME/bin

export PATH
```

.bashrc

- Executed by each new shell, including your login shell via `.bash_profile`
- Add lines to create aliases and bash functions after the comment line in red

```
[(it_css:traine)@farber ~]$ more .bashrc
# .bashrc

# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi

# User specific aliases and functions
```

.bash_udit

- Executed by each new shell
- Opt into IT suggested environment changes

```
##
## Change from "no" to "yes" to enable IT's suggested environment changes.
## The behaviors enabled by the remainder of this file are contingent on
## enabling IT_WANT_ENV_EXTENSIONS:
##
IT_WANT_ENV_EXTENSIONS="no"
```

.bash_udit

- Executed by each new shell
- Opt into IT suggested environment changes

```
##
## If you have multiple workgroups available to you, change this to the one
## you want to be the default; otherwise, the first one listed by
## "workgroup -q workgroups" will be your default:
##
IT_DEFAULT_WORKGROUP=""

##
## If you want the "workgroup" command to by default change your working
## directory to the $WORKDIR, change from "no" to "yes".
##
IT_WORKGROUP_CHDIR="no"
```

.bash_udit

- Executed by each new shell
- Opt into IT suggested environment changes

```
##
## By default when you login to the cluster head node you are in the
## "everyone" group and need to issue a "workgroup" command to prepare
## for submitting jobs, etc.
##
## Change this flag from "no" to "yes" if you want your login shell to
## automatically issue the command to change into your default
## workgroup.  Your default workgroup will come from IT_DEFAULT_WORKGROUP
## if set above, or it will be the first group in the list produced by
## the command
##
##   /opt/bin/workgroup --query workgroups
##
IT_SET_WORKGROUP_ON_LOGIN="no"
```

.bash_logout

- Executed at logout from the head (login) node, not the compute node when you use `qlogin`

```
[(it_css:traine)@farber ~]$ more .bash_logout
# ~/.bash_logout
```

Restore your startup files

To restore all your startup files (`.bashrc`, `.bash_profile`, `.bash_udit`, and `.bash_logout`) to the system default, type

```
cp /etc/skel/.bash* $HOME
```

Exercise (.bash_udit)

Exercise (.bash_udit)

Customize our startup file `.bash_udit` to opt into IT suggested environment changes by setting a default workgroup so we only need to type

```
workgroup
```

instead of

```
workgroup -g <investing_entity>
```

Exercise (.bash_udit)

To see what aliases are defined use

```
alias
```

```
[(it_css:traine)@farber ~]$ alias
alias l.='ls -d .* --color=auto'
alias ll='ls -l --color=auto'
alias ls='ls --color=auto'
alias mc='. /usr/libexec/mc/mc-wrapper.sh'
alias vi='vim'
alias which='alias | /usr/bin/which --tty-only --read-alias --show-dot --show-
tilde'
[(it_css:traine)@farber ~]$
```

Exercise (.bash_udit)

Edit (vim) `.bash_udit`

```
[(it_css:traine)@farber ~]$ vim .bash_udit
##
## Change from "no" to "yes" to enable IT's suggested environment changes.
## The behaviors enabled by the remainder of this file are contingent on
## enabling IT_WANT_ENV_EXTENSIONS:
##
IT_WANT_ENV_EXTENSIONS="yes"

##
## If you have multiple workgroups available to you, change this to the one
## you want to be the default; otherwise, the first one listed by
## "workgroup -q workgroups" will be your default:
##
IT_DEFAULT_WORKGROUP="it_css"

##
## If you want the "workgroup" command to by default change your working
## directory to the $WORKDIR, change from "no" to "yes".
##
IT_WORKGROUP_CHDIR="no"
```

Exercise (.bash_udit)

Try out our new `.bash_udit`

- Do not logout! Start a new login session
- Now you only need to type `workgroup` to set the workgroup to `it_css`.

