

Using R on the LSHTM High Performance Computing (HPC)

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Objectives

- Brief overview of the LSHTM HPC
 - What is the HPC?
- Getting started
 - LSHTM wiki page
 - Joining
 - Login: WINSOCP & PuTTY
- Example using R
- Other issues
- Contacts

Brief overview of the HPC

- Also known as 'Cluster', 'super computers' - used interchangeably
- Combined computing power to deliver higher performance
- Performance and processing speed exceeds a typical desktop computer
- Used for computationally intensive tasks
 - Need large memory
 - Large datasets
 - Repetitive tasks
 - Not very useful for small tasks!
- Supports a variety of software (Stata, R, Python)



Accessible
memory per
user = 8GB



Accessible
memory per user
= 200 GB

Getting started – for Windows only

LSHTM HPC wiki page

http://wiki.lshtm.ac.uk/hpc/index.php5/Main_Page

To join:

Send an email to the ITS Helpdesk (servicedesk@lshtm.ac.uk) with name, username, department, brief description of proposed work on cluster, software requirements

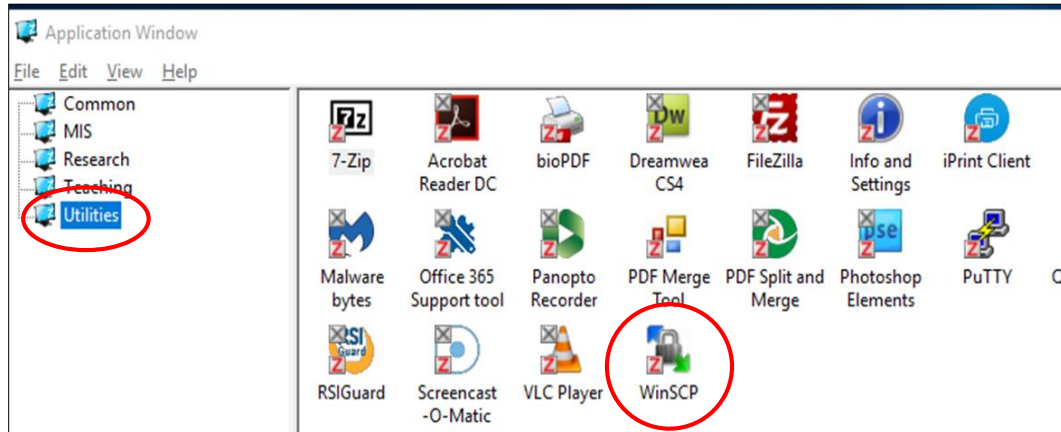
To log in:

