

Running jobs on the HPC

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Questions



Your microphones are all muted



Use the Zoom Q&A to ask questions



Upvote your favourite questions: if we are short on time we will prioritise those with the most votes.

Materials

- Slides and video will be sent out to you after the session

Agenda

- 1 Introduction and admin
- 2 What is the High Performance Cluster?
- 3 Why use the HPC?
- 4 Logging into the HPC and working in an interactive session
- 5 How to create and monitor jobs on the HPC
- 6 Tools and software available and how to load them
- 7 Interactive coding tools
- 8 Bringing in your own tools and software
- 9 Questions



2. What is the High Performance Computing Cluster?

What is High Performance Computing?

High Performance Computing or HPC is set of computing, networking and storage resources integrated with workload orchestration services for HPC applications. Example use cases are:

- Analytics for financial services
- Manufacturing
- Scientific visualization and simulation
- Genomic sequencing and medical research
- Oil & gas
- Weather prediction

GEL's research environment HPC is a number of computers and a Weka storage system linked together by high-speed Local Area Network (LAN). This is all managed by a scheduling software from IBM called Load Sharing Facility (LSF).

Collectively this is known as the 'Helix' Cluster.

Types of cluster hosts/nodes

Management/Master Hosts:

Coordinator of the cluster, scheduling and dispatching of jobs based on cluster configuration and load. Will not run jobs.

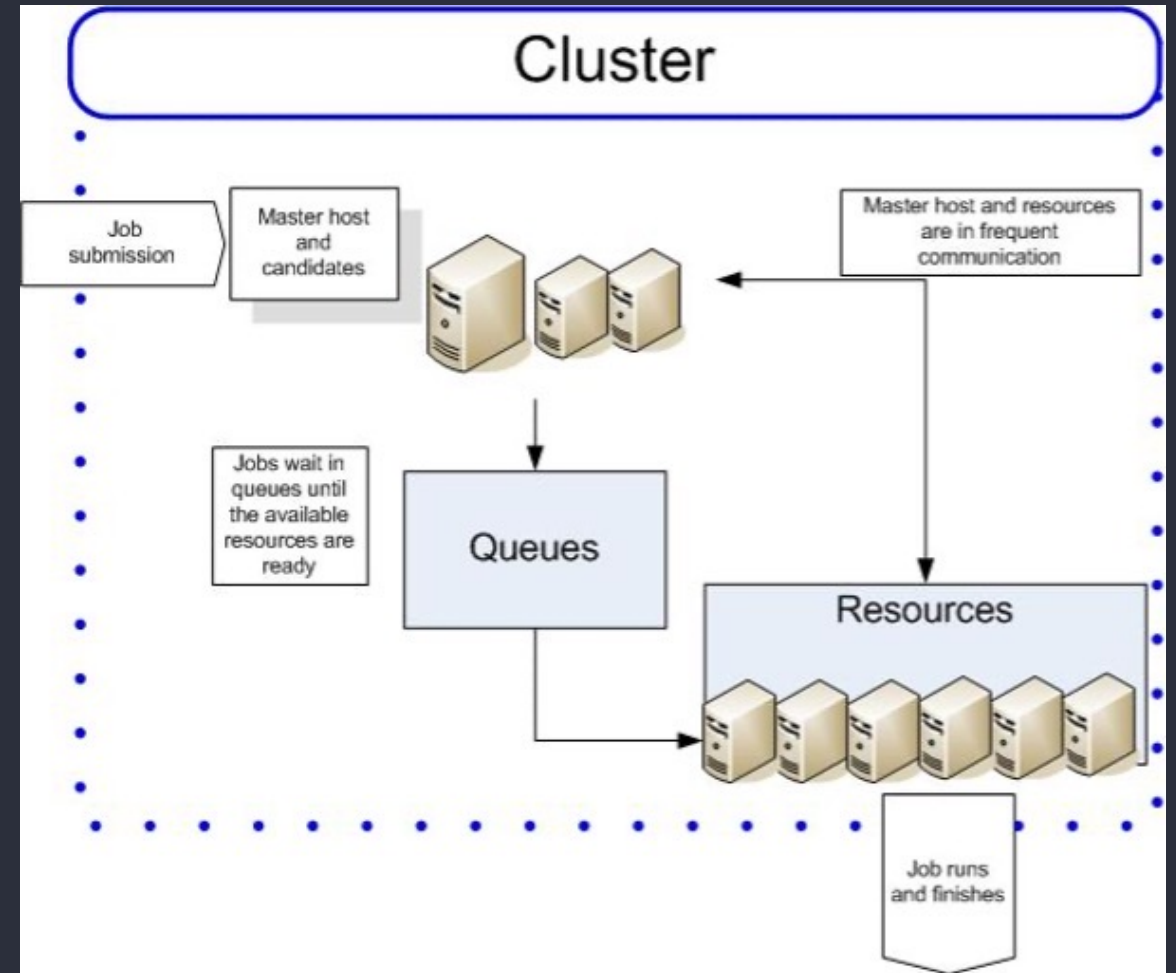
Client/Submission Hosts:

Submits jobs.

