



Introduction to Hartree Centre Resources: IBM iDataPlex Cluster and Training Workstations

Rob Allan

**Scientific Computing Department
STFC Daresbury Laboratory**

also ack: Crispin Keable (IBM)

Agenda

09:30 - 10:00 Coffee (*In the breakout room next door to the training suite*)

10:00 - 10:15 Roger BARLOW - Introduction to the Workshop - Day 1

10:15 - 10:30 Rob ALLAN - Basic use of the system and job submission

10:30 - 10:40 Peter WILLIAMS Introduction to running ELEGANT on Sid

10:40 - 10:50 David DUNNING Introduction to using GENESIS on Sid

10:50 - 13:00 Practical session for ELEGANT and GENESIS

13:00 - 14:00 Lunch (*In the breakout room next door to the training suite*)

14:00 - 14:15 Jonny SMITH Introduction to running VORPAL on SID

14:15 - 17:30 Practical session running VORPAL (also ELEGANT and GENESIS if desired)

Coffee is also available at 11:00 and 15:00 in the breakout room next door to the training suite for anyone that needs some refreshment during the practical sessions. Please note that no food or drink is allowed in the training suite at any time!

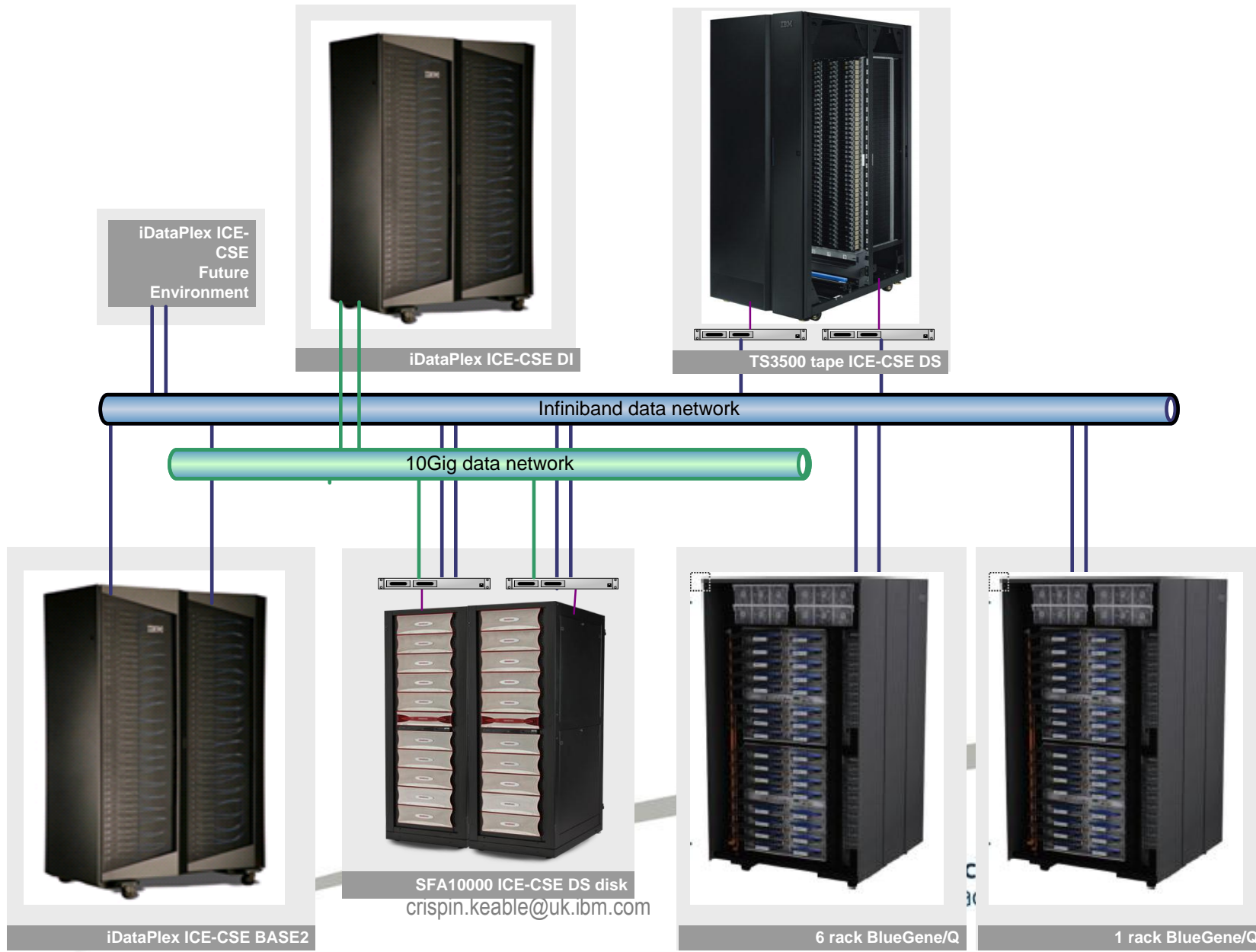


Hartree Centre Resources

- Modern Data Centre with water cooling – room for expansion
- 7 racks of IBM BlueGene/Q with 114,688 cores – 1.46 Pflop/s peak (#13 in Top500)
- IBM iDataPlex with 8,192 cores – 170 Tflop/s peak (#114 in Top500)
 - including 8x 4 TB ScaleMP virtual shared memory systems
- ~6 PB of DDN disk storage with GPFS
- ~15 PB Tape library
- Visualisation systems at Daresbury and Rutherford Appleton Laboratories – to complement the Virtual Engineering Centre
- Training and conference facilities



Hartree Centre HPC Resources



How to Log On

Log on to a workstation:

- 1) in “other” enter your course id, e.g. xxxyy-jpf03
- 2) enter the login password that you have been given

Log on to the iDataPlex:

- 1) Open the iDataPlex window
- 2) Or open a terminal (right click the mouse) and type:

```
ssh idpxlogin3
```

From home (using your SSH keys):

```
ssh xxxyy-jpf03@wonder.hartree.stfc.ac.uk
```