A new user account on the HPC + a new home directory

Use your usual LSHTM username and password

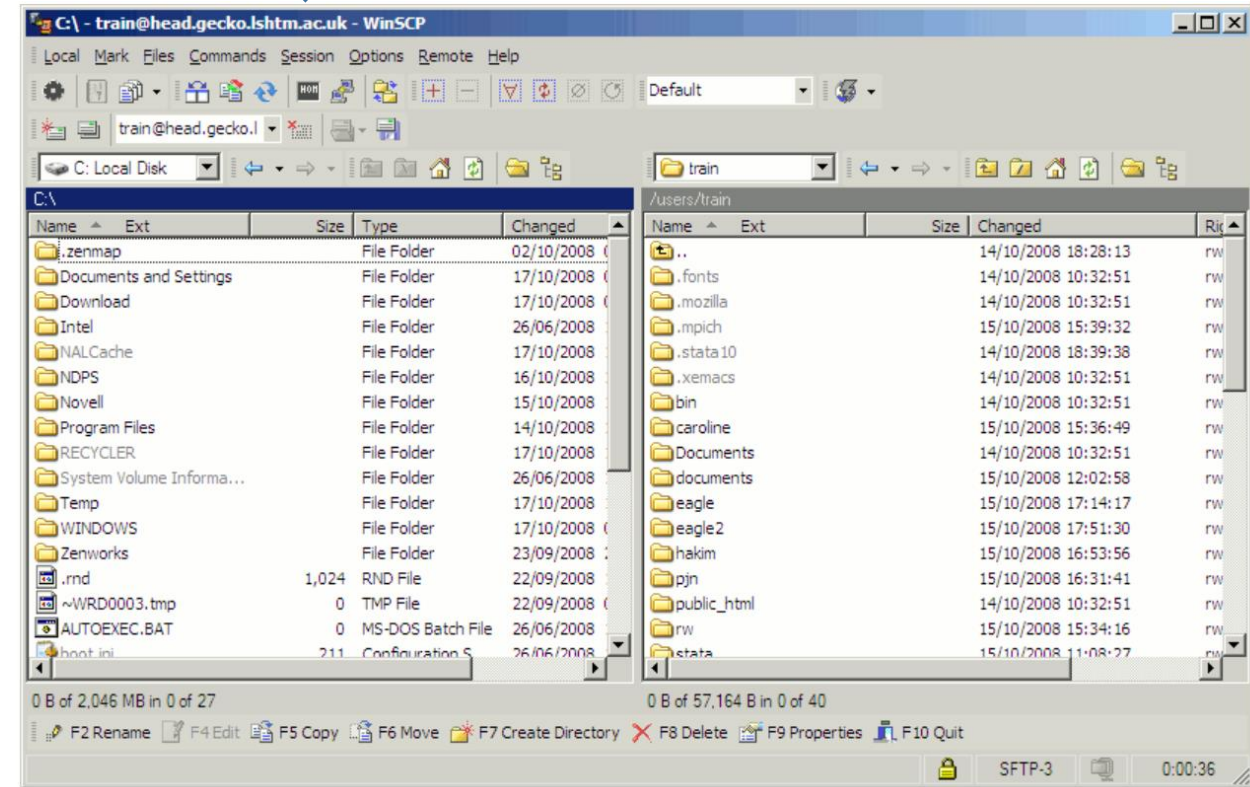
Copy files to and from HPC using WinSCP