Execution/Server Hosts:

Runs jobs. These are the resources in the diagram.

Host and Node mean the same and can be used interchangeably.



Helix

Three master nodes, primary, secondary and tertiary. Multi master setup in an active/passive configuration, automatic failover.

Four login nodes, used for different groups.

Three server nodes for interactive jobs. 50 job slots per node, maximum of five jobs per user.

54 server nodes for all other jobs. 34 job slots per node, maximum of 600GB memory per job.

Helix

- Each server node has dual 50Gb/s connections to the LAN
- Weka backend servers are connected via dual 100Gb/s
- LAN is non-blocking architecture
- Each connected host can run at full speed without the network throttling

Queues

Inter – Interactive jobs only

Pipeline – Pipeline divisional queue

Short – For jobs running up to four hours.

Medium – For jobs running up to 24 hours.

Long - For jobs running up to one week.

Job scheduling

When a job is submitted to the cluster the management node will allocate the job to a server immediately if the resources are available otherwise, they get placed into a queue waiting for dispatch.

There are many scheduling configurations and submission options which affect how long your job takes to get dispatched to a server node for execution.

Resource requirements can affect the time it takes for the job to be submitted to an execution host. More resources requested, busier the cluster, the longer it will take to be dispatched. We have configured the cluster such that a job should never be permanently waiting for resources. Nonetheless it is recommended to be conservative with jobs resource requirements and review usage in the job output file.

Queue prioritisation

Queues in order of dispatch priority:
Inter, Pipeline, Short, Medium, Long

Fairshare

LSF will dispatch jobs from queues based on user shares, most users have equal share. There are some exceptions who have slightly more.

Pre-emption

Pending jobs in higher priority queues can pre-empt and suspended (SSUP status) running jobs in lower priority queues in order of preference:

Pipeline -> Long, Medium then Short

Short -> Long then Medium

Medium -> Long

Guaranteed Resource Pool

Helix queues have a guaranteed minimum number of hosts for running jobs:

Pipeline: 5

Short: 20

Medium: 15

Long: 15

Connecting to the cluster for the first time

Create ssh keys:

```
ssh-keygen
```

Copy over the ssh key to the Helix login node:

```
ssh-copy-id  
<username>@corp.gel.ac@<login node>.int.corp.gel.ac
```

Enter password

Create ssh config file:

```
nano ~/.ssh/config
```

Add the following:

```
host helix-login  
    Hostname <login node>.int.corp.gel.ac  
    User <username>@corp.gel.ac  
    IdentityFile ~/.ssh/id_rsa  
ssh helix-login
```

Save file you will then be able to login via:

3. Why use the HPC?

Why use the HPC?

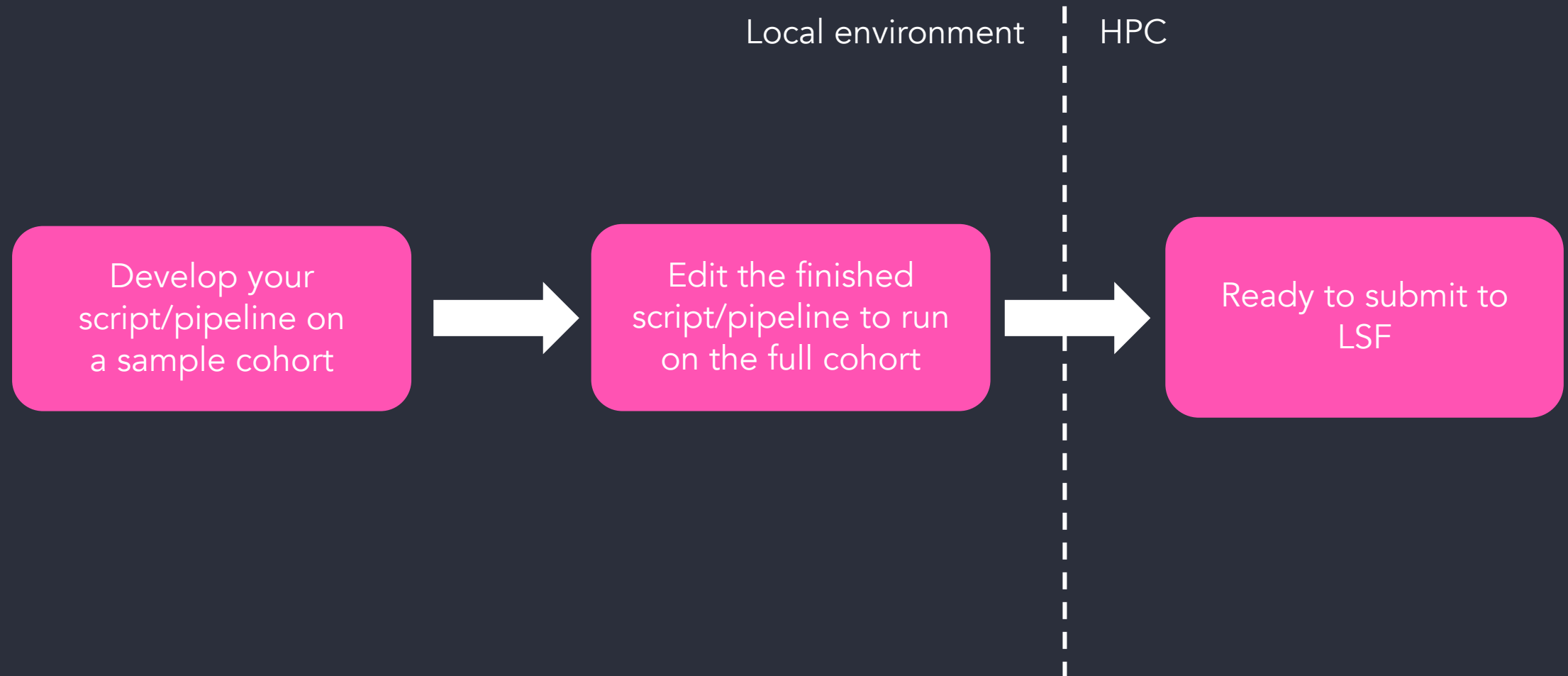
The HPC enables you to solve larger, more complex problems in far less time...