Transferring Files

Open a terminal (right click the mouse) and type:

```
cd ~
```

This should take you to, e.g. /gpfs/home/training/jpf03/xxxxy-jpf03

To copy a file from the iDataPlex do:

```
scp idpxlogin3:<filename> .
```

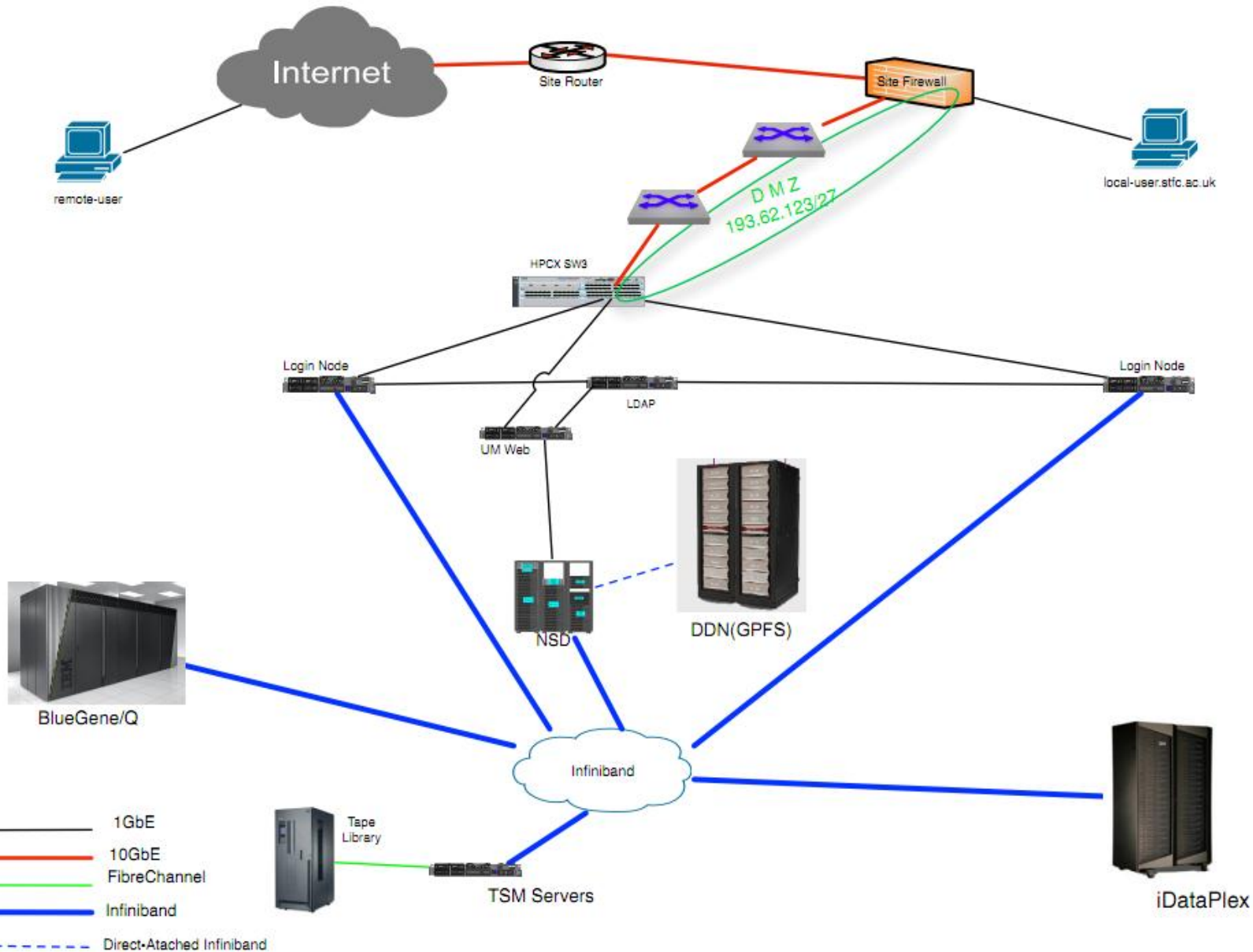
Data can be copied from USB memory sticks by plugging them into the keyboard port on the workstation. They should automount as /media/???. You can copy data to the shared training file system or to the iDataPlex.

From home (using your SSH keys) e.g.