```
[traine@farber ~]$ alias
alias l.='ls -d .* --color=auto'
alias ll='ls -l --color=auto'
alias ls='ls --color=auto'
alias mc='. /usr/libexec/mc/mc-wrapper.sh'
alias vi='vim'
alias which='alias | /usr/bin/which --tty-only --read-alias --show-dot --show-
tilde'
alias workgroup='/opt/bin/workgroup  -g it_css'
[traine@farber ~]$ workgroup
[(it_css:traine)@farber ~]$
```

Exercise (.bash_udit)

Edit (vim) `.bash_udit`

```
[(it_css:traine)@farber ~]$ vim .bash_udit
##
## By default when you login to the cluster head node you are in the
## "everyone" group and need to issue a "workgroup" command to prepare
## for submitting jobs, etc.
##
## Change this flag from "no" to "yes" if you want your login shell to
## automatically issue the command to change into your default
## workgroup.  Your default workgroup will come from IT_DEFAULT_WORKGROUP
## if set above, or it will be the first group in the list produced by
## the command
##
##   /opt/bin/workgroup --query workgroups
##
IT_SET_WORKGROUP_ON_LOGIN="yes"
```

Exercise (.bashrc)

Exercise (.bashrc)

Customize our startup file `.bashrc` to create aliases for whatis, workgroups and other file storage directories

- Create a new alias whatis
- Create a new alias for each <***investing_entity***> to define a workgroup
- Create a new alias for each file storage personal work directory and change to it

Exercise (whatis)

Create an alias to determine what is the type of a command.

Example line shown in red

```
[(it_css:traine)@farber ~]$ vim .bashrc
  1 # .bashrc
  2
  3 # Source global definitions
  4 if [ -f /etc/bashrc ]; then
  5         . /etc/bashrc
  6 fi
  7
  8 # User specific aliases and functions
  9
 10 alias whatis='builtin type -t'
```

Exercise (whatis)

Try out our new .bashrc

- Do not logout! Start a new login session.

```
[traine@farber ~]$ alias
alias l.='ls -d .* --color=auto'
alias ll='ls -l --color=auto'
alias ls='ls --color=auto'
alias mc='. /usr/libexec/mc/mc-wrapper.sh'
alias vi='vim'
alias whatis='builtin type -t'
alias which='alias | /usr/bin/which --tty-only --read-alias --show-dot --show-
tilde'
alias workgroup='/opt/bin/workgroup  -g it_css'
[traine@farber ~]$ which vpkg_require
/usr/bin/which: no vpkg_require in
(/opt/bin:/opt/shared/valet/2.0/bin/bash:/opt/shared/valet/2.0/bin:/opt/shared/uni
va/current/bin/lx-amd64:/usr/lib64/qt-
3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sbin:/opt/ibutils/
bin:/home/1201/bin)
[traine@farber ~]$ whatis vpkg_require
function
[traine@farber ~]$
```

Exercise (workgroup)

Create an alias for each <***investing_entity***> to set the workgroup

Example lines shown in red for `it_css`

```
[(it_css:traine)@farber ~]$ vim .bashrc
  1 # .bashrc
  2
  3 # Source global definitions
  4 if [ -f /etc/bashrc ]; then
  5         . /etc/bashrc
  6 fi
  7
  8 # User specific aliases and functions
  9
 10 alias whatis='builtin type -t'
 11 alias it_css='\workgroup -g it_css'
```

Exercise (workgroup)

Try out our new .bashrc

- Do not logout! Start a new login session
- Now `it_css` and `workgroup` work the same.

```
[traine@farber ~]$ alias
alias it_css='\workgroup -g it_css'
alias l.='ls -d .* --color=auto'
alias ll='ls -l --color=auto'
alias ls='ls --color=auto'
alias mc='. /usr/libexec/mc/mc-wrapper.sh'
alias vi='vim'
alias whatis='builtin type -t'
alias which='alias | /usr/bin/which --tty-only --read-alias --show-dot --show-
tilde'
alias workgroup='/opt/bin/workgroup  -g it_css'
[traine@farber ~]$ it_css
[(it_css:traine)@farber ~]$ exit
exit
[traine@farber ~]$ workgroup
[(it_css:traine)@farber ~]$
```

Exercise (file storage)

Make sure you have a your own personal directory created for each file storage area. This may vary for each <***investing_entity***> research group (eg. `users` or `projects` subdirectory may exist).

These exercises assume your username will be in the base work directories

- `/home/work/<`***investing_entity***`>/`
- `/lustre/scratch/`

Exercise (/home/work)

Check for your username in `/home/work/<`***investing_entity***`>` or `$WORKDIR`

Example shows creating a personal directory for `traine` in `/home/work/it_css`