1. Increased performance when running complex scripts
2. Avoid usage capping in the Research Environment
 - Previously RE configuration has allowed researchers to use a disproportionate amount of memory, and consequently to cause stability issues for other researchers.
 - We now implement a resource cap which limits the maximum RAM to 12GB per user/RE session to improve the overall stability of the RE.

The local environment of the RE is designed for exploratory work.

The HPC is provided for "heavyweight" batch research.

Why use the HPC?



4. Logging into the HPC and working in an interactive session

Logging into the HPC: the Login nodes

When you log into our HPC , you will be connected to one of the **log in nodes**:

```
ssh username@corp.gel.ac@phpgridzLogn001.int.corp.gel.ac
```

username@corp.gel.ac@phpgridzLogn001.int.corp.gel.ac's password:

```
>[username@corp.gel.ac@phpgridzLogn001]$
```

Name	Who
phpgridzlogn001.int.corp.gel.ac	<u>GECIP & Clinical Researchers</u>
phpgridzlogn002.int.corp.gel.ac	<u>GECIP & Clinical Researchers</u>
phpgridzlogn004.int.corp.gel.ac	Commercial (Discovery Forum)
phpgridzlogn003.int.corp.gel.ac	Internal users

A word of caution...

- The login nodes act as a portal to the HPC for navigating our folders and submitting your jobs
- They have not been designed to handle the processing of data directly
- Unauthorised tools will not be permitted to run on the login nodes and may be terminated without warning



Command line coding on the HPC: the Interactive nodes

- Inter nodes: Access to HPC compute through a familiar terminal interface
- Useful for exploratory analysis and developing scripts that will later be scaled up

To start an interactive bash session:

```
bsub -Is -q inter -P <project code> bash
```

```
Job <931873> is submitted to queue <inter>.
```

```
<<Waiting for dispatch ...>>
```

```
<<Starting on phpgridzlsfe031>>
```

```
[username@corp.gel.ac@phpgridzlsfe031 ~]$
```

DEMO #1

5. How to create and monitor jobs on the HPC

Running larger analyses: LSF and the HPC Queues

- For most HPC use cases, your full analysis scripts should be submitted as "jobs" to the LSF
- The **Load Sharing Facility** balances job load, providing access to the HPCs full compute
 - Mature, commercial job scheduler by IBM
 - Takes your job requirements
 - Finds the best resources to run the job
 - Monitors its progress and provides detailed logging
- LSF jargon:
 - **Job**: A logical unit for application, environment and resources when computing a task
 - **Cluster**: A group of hosts running LSF that work together as a single unit
 - **Queue**: A scheduling entity where to-be-run and running jobs reside
 - **Execution host**: The actual compute resource (node) that runs a job
 - **Priority**: Priority at a technical level (not implying a job is more important than another)

Running larger analyses: LSF and the HPC Queues

- There are four available queues you may specify to the LSF, select according to expected job length:

Inter

Interactive jobs:

- Lightweight interactive or GUI tools
- Require constant connection to the submission shell
- Auto-killed after 2 weeks