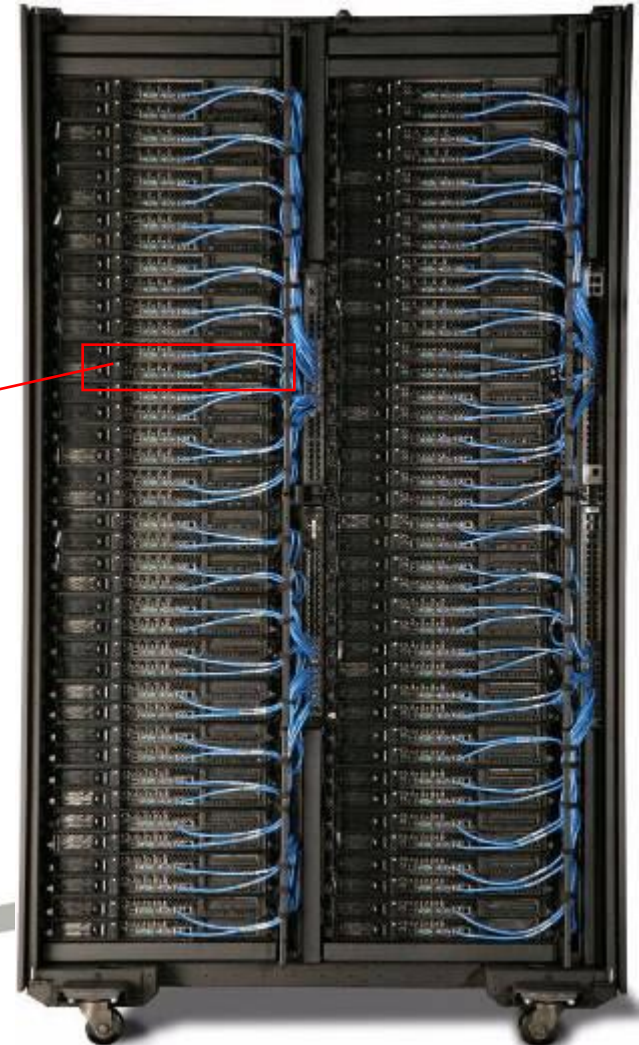
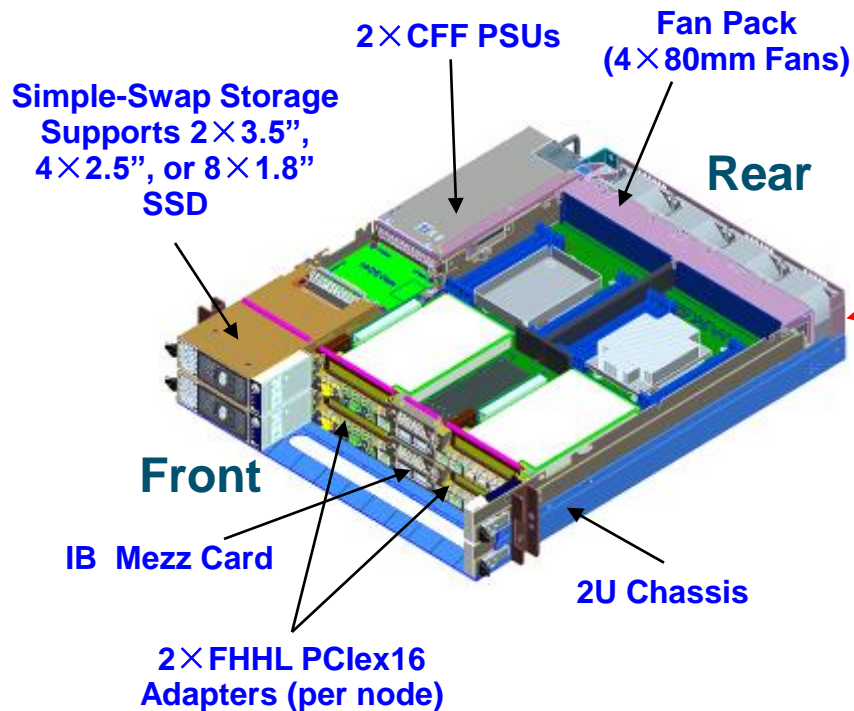
```
scp xxxyy-jpf03@wonder.hartree.stfc.ac.uk:<filename> .
```



