BROWN UNIVERSITY CENTER FOR
COMPUTATION & VISUALIZATION

Getting Started With CCV

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User Services & Support

This talk...

- Assumes you have some familiarity with a Unix shell
- Provides examples and best practices for typical usage of CCV systems
- Is a condensed form of the documentation available at:

  http://brown.edu/ccv/doc

Overview

- Connecting to CCV
- Transferring files
- Available software
- Running and monitoring jobs
- Compiling and linking your own code

Logging in

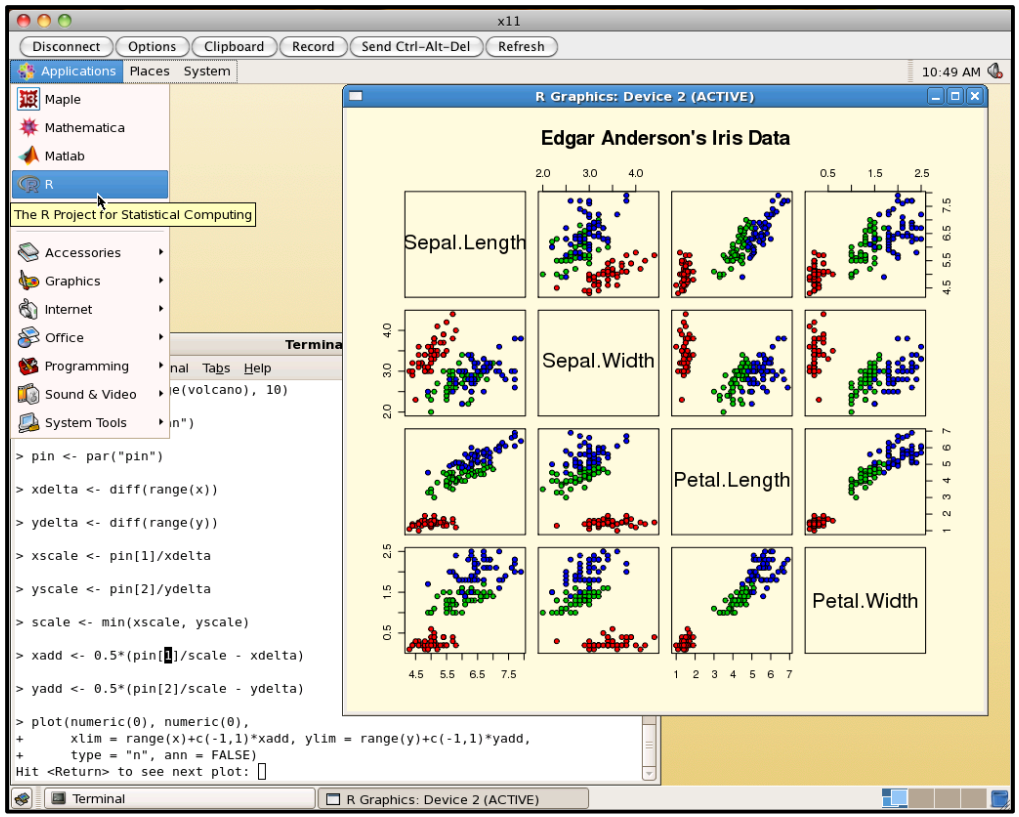
- CCV uses the Secure Shell (SSH) protocol
- You will need an SSH client
  - Linux / OS X comes with a command-line client
  - Windows: try PuTTY or Cygwin
- Connect to the “ssh” server
  - Linux / OS X / Cygwin:
    `ssh username@ssh.ccv.brown.edu`
  - PuTTY: enter `ssh.ccv.brown.edu` in “Host Name”

Login nodes

- When you ssh to Oscar, you are placed on either login001 or login002
  - The login nodes are intended for tasks like:
    - writing, compiling, and debugging code
    - transferring and managing files
    - submitting and managing jobs
  - They are shared by all users logged into CCV
  - Please don't run your jobs directly on the login nodes!
    - It disrupts other users
    - Start an interactive or batch job instead

Virtual Network Computing

- OR connect through CCV's Virtual Network Computing client, available here:
  - http://brown.edu/ccv/vnc



File systems

~ → /home/<user>	Your home directory: • optimized for many small files (<1MB) • nightly backups • 10GB quota
~/data → /gpfs/data/<group>	Your data directory: • optimized for reading large files (>1MB) • nightly backups • quota is by group (usually >=256GB)
~/scratch → /gpfs/scratch/<user>	Your scratch directory: • optimized for reading/writing large files (>1MB) • NO BACKUPS • purging: files older than 30 days may be deleted • 512GB quota

Note: class or temporary accounts may not have a ~/data directory!