Short

<4hrs

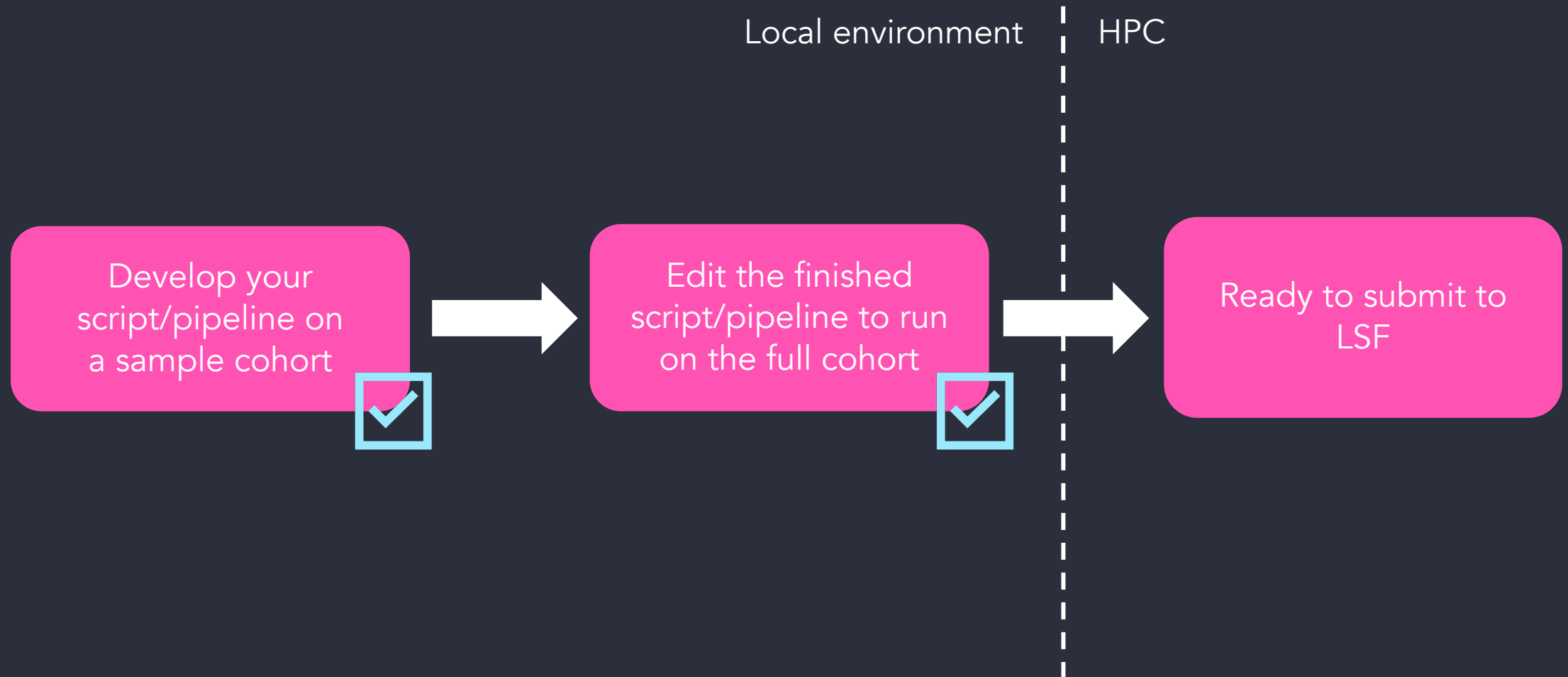
Medium

<24hrs

Long

<7days (or longer if explicitly configured)

Running larger analyses: LSF and the HPC Queues



Typical LSF submission

```
1  #!/bin/bash
2  #BSUB -q <your_queue>
3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName>
17
18 script
```

bsub < submission_script.sh

Typical LSF submission

```
1  #!/bin/bash
2  #BSUB -q <your_queue> short, medium, long
3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir">
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15
16 module load <moduleName>
17
18 script
```

bsub < submission_script.sh

Typical LSF submission

```
1  #!/bin/bash
2  #BSUB -q <your_queue>
3  #BSUB -P <yourProject> re_gecip_XXX / re_df_XXX
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
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18 script
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Typical LSF submission

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6 #BSUB -J <jobName>
7 #BSUB -R "rusage[mem=10000] span[hosts=1]"
8 #BSUB -M <max_memory_in_mb>
9 #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName>
17
18 script
```

paths to output error messages

bsub < submission_script.sh

Typical LSF submission

```
1  #!/bin/bash
2  #BSUB -q <your_queue>
3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName> the name of your job, helpful for monitoring
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
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17
18 script
```

bsub < submission_script.sh

Typical LSF submission

```
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2 #BSUB -q <your_queue>
3 #BSUB -P <yourProject>
4 #BSUB -o <path_to/job.%J.out>
5 #BSUB -e <path_to/job.%J.err>
6 #BSUB -J <jobName>
7 #BSUB -R "rusage[mem=10000] span[hosts=1]" requested resources - memory in MB, span = number of hosts
8 #BSUB -M <max_memory_in_mb>
9 #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
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16 module load <moduleName>
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bsub < submission_script.sh

Typical LSF submission

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3 #BSUB -P <yourProject>
4 #BSUB -o <path_to/job.%J.out>
5 #BSUB -e <path_to/job.%J.err>
6 #BSUB -J <jobName>
7 #BSUB -R "rusage[mem=10000] span[hosts=1]"
8 #BSUB -M <max_memory_in_mb> max memory usage (exceeding this will terminate the job)
9 #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName>
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18 script
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bsub < submission_script.sh

Typical LSF submission

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2  #BSUB -q <your_queue>
3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2 number of CPU nodes (each can cope with 16GB, so remember to update this)
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName>
17
18 script
```

bsub < submission_script.sh

Typical LSF submission

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3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir"> your current working directory (paths are relative to this)
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName>
17
18 script
```

bsub < submission_script.sh

Typical LSF submission