```
[(it_css:traine)@farber ~]$ cd $WORKDIR
[(it_css:traine)@farber it_css]$ ls -lad traine
ls: cannot access traine: No such file or directory
[traine@farber it_css]$ mkdir traine
[traine@farber it_css]$ ls -lad traine
drwxr-sr-x 2 traine it_css 2 Sep 29 00:10 traine
```

Exercise (/lustre/scratch)

Check for your username in `/lustre/scratch/`

Example shows a personal directory exists for `traine` in `/lustre/scratch`

```
[(it_css:traine)@farber ~]$ cd /lustre/scratch
[(it_css:traine)@farber scratch]$ ls -lad traine
drwxr-sr-x 2 traine it_css 4096 Sep 29 00:13 traine
[(it_css:traine)@farber scratch]$
```

Exercise (file storage)

Create an alias for each file storage to change to that work directory

Example lines shown in red for `traine` and `it_css`

```
[(it_css:traine)@farber ~]$ vim .bashrc
  1 # .bashrc
  2
  3 # Source global definitions
  4 if [ -f /etc/bashrc ]; then
  5         . /etc/bashrc
  6 fi
  7
  8 # User specific aliases and functions
  9
 10 alias whatis='builtin type -t'
 11 alias it_css='\workgroup -g it_css'
 12 alias cdwork='cd /home/work/it_css/traine'
 13 alias cdscratch='cd /lustre/scratch/traine'
```

Exercise (file storage)

Try out our new .bashrc

- Do not logout! Start a new login session

```
alias cdscratch='cd /lustre/scratch/traine'
alias cdwork='cd /home/work/it_css/traine'
alias it_css='\workgroup -g it_css'
alias l.='ls -d .* --color=auto'
alias ll='ls -l --color=auto'
alias ls='ls --color=auto'
alias mc='. /usr/libexec/mc/mc-wrapper.sh'
alias vi='vim'
alias which='alias | /usr/bin/which --tty-only --read-alias --show-dot --show-
tilde'
alias workgroup='/opt/bin/workgroup  -g it_css'
[(it_css:traine)@farber traine]$ cdwork
[(it_css:traine)@farber traine]$ pwd
/home/work/it_css/traine
[(it_css:traine)@farber traine]$ cdscratch
[(it_css:traine)@farber traine]$ pwd
/lustre/scratch/traine
```

Compiling, Running and Monitoring Jobs

C Example

C program example using a library called gsl (Gnu Scientific Library)

- `clib`

Compile scripts for valid compilers

- `compile-intel` and `compile-gcc`

Batch job scripts for each compiler

- `serial-intel.qs` and `serial-gcc.qs`

VALET

- Using VALET to set our environment

```
vpkg_versions gsl
```

- Only available for Intel and GCC

```
[(it_css:traine)@farber ~]$ vpkg_versions gsl
Available versions in package (* = default version):

[/opt/shared/valet/2.0/etc/gsl.vpkg_json]
gsl              GNU Scientific Library
  1.16-intel64  Version 1.16 Intel64(2015) compilers
* 1.16           Version 1.16 with GCC(system) compilers
  intel64        alias to gsl/1.16-intel64
```

Exercise

Exercise

Using our workgroup storage, compile and batch run the C program in `clib` for

- Intel

```
source compile-intel
qsub serial-intel.qs
```

- GCC

```
source compile-gcc
qsub serial-gcc.qs
```

Copy Examples

Use your new alias, `cdwork`, to get you to your workgroup storage and copy the examples.

```
cdwork
cp -r ~trainf/fhpcII .
cd fhpcII/clib
```

```
[(it_css:traine)@farber traine]$ cdwork
[(it_css:traine)@farber traine]$ pwd
/home/work/it_css/traine
[(it_css:traine)@farber traine]$ cp -r ~trainf/fhpcII .
[(it_css:traine)@farber traine]$ cd fhpcII/clib
[(it_css:traine)@farber clib]$ pwd
/home/work/it_css/traine/fhpcII/clib
[(it_css:traine)@farber clib]$ ls
compile-gcc  compile-intel  example.c  serial-gcc.qs  serial-intel.qs
```

Compile (intel)

Compile using script `compile-intel`
to generate executable `example-intel`