Login in to HPC – Windows example



Your local drive

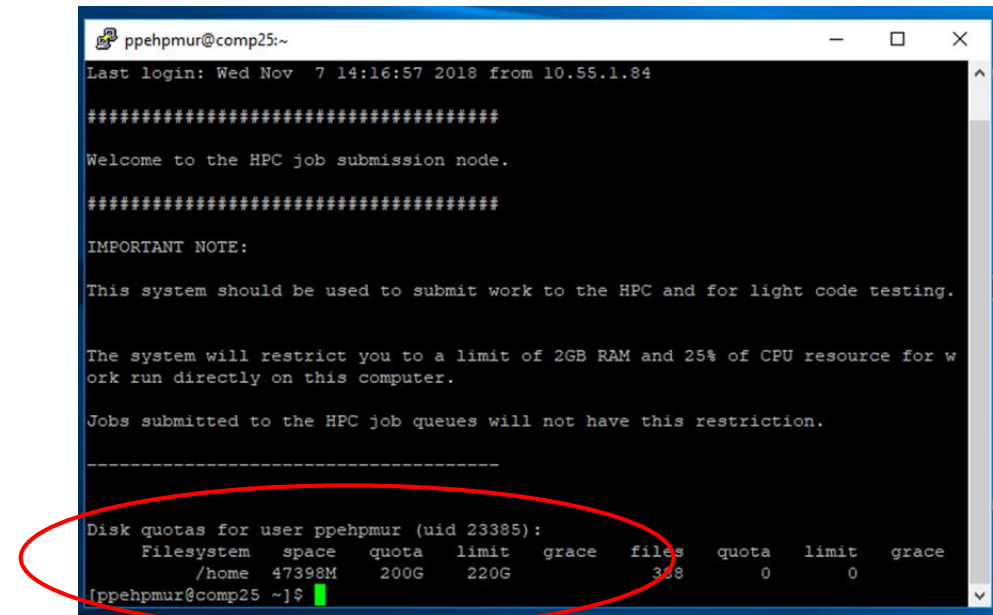
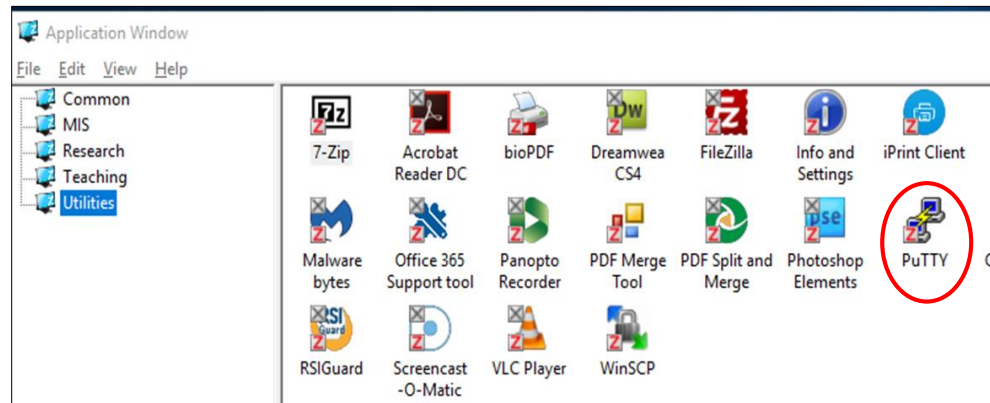
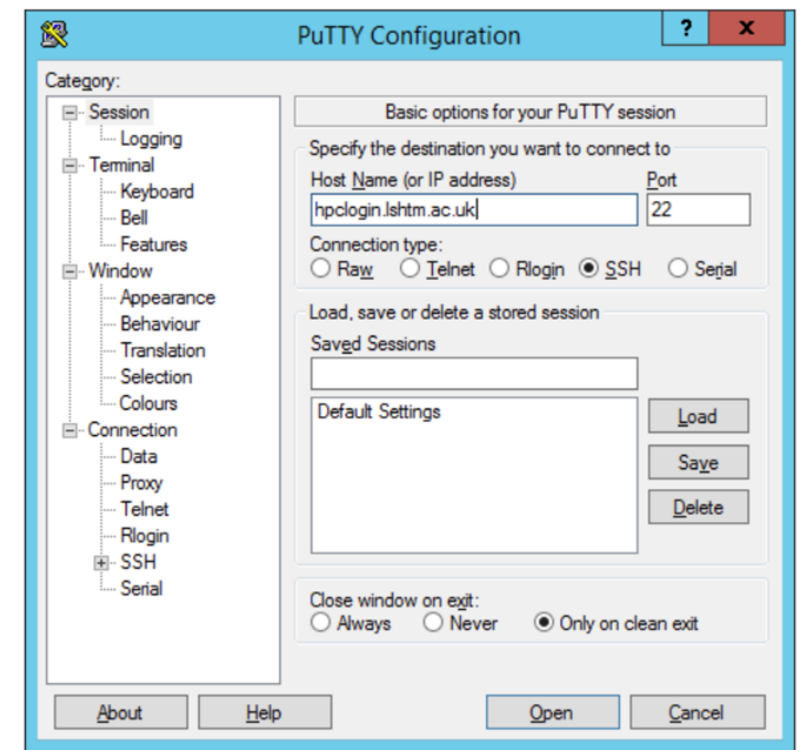
Your HPC drive