```
1  #!/bin/bash
2  #BSUB -q <your_queue>
3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName>
17
18 script
```

Set path to temporary directories i.e. your scratch space

bsub < submission_script.sh

Typical LSF submission

```
1  #!/bin/bash
2  #BSUB -q <your_queue>
3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName> load the module dependencies for your script (incl. languages, software)
17
18 script
```

bsub < submission_script.sh

Typical LSF submission

```
1  #!/bin/bash
2  #BSUB -q <your_queue>
3  #BSUB -P <yourProject>
4  #BSUB -o <path_to/job.%J.out>
5  #BSUB -e <path_to/job.%J.err>
6  #BSUB -J <jobName>
7  #BSUB -R "rusage[mem=10000] span[hosts=1]"
8  #BSUB -M <max_memory_in_mb>
9  #BSUB -n 2
10 #BSUB -cwd <"your_dir">
11
12 # Only retain the TMPDIR corresponding to your GECIP or Discovery Forum membership
13 export TMPDIR=/re_scratch/re_GECIP/<your_GECIP>/<your_username>
14 export TMPDIR=/re_scratch/re_discovery_forum/<your_discovery_forum_folder>/<your_username>
15
16 module load <moduleName>
17
18 script run your script!
```

bsub < submission_script.sh

Advice for more advanced jobs

Multicore jobs:

- A parallel job may span multiple hosts, with a number of processes allocated to each host.
- Specify number of CPUs with `-n`
- Schedule on to a single host to take advantage of its efficient shared memory: `span[hosts=1]`
- Spread out on to multiple hosts to take advantage of aggregate memory: `span[hosts=>1]`

Job dependencies:

- Sometimes, whether a job should start depends on the result of another job.
- To submit a job that depends on another job: use the `-w` option to `bsub` (it is lowercase `w`)

Job arrays:

- Allows a sequence of jobs to share the same executable and have different inputs and outputs
- Syntax: `bsub -J "ArrayName[index]" -i in.%I myjob`

Throttling jobs:

- Control the number of concurrent running jobs, being mindful of other users in the cluster.
- `bsub -q medium -J "myArray[1-1000]%50" <rest of the submission>`

Monitoring your job

command	description
<code>bsub</code>	submits a job to the cluster
<code>bqueues</code>	shows info on the cluster queues
<code>bjobs</code>	shows info on the cluster jobs
<code>bhosts</code>	shows info on the cluster hosts
<code>bhist</code>	shows info on the finished cluster jobs
<code>bacct</code>	shows statistics and info on finished cluster jobs
<code>bkill</code>	removes a job from the cluster
<code>lshosts</code>	shows static resource info