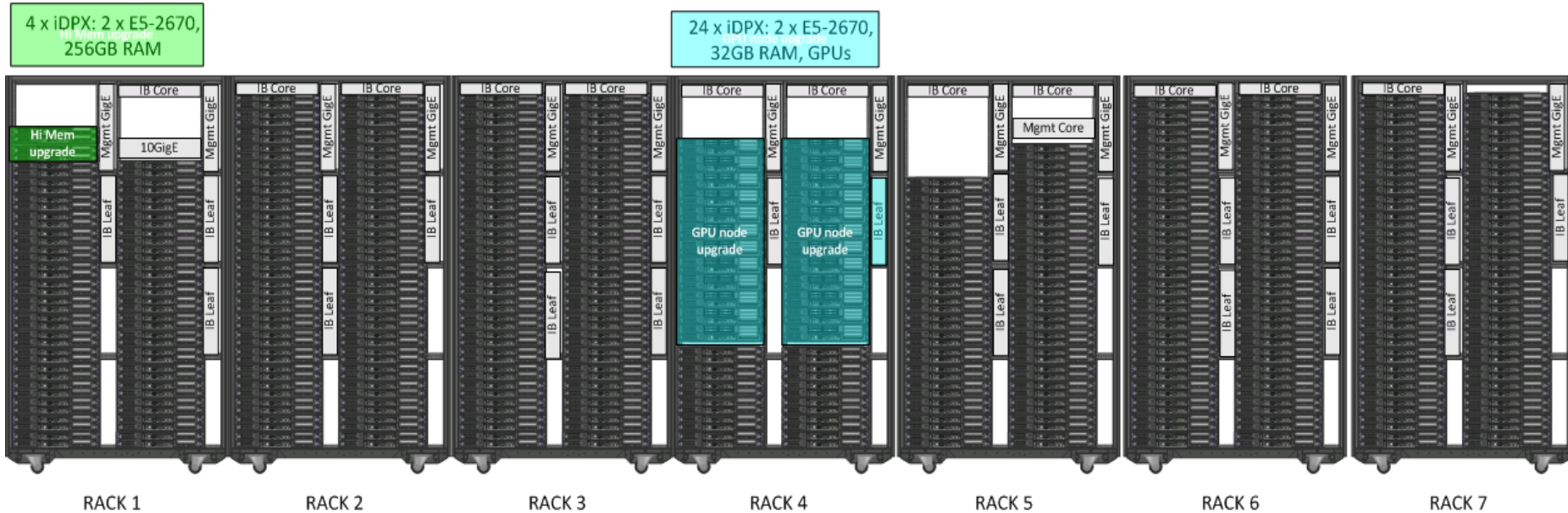
Remote Connectivity



Base & Data Intensive systems (IBM iDataPlex)



June MES upgrade



7 racks

512 nodes – 2 processors = 16 cores per node (Intel SandyBridge)

8192 cores in total

InfiniBand communication network

GPFS file system

Managed Applications

We use environment modules to manage installed applications on the iDataPlex.

Try:

`module avail`

Of interest here might be:

`genesis/2.0` `pelegant-gcc/25.1.0` `vorpal/5.2.2` `vorpal/6.0`

To use Genesis do:

`module load genesis/2.0`

`module list`

Should show you that its correctly loaded.



Using the LSF Batch Queues

Using `idpxlogin3` or `wonder.hartree.stfc.ac.uk` will take you to a login node on the iDataPlex cluster. You can only edit files (using `emacs` or `vi`) and compile programs there. To run jobs you need to use the LSF batch queues which submit jobs to the 512 compute nodes using a fair share method.

“`bqueues`” – shows what queues are available

“`bsub < testjob.bsub`” – submits a job as defined in the script “`testjob.bsub`”.
Note: be careful to remember the “`<`” re-direction symbol

“`bjobs -u all -w`” - shows all jobs, their jobid and their status, PEND, RUN, etc.

“`bjobs -l <jobid>`” - shows detailed information about a job

“`bkill <jobid>`” - kills the job if you've made a mistake or its hung.

To get more information type “`man bjobs`” etc.



BSUB - Job Description Syntax

The following tutorials will give detailed examples for each application.
Here are some general notes based on the Genesis example.

```
#!/bin/bash # use the bash shell
```

```
#BSUB -o stdout.%J.txt # stdout file, %J puts the jobid as a string
```

```
#BSUB -e stderr.%J.txt # stderr file
```

```
#BSUB -r [ptile=16] # tell the scheduler to put 16 processes per node
```

```
#BSUB -n 32 # tells the scheduler a total of 32 processes are required (i.e.  
2 nodes in this case)
```

```
#BSUB -J Genesis # use "Genesis" as the display name for bjobs
```

```
#BSUB -W 30 # job expected to run in less than 30 minutes wall time
```

Other commands in the script file use bash shell syntax.

For more information try `"man bsub"`.



More Information

Web site: <http://www.stfc.ac.uk/hartree>

Community Portal: <http://community.hartree.stfc.ac.uk>

Document Repository: <http://community.hartree.stfc.ac.uk> “Documents”

Status and User Guide:

<http://community.hartree.stfc.ac.uk/wiki/site/admin/home.html>

Training and Events: <http://community.hartree.stfc.ac.uk> “Clearing House”

JISCMail group: <http://www.jiscmail.ac.uk/HARTREE-USERSGROUP>

Help desk e-Mail: hartree@stfc.ac.uk