Transferring files

- RData: mount your home, data, and scratch directories on your local system over CIFS (Brown network only)
  - http://brown.edu/ccv/doc/cifs
- scp: a command used from the terminal
  - Copy from Oscar:
    ```
    scp username@ssh.ccv.brown.edu:/remote/path /local/path
    ```
  - Copy to Oscar:
    ```
    scp /local/path username@ssh.ccv.brown.edu:/remote/path
    ```
- rsync: a command like scp but with more features
- GUI "Secure Copy" programs
  - e.g. WinSCP, Fugu (Mac), CyberDuck (Mac)

Available software

- Software is organized using Environment Modules
- Load a software module with `module load <name>`
- Loading a module alters your environment, paths, etc:

```
[user@login001 ~]$ module display intel
-------------------------------------------------------------------
/gpfs/runtime/modulefiles/intel/12.0.4:
setenv          MKL -L/gpfs/runtime/opt/intel/12.0.4/mkl/lib/intel64 -
lmkl_rt -liomp5 -lpthread
prepend-path     PATH /gpfs/runtime/opt/intel/12.0.4/bin
prepend-path     MANPATH /gpfs/runtime/opt/intel/12.0.4/man/en_US
prepend-path     LD_LIBRARY_PATH /gpfs/runtime/opt/intel/12.0.4/lib/
intel64:/gpfs/runtime/opt/intel/12.0.4/mkl/lib/intel64
…

[user@login001 ~]$ module load intel

[user@login001 ~]$ which icc
/gpfs/runtime/opt/intel/12.0.4/bin/icc
```

Available software (Cont'd)

- View available modules with `module avail`
  - Or search for a specific package with `module avail <package>`
- View your loaded modules with `module list`
- Module commands in your ~/.modules file will automatically execute when you login
  - Add a module to your default list with `echo "module load <name>" >>~/.modules`
- If you need software that is not installed, submit a request at http://brown.edu/ccv/protected/software

Running jobs

- An interactive job allows you to:
  - Interact with a program by typing input, using a GUI, etc.
    - But if your connection is interrupted, the job will abort
  - Quickly stop and restart a program, e.g. to test out different parameters or for debugging
  - Run on resources shared with other users
- A batch job allows you to:
  - Submit a script that will run without any intervention
  - Access dedicated resources for your job
  - Run for long periods of time without worrying about other users interfering with your job, or your connection dying

Queues on Oscar

- Oscar's compute nodes are organized into queues
- Choose the queue that best matches the needs of your job
- Nodes are packed by user: if you have multiple jobs that request less than a full node, the jobs can share a node
  - But other users' jobs will not run on that same node as yours

dq	Default queue with most of the compute nodes: 8-, 12-, or 16-core; 24GB to 48GB of memory; all Intel based
gpu	Specialized compute nodes (8-core, 24GB, Intel) each with 2 NVIDIA GPU accelerators
timeshare	Large memory nodes that are shared by multiple users: 12-, 16-, or 32-core; 64GB to 128GB of memory; both Intel and AMD
debug	Dedicated nodes for fast turn-around, but with a short time limit of 40 node-minutes

Interactive jobs

- You can start an interactive job from the login node with:

```
interact [-n cores] [-t walltime]
         [-m memory] [-q queue] [-X]
```

- Defaults are 1 core, 30:00, 4GB, timeshare queue:

```
[user@login001 ~]$ interact
```

- To request more cores/time/memory:

```
[user@login001 ~]$ interact -n 8 -m 64g -t 4:00:00
```

- To enable X forwarding (e.g. to run a GUI program):

```
[user@login001 ~]$ interact -X
```

- To request a different queue:

```
[user@login001 ~]$ interact -q debug
```

Batch jobs

- Specify resources and the commands to run in a file called a batch script

```
#!/bin/bash
#PBS -N MyJobName
#PBS -l walltime=2:00:00

# execute your commands:
my_program <args>
```

- Submit the script to a queue with:

```
qsub myjob.sh
qsub -q timeshare myjob.sh
```

- Default resources are:
  - 1 node, 1 core, 1 minute (e.g. always specify a walltime!)