<code>lsload</code>	shows dynamic resource info

Useful link to all the LSF commands:

<https://www.ibm.com/docs/en/spectrum-lsf/10.1.0?topic=started-quick-reference>

DEMO #2

6. Tools and software available and how to load them

Modules

- Allows the HPC Helix to have **multiple versions of software** available
- **Dynamic modification** of a user's environment via *module files*
- **Chain module load commands** to set up your environment for your research
- >1,000 different set of tools and versions available

For quick guidance: `module help`

To list available modules: `module avail`

To load a module: `module load XXX`

e.g. `module load Lang/R/4.0.2-foss-2019b`

A quick mention on R versions & Libraries



- Several versions of R available (module avail): 3.6/4.0/4.1
- Each version has its own range of centrally installed packages
- `>library(<package_name>)`
- Rstudio is installed in the Research Environment for script development
- More from Ken in a moment...

Python packages & conda environments



- Several versions of python available (module avail): 2.7, 3.7, 3.10
- `import <package> // import <package> as <alias>`
- Conda* envs: `/re_gecip/shared_allGeCIPs/mvizueteForster/catalogues`
- ^ See the README files for usage
- Create your own! (see user guide)
 1. Copy `.condarc` to your working directory
 2. `conda create python==<version_number> --prefix /path/to/env/location`
 3. `source /resources/conda/miniconda3/bin/activate`
 4. `conda activate /path/to/env/location`
 5. `conda install -c conda-main <package_1>`
 6. `pip install <package_name> --index-url https://artifactory.aws.gel.ac/artifactory/api/pypi/pypi/simple`

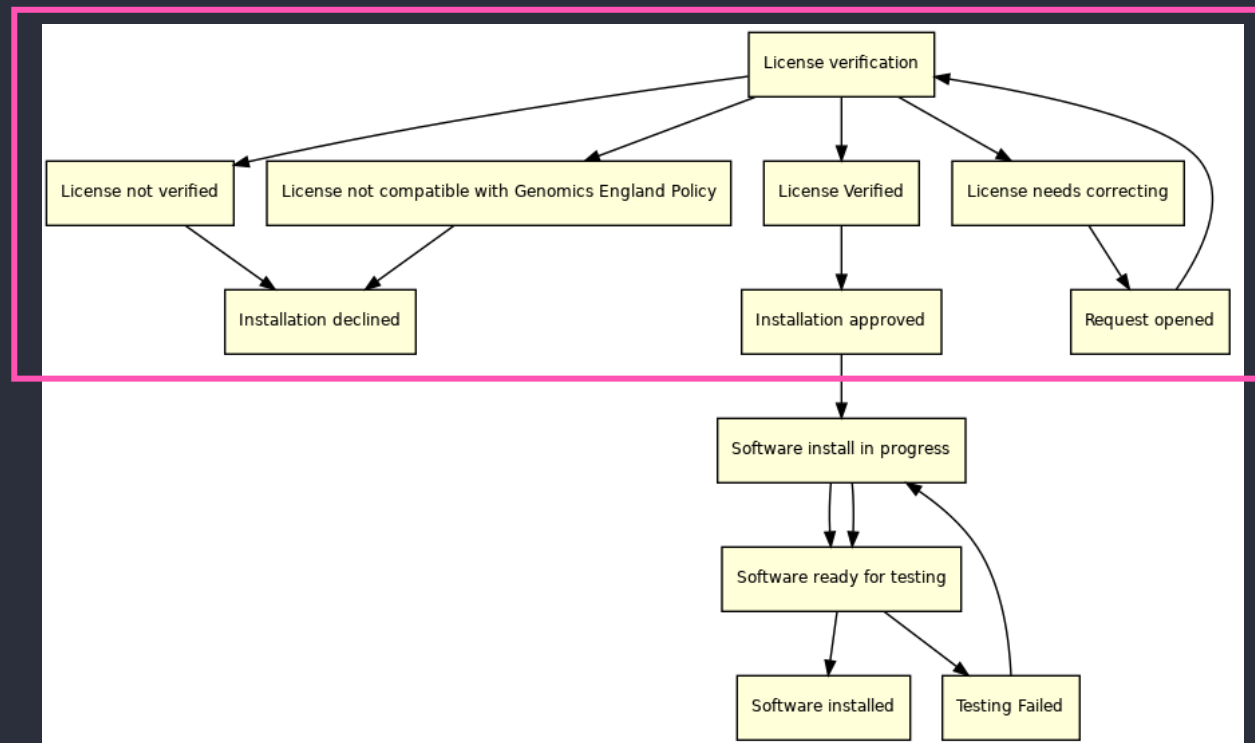
*Conda env = a ring-fenced environment that allows access to a specific set of python packages

DEMO #3

Software Requests

<https://research-help.genomicsengland.co.uk/display/GERE/How+to+request+Software+installation+within+the+Research+Environment>

- Software search catalogue is in development... watch this space
- Software not already available? Self-installation not possible?
- Raise a ticket: <https://jiraservicedesk.extge.co.uk/plugins/servlet/desk>

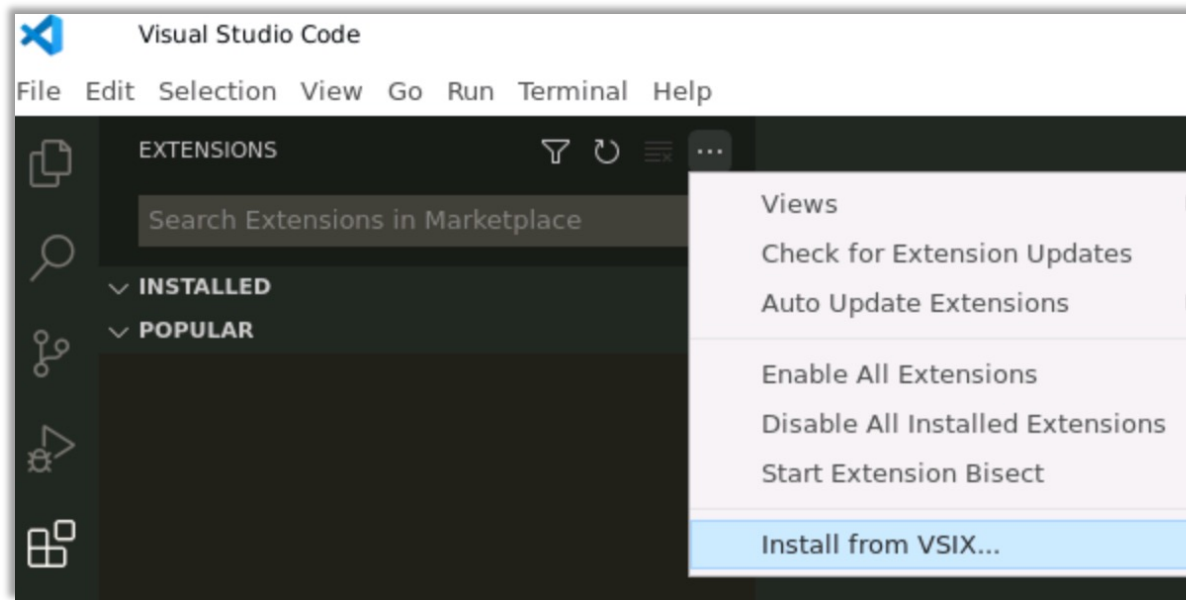


7. Interactive coding tools

Text editors/ IDEs

- several text editors/ IDEs available
- any can be used to write and develop scripts for submission to the HPC
 - scite, atom, gvim, vscode*, ...
 - *no direct access to vscode marketplace
 - curated set of extensions ~/public_data_resources/vscode_extensions/vsix