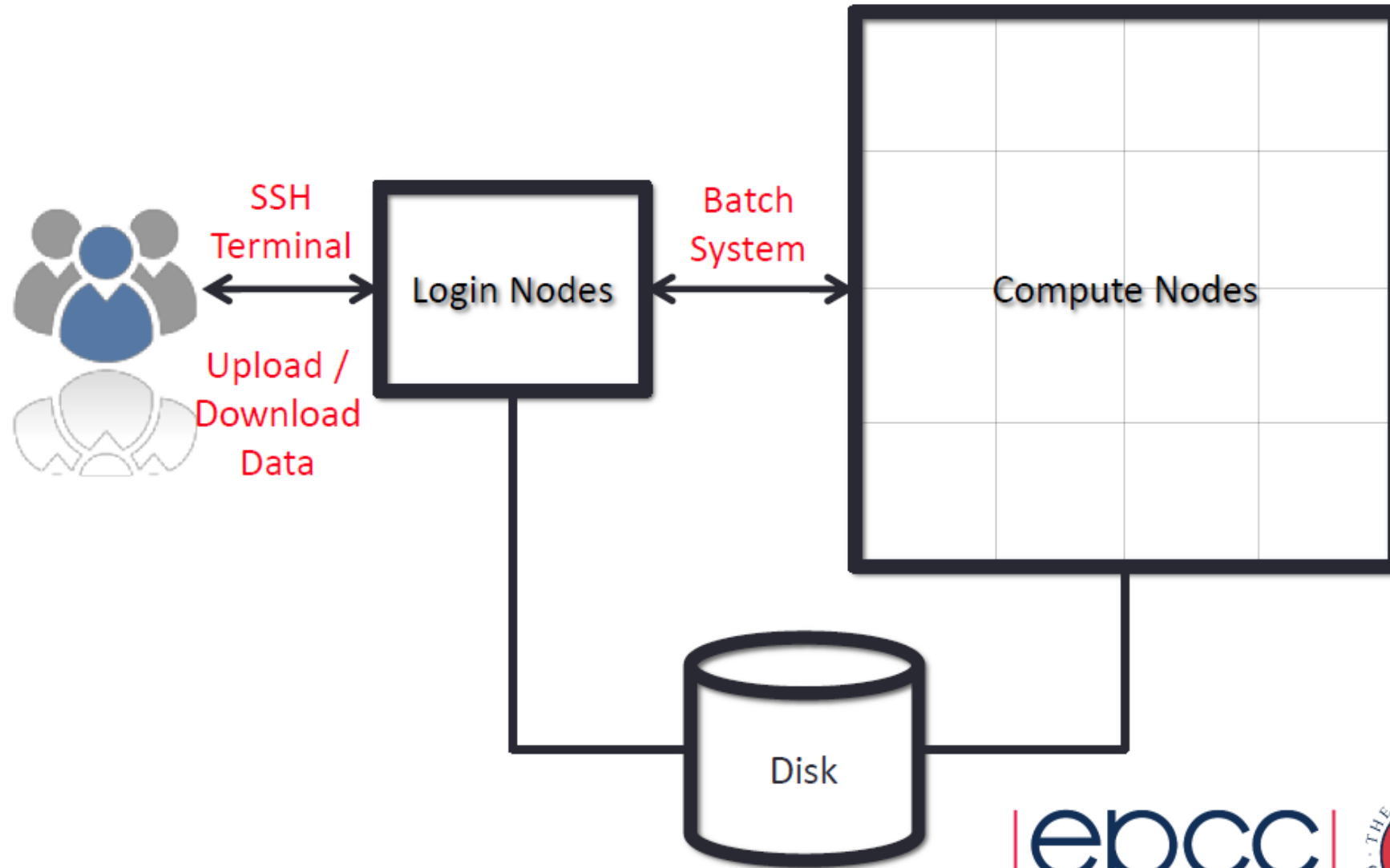
Getting started

To submit a job:

- PuTTY software provides remote terminal access to the HPC
- Check LSHTM wiki page on how to configure PuTTY
- Once again use your usual LSHTM username and password



