



Introduction to NeSI HPC Platforms

New Zealand eScience Infrastructure

Support

- Expert knowledge in multiple domains



Consultancy

- Analysis, debug and optimization of user applications



Training

- Software Carpentry / Data Carpentry
- Intro & advanced HPC training



NeSI

New Zealand eScience Infrastructure



Data transfer

- high speed data input/output
- Partnership with Globus (global data management platform)



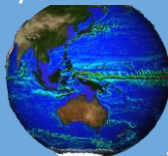
Hardware and software for compute and analysis

- ~700 compute nodes
- hundreds of software packages



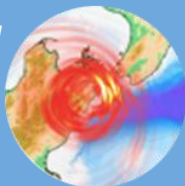
**Dr Olaf Morgenstern and
Dr Erik Behrens (Earth Science)**

*Deep South Challenge project using
NeSI supercomputers for climate
modelling, incorporating regional
and global scales.*



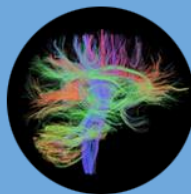
**Yoshihiro Kaneko
(Seismology)**

*GNS Science using NeSI
supercomputers to
recreate earthquake
events to better
understand their
processes and
aftermath effects.*



**Dr Richie Poulton
(Psychology)**

*Using NeSI Data
Transfer platform to
send MRI scan images
from Dunedin
Multidisciplinary Health
& Development Study
Research Unit to a
partner laboratory in
the United States for
analysis.*



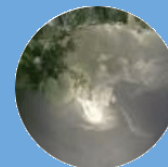
Andrew Chen (Engineering)

*Using NeSI supercomputers for advancing image
processing capabilities using computer vision*



**Dr Kim Handley
(Biological
Sciences)**

*Genomics Aotearoa
project using NeSI
supercomputers to
better understand
environmental
processes on a
microbial level*



**Dr Sarah Masters,
Dr Deborah Crittenden,
Nathaniel Gunby
(Chemistry)**

*Using NeSI supercomputers to
develop new analysis tools for
studying molecules' properties.*



 Location of our team



Definining High Performance Computing

While modern computers can do a lot (and a lot more than their equivalents 10-20 years ago), there are limits to what they can do and the speed at which they are able to do this. One way to overcome these limits is to pool computers together to create a cluster of computers. These pooled resources can then be used to run software that requires more total memory, or need more processors to complete in a reasonable time.

One way to do this is to take a group of computers and link them together *via* a network switch. Consider a case where you have five 4-core computers. By connecting them together, you could run jobs on 20 cores, which could result in your software running faster.

So, this will do it ?



Not exactly

Mahuika: 8980 cores

These will

Maui: 18,560 cores



Shared Storage

- IBM ESS GL4S and GL6S disk storage (8.7PB, 140 GB/s), Spectrum Scale (aka GPFS)
- EDR Infiniband network to storage
- Spectrum Protect Hierarchical Storage Management system (capable of storing up to ~60PB)

HPC for Life Scientists

Genomics



Image courtesy of <http://www.journaloia.org/blog/what-is-the-purpose-of-genomics-4581.html>

Molecular Dynamics

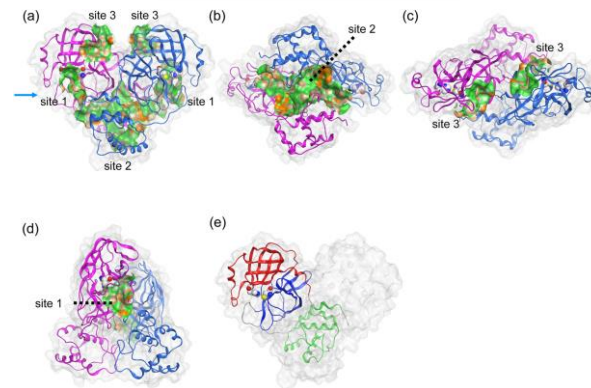


Image courtesy of <http://www.journaloia.org/blog/what-is-the-purpose-of-genomics-4581.html>