```
ls ~/public_data_resources/vscode_extensions/vsix
```



R configuration



- copy config files to your home directory (from Terminal)

on Inuvika Desktop

```
cp -a ~/gel_data_resources/example_config_files/Inuvika/. ./
```

on Helix HPC

```
ssh <username>@corp.gel.ac@phpgridzlogn00<N>.int.corp.gel.ac  
cp -a /gel_data_resources/example_config_files/Helix/. ./
```

- copies 3 files: .Renviron, .Rprofile, .netrc
 - edit **.netrc**

```
machine labkey-embassy.gel.zone  
login <username>  
password <password>
```

⚠ set permission to user only access, (i.e. -rw----- <username> <username> .netrc)

```
chmod 600
```

R/RStudio



- select R version

```
# on Inuvika Desktop
module avail R/
module load R/4.0.2
R # or rstudio
```

```
# on Helix HPC
ssh <username>@corp.gel.ac@phpgridzlogn00<N>.int.corp.gel.ac
bsub -Is -q inter -P <project_code> bash
module avail lang/R
module load lang/R/4.0.2-foss-2019b
R
```

- use RStudio on Helix HPC
 - open RStudio (double-click desktop icon)
 - open a Terminal (**T**ools > **T**erminal > **N**ew Terminal or Alt+Shift+R)

R/RStudio



(from Terminal inside RStudio)

- log into Helix HPC

```
ssh <username>@corp.gel.ac@phpgridzlogn00<N>.int.corp.gel.ac
```

- start an interactive session (RE sessions are capped at 12GB)

```
bsub -q inter -P <project_code> -Is -n 1 -R rusage[mem=16000] -M 16000 /bin/bash
```

- select R version and start R

```
module load lang/R/4.0.2-foss-2019b  
R
```

- open new (File > New File > R Script or Ctrl+Shift+N) or existing script
- send code to Terminal
 - optional keyboard shortcut change, recommended for Mac users (Tools > Modify Keyboard Shortcuts...)
 - change "**Send Selection to Terminal**" (suggested: Ctrl+Cmd+Enter)

R/RStudio



- make a common folder to store packages, e.g., ~/re_gecip/<domain>/R_packages
- **install / load** on Inuvika Desktop: ~/re_gecip/<domain>/ or ~/re_df/<domain>/
- **load only** on Helix HPC: /re_gecip/<domain>/ or /re_df/<domain>/

Install and load on Inuvika desktop

```
install.packages("<package>", lib = "~/re_gecip/yourDomain/R_packages")  
library("<package>", lib = "~/re_gecip/yourDomain/R_packages")
```

- raise a service desk ticket for dependency failures or packages not in artifactory
- all R packages located on GitHub require GEL admins to install them
- * Bioconductor access unstable; look out for announcements

Load (only) on Helix HPC

```
library("<package>", lib = "/re_gecip/yourDomain/R_packages")
```



Jupyter Notebook/ Lab

- login to Helix HPC, start an interactive session

```
ssh <username>@corp.gel.ac@phpgridzlogn00<N>.int.corp.gel.ac  
bsub -P <project_code> -M 25G -Is -q inter bash
```

- start Jupyter Lab in the conda environment 2021_base_clone (note URL*)

```
source /resources/conda/miniconda3/bin/activate  
conda activate 2021_base_clone  
jupyter lab --no-browser --ip="*" --port=<remote_port>
```

- connect to your Jupyter Lab session (from another terminal)

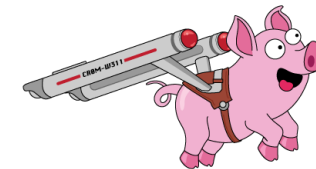
```
# Set host and remote ports to the same value. Don't use: 8888, 5000, 8000 or 9000  
# (NB. this is one line, just wrapped)  
ssh -4 -L <host_port>:phpgridzlsfe<N>.cluster:<remote_port>  
<username>@corp.gel.ac@phpgridzlogn00<N>.int.corp.gel.ac
```

- start a browser, paste URL*

8. Bringing in your own tools and software

Software/ Containers

nextflow



- **typical software installation raise a service desk ticket**

Containers

- to use containerised software with `singularity`

on Helix HPC