```
[(it_css:traine)@farber clib]$ more compile-intel
touch example.c
vpkg_rollback all
vpkg_devrequire gsl/intel64
export CC=icc
export CFLAGS="-Wall"
export LDLIBS='-lgsl -lgslcblas -lm'
make example && mv example example-intel
[(it_css:traine)@farber clib]$ source compile-intel
Adding dependency `intel/2015.0.090` to your environment
Adding package `gsl/1.16-intel64` to your environment
icc -Wall -I/opt/shared/gsl/1.16-intel64/include -L/opt/shared/gsl/1.16-
intel64/lib  example.c  -lgsl -lgslcblas -lm -o example
```

Batch job script

```
[(it_css:traine)@farber clib]$ more serial-intel.qs
#
# Template:  Basic Serial Job
# Revision:  $Id: serial.qs 523 2014-09-16 14:29:54Z frey $
#
# Change the following to #$ and set the amount of memory you need
# per-slot if you're getting out-of-memory errors using the
# default:
# -l m_mem_free=2G
#
# If you want an email message to be sent to you when your job ultimately
# finishes, edit the -M line to have your email address and change the
# next two lines to start with #$ instead of just #
# -m eas
# -M my_address@mail.server.com
#

# Add vpkg_require commands after this line:
vpkg_require gsl/intel64

# Now append all of your shell commands necessary to run your program
# after this line:

echo ""
echo "---- Run Test ----------"
time ./example-intel
```

Batch Run (intel) and monitor

`qsub` and `qstat`

```
[(it_css:traine)@farber clib]$ qsub serial-intel.qs
Your job 615 ("serial-intel.qs") has been submitted
[(it_css:traine)@farber clib]$ qstat
job-ID    prior   name       user      state submit/start at        queue
          jclass                       slots ja-task-ID
-----------------------------------------------------------------------------------------
-----------------------------------------
          615 0.00000 serial-int traine           qw        09/29/2014 01:03:28
```

More monitoring

`qstat -j <job_id>`

```
[(it_css:traine)@farber clib]$ qstat -j 615
==============================================================
job_number:                 615
jclass:                     NONE
exec_file:                  job_scripts/615
submission_time:            09/29/2014 01:03:28.083
owner:                      traine
uid:                        1201
group:                      it_css
gid:                        1002
sge_o_home:                 /home/1201
sge_o_log_name:             traine
sge_o_path:                 /opt/shared/gsl/1.16-
intel64/bin:/opt/shared/intel/composer_xe_2015.0.090/bin/intel64:/opt/shared/intel/composer_xe_2
015.0.090/mpirt/bin/intel64:/opt/shared/intel/composer_xe_2015.0.090/debugger/gdb/intel64_mic/bi
n:/opt/bin:/opt/shared/valet/2.0/bin/bash:/opt/shared/valet/2.0/bin:/opt/shared/univa/current/bi
n/lx-amd64:/usr/lib64/qt-
3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sbin:/opt/ibutils/bin:/home/1201
/bin
sge_o_shell:                /bin/bash
sge_o_workdir:              /home/work/it_css/traine/fhpcII/clib
sge_o_host:                 login000
...
[(it_css:traine)@farber clib]$
```

Batch Run (intel) output

Look at batch run output

```
[(it_css:traine)@farber clib]$ more serial-intel.qs.o615

[CGROUPS] UD Grid Engine cgroup setup commencing
[CGROUPS] Setting 1073741824 bytes (vmem 1073741824 bytes) on n038 (master)
[CGROUPS]   with 1 core = 0
[CGROUPS] done.

Adding dependency `intel/2015.0.090` to your environment
Adding package `gsl/1.16-intel64` to your environment

---- Run Test ----------
J0(5) = -1.77596771314338264e-01

real     0m0.005s
user     0m0.001s
sys      0m0.001s
```

Local (non-standard) Commands

Local Commands

Check `/opt/bin` for local commands.

These are "non-standard" commands that are specific to the Farber cluster; UD community clusters.

Local Commands

`hpc-user-info -a` ***username***

`hpc-user-info -h`

display information about ***username***

```
[(it_css:traine)@farber ~]$ hpc-user-info -a traine
full-name = Student Training
last-name = Student Training
home-directory = /home/1201
email-address = traine@udel.edu
clusters = Mills, Farber
[(it_css:traine)@farber ~]$
```

Local Commands

`qnodes`

`qnodes -g <`***investing_entity***`>`

will display the compute nodes based on the current workgroup or specified with `-g`