Monitoring jobs

`allq`	List all jobs in all queues Hint: page through the list with `allq | more`
`allq <queue>`	List all jobs in the specified queue
`myq`	List only your own jobs in all queues
`myq <user>`	List another user's jobs
`qdel <jobid>`	Delete a job (the batch script is terminated)
`qstat -f <jobid>`	See full details for a job
`checkjob <jobid>`	Diagnose a blocked job

The output of a running job is spooled to a file that you can view with:

```
tail <jobid>.mgt.OU
```

To receive an email when your job begins, ends, or aborts add the PBS options:

```
#PBS -m abe
#PBS -M oscar_user@brown.edu
```

Batch jobs for threaded programs

- A threaded program can use additional cores on a node
- The ppn property controls the *p*rocessors (cores) *p*er *n*ode
- The $PBS_NP shell variable is a shortcut for the total *n*umber of *p*rocessors (cores) = nodes x ppn

```
#!/bin/bash
#PBS -N MyJobName
#PBS -l walltime=2:00:00
#PBS -l nodes=1:ppn=8

# execute your (threaded) commands:
my_program -t $PBS_NP <args>
```

Batch jobs for MPI programs

- An MPI program can communicate among multiple nodes
- Use the nodes property and the $PBS_NP shell variable

```
#!/bin/bash
#PBS -N MyJobName
#PBS -l walltime=2:00:00
#PBS -l nodes=4:ppn=8

# execute your MPI command on 32 cores
# across 4 nodes:
mpirun -n $PBS_NP my_mpi_program <args>
```

Job arrays

- Job arrays are a special feature for running parameter sweeps
- Add `#PBS -t <range>`
  - Where range is of the form *1-N* or *0,2,4-8* etc.
  - A job with the name `<jobname>[i]` is created for each value in the range
  - Each job is given a different `$PBS_ARRAYID` value from the range

Job arrays

- This job will use 32 cores to sweep over 32 parameters
  - The parameters are located in 32 different files named: input_file_1, input_file_2, etc.
  - In the queue, you will see 32 individual jobs named: MySweep[1], MySweep[2], etc.

```
#!/bin/bash
#PBS -N MySweep
#PBS -l walltime=1:00:00
#PBS -t 1-32
#PBS -l nodes=1:ppn=1

echo "Starting sweep $PBS_ARRAYID on $HOSTNAME:$PBS_VNODENUM"
my_program "input_file_$PBS_ARRAYID"
```

Compiling

- GNU compiler suite is the default on Oscar
- Compile a single source file with:

```
gcc -g -O2 -o myprogram myprogram.c
g++ -g -O2 -o myprogram myprogram.cpp
gfortran -g -O2 -o myprogram myprogram.f90
```

- -g flag = generate debugging symbols
- -O2 flag = use a higher level of optimization

Intel and PGI Compilers

- The Intel compiler suite is available with

```
module load intel
icc
icpc
ifort
```

- The Portland Group compilers are available with

```
module load pgi
pgcc
pgCC
pgf77
pgf90
```

Linking

- Many modules include environment variable shortcuts that contain linking directions, e.g.

FFTW

```
gcc -o fftw-app fftw-app.c $FFTW

$FFTW = -I/gpfs/runtime/opt/fftw/3.2.2/include -L/
  gpfs/runtime/opt/fftw/3.2.2/lib -lfftw3
```

GotoBLAS

```
gcc -o blas-app blas-app.c $GOTO

$GOTO = -I/gpfs/runtime/opt/gotoblas2/1.13/include
  -L/gpfs/runtime/opt/gotoblas2/1.13/lib -lgoto2 -
  lpthread -lgfortran
```

Contact Info

- For help or support:
  - (401) 863-7557
  - support@ccv.brown.edu
  - Hours:
    8:30 – 5:00 (Academic Year)
    8:00 – 4:00 (Summer)
- Keeping in touch:
  - System updates from Twitter: ccv_brown
  - User mailing list: users@ccv.brown.edu
  - Website: http://brown.edu/ccv