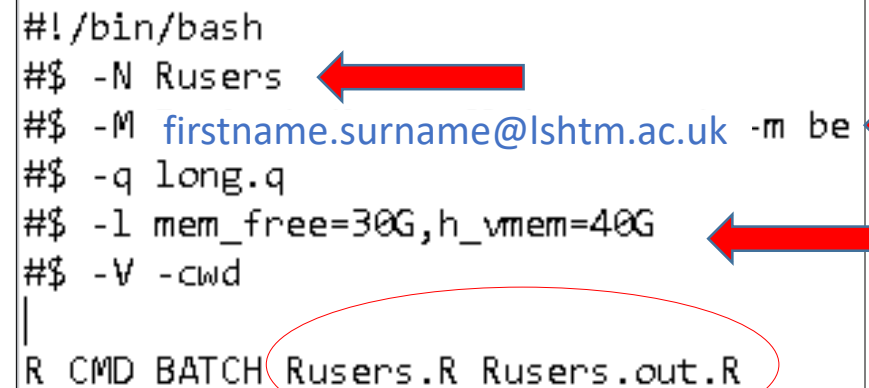
Typical HPC system layout



Brief example

- Preparing a task/job
 - Transfer files to your new HPC drive
 - Check that the job works ...run part of the job interactively or on own PC
- Brief description of my task
save R scripts on HPC drive
- Submitting a “simple” job
 - batch/ shared system
 - use a ‘.txt file’ – specify required memory
 - running the script on PuTTY
 - example of script –
 - running a job = *qsub myjob.txt*
 - every job is issued a jobId
 - deleting a job = *qdel jobId*

```
#!/bin/bash
#$ -N Rusers
#$ -M firstname.surname@lshtm.ac.uk -m be
#$ -q long.q
#$ -l mem_free=30G,h_vmem=40G
#$ -V -cwd
|
R CMD BATCH Rusers.R Rusers.out.R
```

A terminal window showing a qsub command. Red arrows point to the job name 'Rusers', the email address 'firstname.surname@lshtm.ac.uk', and the memory limit 'mem_free=30G,h_vmem=40G'. A red oval highlights the script name 'Rusers.R' in the command 'R CMD BATCH Rusers.R Rusers.out.R'.

Brief example using R

- Email notifications
 - Job started
 - Job completed
- Submit one jobs with multiple tasks
E.g. process 5 tasks using 5 different data files
Run job on one textfile 'txt'

```
#!/bin/bash
#$ -N merge_hpc
#$ -M Peninah.Murage@lshtm.ac.uk -m be
#$ -q short.q
#$ -l mem_free=90G,h_vmem=100G
#$ -t 1-5

R CMD BATCH merge_hpc${SGE_TASK_ID}.R merge_hpcout${SGE_TASK_ID}.out.R
```

-t 1:5 specifies the number of sequential tasks
The job is submitted in 5 tasks and will create 5 R output files

- Parallel processing?

```
Job 3129103 (Rusers) Started
User   = ppehpmur
Queue  = short.q
Host   = comp34.cluster
Start Time = 11/28/2018 22:12:22
```

```
Job 3129102 (Rusers) Complete
User      = ppehpmur
Queue     = short.q@comp35.cluster
Host      = comp35.cluster
Start Time = 11/28/2018 18:28:43
End Time   = 11/28/2018 18:57:10
User Time  = 00:24:12
System Time = 00:04:14
Wallclock Time = 00:28:27
CPU        = 00:28:27
Max vmem   = 62.127G
Exit Status = 1
```

Other issues

- Queuing
show all your on jobs, *qstat*
other jobs on queue *qstat -u '*'*
details of specified job *qstat -j jobid*
- Installing packages
Login to 'PuTTY' and run R interactively
- Loading different versions of R
Presently not possible at LSHTM!
See University of Sheffield example here
<http://docs.hpc.shef.ac.uk/en/latest/sharc/software/apps/R.html>
- Service desk and LSHTM wiki page contacts
Steven Whitbread (Datacentre and Infrastructure Manager)

```
R

Install Library from Cran

install.packages('packageName')

You should be prompted to choose a cran repository mirror. If you have problems choosing, you

install.packages('packageName', repos="http://cran.ma.imperial.ac.uk/🔗")
```