```
[(it_css:traine)@farber ~]$ qnodes
n036 n037 n038 n039 n040
[(it_css:traine)@farber ~]$ exit
exit
[traine@farber ~]$ qnodes
Host group "@everyone" does not exist
[traine@farber ~]$ qnodes -g it_css
n036 n037 n038 n039 n040
```

Local Commands

`qhostgrp`

`qhostgrp -g <`***investing_entity***`>`

will display compute nodes system information for the current workgroup or specified with `-g`

```
[(it_css:traine)@farber ~]$ qhostgrp
HOSTNAME                ARCH         NCPU NSOC NCOR NTHR NLOAD  MEMTOT  MEMUSE  SWAPTO  SWAPUS
----------------------------------------------------------------------------------------------
global                  -               -    -    -    -     -       -       -       -       -
n036                    lx-amd64       20    2   20   20  0.00   63.0G    1.1G    2.0G     0.0
n037                    lx-amd64       20    2   20   20  0.00   63.0G    1.1G    2.0G     0.0
n038                    lx-amd64       20    2   20   20  0.00   63.0G    1.1G    2.0G     0.0
n039                    lx-amd64       20    2   20   20  0.00   63.0G    1.1G    2.0G     0.0
n040                    lx-amd64       20    2   20   20  0.00   63.0G    1.1G    2.0G     0.0
```

Local Commands

`qhostgrp -j`

`qhostgrp -g <`***investing_entity***`> -j`

will display compute nodes system information for the current workgroup or specified with `-g` and all the jobs running on each node including standby

```
[(it_css:traine)@farber ~]$ qhostgrp -j
HOSTNAME                ARCH         NCPU NSOC NCOR NTHR NLOAD  MEMTOT  MEMUSE  SWAPTO  SWAPUS
----------------------------------------------------------------------------------------------
global                  -               -    -    -    -     -       -       -       -       -
n036                    lx-amd64       20    2   20   20  0.05   63.0G    8.0G    2.0G    1.7M
   job-ID     prior   name       user         state submit/start at     queue      master ja-task-ID
   ------------------------------------------------------------------------------------------------
       385547 0.25590 openmpi-ib zzhou        r     12/18/2015 09:07:12 standby-4h SLAVE
n037                    lx-amd64       20    2   20   20  1.01   63.0G    5.9G    2.0G   25.4M
       385261 0.25632 JobArray   rpatet       r     12/18/2015 03:52:41 standby.q@ MASTER 31
                                                                        standby.q@ SLAVE  31
                                                                        standby.q@ SLAVE  31
                                                                        standby.q@ SLAVE  31
                                                                        standby.q@ SLAVE  31
                                                                        standby.q@ SLAVE  31
.......
```

Local Commands

```
qjobs
qjobs -g <investing_entity>
qjobs -a
```

will display the status of jobs submitted by your research group or specified workgroup with `-g` or all jobs with `-a`.

Local Commands

`qstatgrp`

`qstatgrp -g <`***investing_entity***`>`

will display queue information for the current workgroup or specified with `-g`

```
[(it_css:traine)@farber ~]$ qstatgrp
CLUSTER QUEUE                   CQLOAD   USED    RES  AVAIL  TOTAL aoACDS  cdsuE
it_css.q                          0.00      0      0    100    100       0      0
standby-4h.q                      0.07      0      0   1680   1800     120      0
standby.q                         0.07      0      0   1680   1800     120      0
```

Local Commands

```
qstatgrp -j
qstatgrp -g <investing_entity> -j
```

will display queue information for the current workgroup or specified with `-g` and all jobs running or queued by workgroup members

```
[(it_css:traine)@farber ~]$ qstatgrp -j
job-ID     prior   name       user         state submit/start at     queue
jclass                         slots ja-task-ID
-----------------------------------------------------------------------------------------
-----------------------------------------------
    385557 0.50000 openmpi-ib traine        r    12/18/2015 10:07:41 it_css.q@n040
30
    377224 0.50429 script2    trainf       qw    12/09/2015 15:06:59
2
    377225 0.50429 script3    trainf       qw    12/09/2015 15:09:23
```

Need Help?

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