```
module load tools/singularity/3.8.3
```

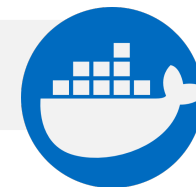
- default image cache dir `/home/<username>/.singularity/`
- for batch jobs running on compute nodes set the environment variable `SINGULARITY_CACHEDIR`
 - **Recommended:** add the following to `~/.bashrc`

```
SINGULARITY_CACHEDIR="/re_gecip/<my_gecip>/<username>/singularity_cache/"
```

- run, e.g., `bcftools`

```
singularity exec docker://quay.io/biocontainers/bcftools:1.13--h3a49de5_0 bcftools --version
```

 **read about software licensing** (tl;dr, it's your responsibility) *



GEL Workflows

- we provide workflows to our users targeting different areas of research and data
- some are written in WDL/Cromwell, and some in Nextflow DSL1

Aggregate Variant Testing workflow

Assess the cumulative effects of multiple rare variants on a gene or region for a cohort of case vs control

Functional Annotation workflow

Simplify the process of annotating VCFs using VEP

Gene-Variant workflow

Extract variants within a gene(s), aggregate and annotate with VEP

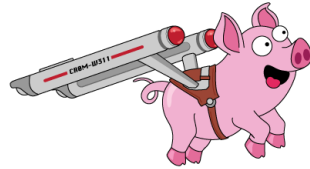
GWAS workflow

Produce GWAS summary statistics, manhattan and qqplot figures

SV/CNV workflow

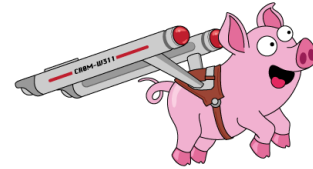
Extract large structural and copy number variants for a gene or region

nextflow



GEL Workflows

nextflow



- for **WDL/Cromwell workflows**, copy the directory, run the shell script

```
cp -R /gel_data_resources/workflows/BRS_tools_geneVariantWorkflow/v1.7/ ~/my_workflows
bsub < ./submit_workflow.sh
```

- for **Nextflow workflows**, load nextflow and singularity, run w/ nextflow CLI

```
module load bio/Nextflow/21.10.6 singularity/3.2.1

nextflow run /pgen_int_data_resources/workflows/BRS_tools_GWAS_nf/v1.1/main.nf \
--phenoFile 'example.pheno' \
--unrelatedFile 'example.unrel' \
--pgenlist 'example.csv' \
--HQplinkfile 'example.{bed,bim,fam}' \
--sampleIDCol 'platekey' \
--sexCol 'sex' \
--phenoCol 'pheno'
```



Best practices for using the HPC

DO...

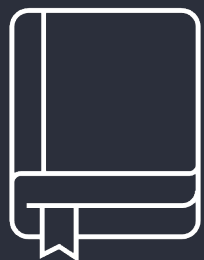
- make use of interactive sessions for lightweight analysis and script development
- estimate the length of your job and choose the most appropriate queue
- consider queue priority/scheduling when requesting resources through LSF
- use singularity containers to import software to improve your analysis
- utilise the GEL workflows if they will help you achieve your research goals
- raise a "software request" if you are unable to install your own software
- raise a "service request" if we can help you with anything
- use '-o' and '-e' options with job submissions as offers resource usage any output and errors for troubleshooting

DO NOT...

- use the log in nodes to run any analysis
- request excessive resources to run your jobs

9. Getting help and questions

Getting help



Check our documentation:

- <https://research-help.genomicsengland.co.uk/>
- Click on the documentation icon in the environment
- Advice for getting help: <https://research-help.genomicsengland.co.uk/display/GERE/8.+Getting+help+and+resolving+problems>



Contact our Service Desk:

- ge-servicedesk@genomicsengland.co.uk
- Self-service portal: <https://jiraservicedesk.extge.co.uk/plugins/servlet/desk>

Questions



Your microphones are all muted



Use the Zoom Q&A to ask questions



Upvote your favourite questions: if we are short on time we will prioritise those with the most votes

Future sessions

17 th January	Introduction to the Research Environment	Virtual
21 st February	Using the Research Environment for clinical analysis	Virtual
21 st March	Importing tools and data to use in the Research Environment	Virtual
18 th April	New datasets in the RE: GMS, Covid and pilot data	Virtual
May TBC	Building cancer cohorts and survival analysis	TBC
June TBC	Building rare disease cohorts with matching controls	TBC
July TBC	Finding participants based on genotypes	TBC
August TBC	Getting medical records for participants	TBC
September TBC	Tools created by researchers – a showcase	TBC
October TBC	Using GEL data for publications and reports	TBC
November TBC	What tools and workflows should I use to fulfil an overall goal?	TBC
December TBC	Running workflows on the HPC and Cloud	TBC

Past training

In the User Guide:

- Redacted slides and videos
- Q&A from sessions

Sessions:

- Introduction the Research Environment, March
- Building a cohort based on phenotypes, May
- Finding participants based on genotypes, July
- Getting medical history for participants, September

Feedback

Thank you