Precision Medicine

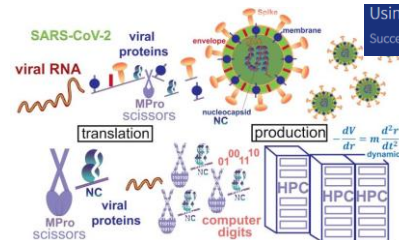


Image courtesy of : <https://www.deepgenomics.com>

Conservation



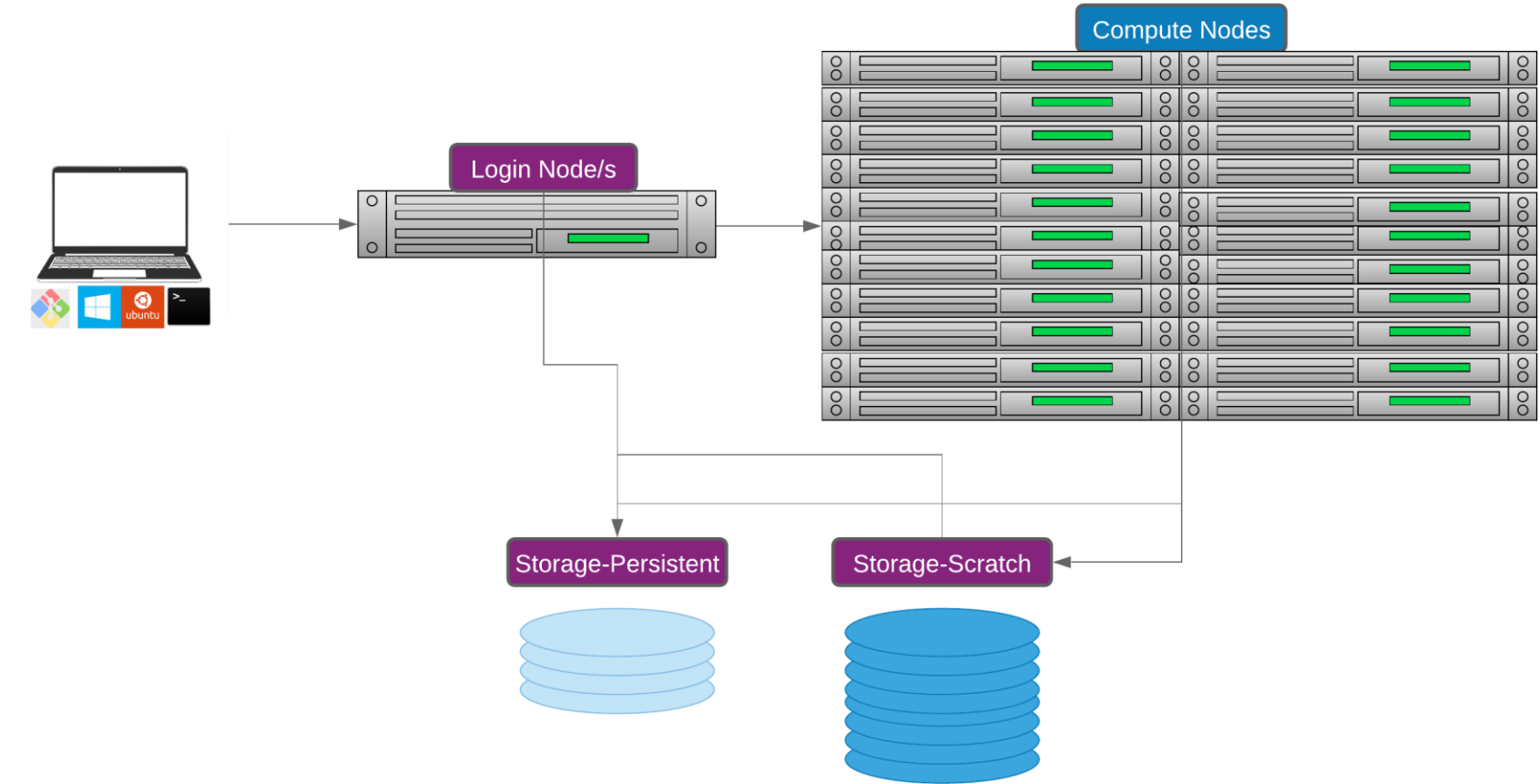
Virtual Drug Screens



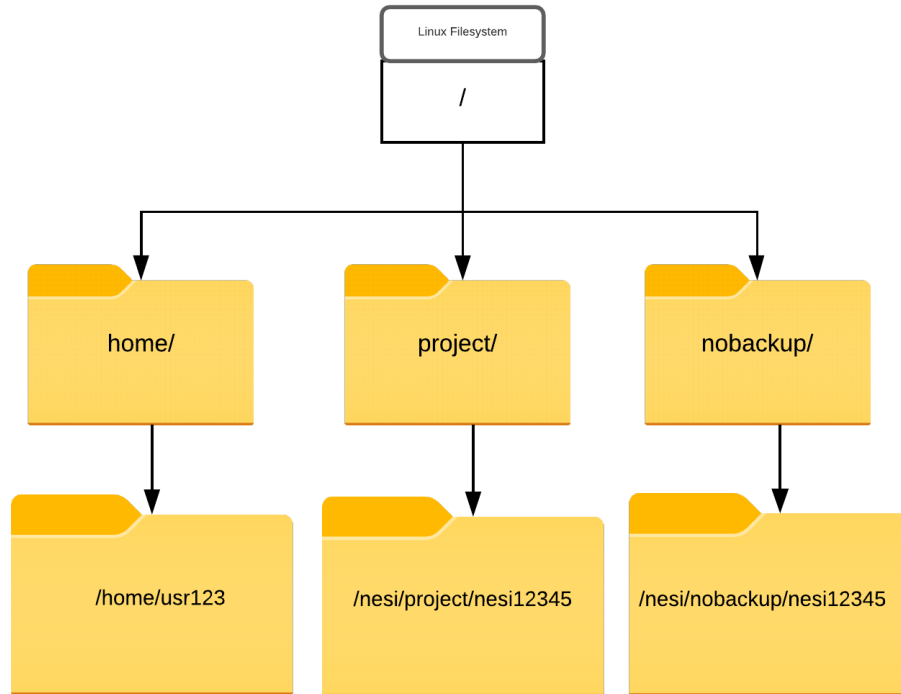
Using Molecular Dynamics To Find Drugs And Vaccines For COVID-19
Success Stories

Image courtesy of : <https://prace-ri.eu/using-molecular-dynamics-to-find-drugs-and-vaccines-for-covid-19/>

HPC Architecture



NeSI Filesystems

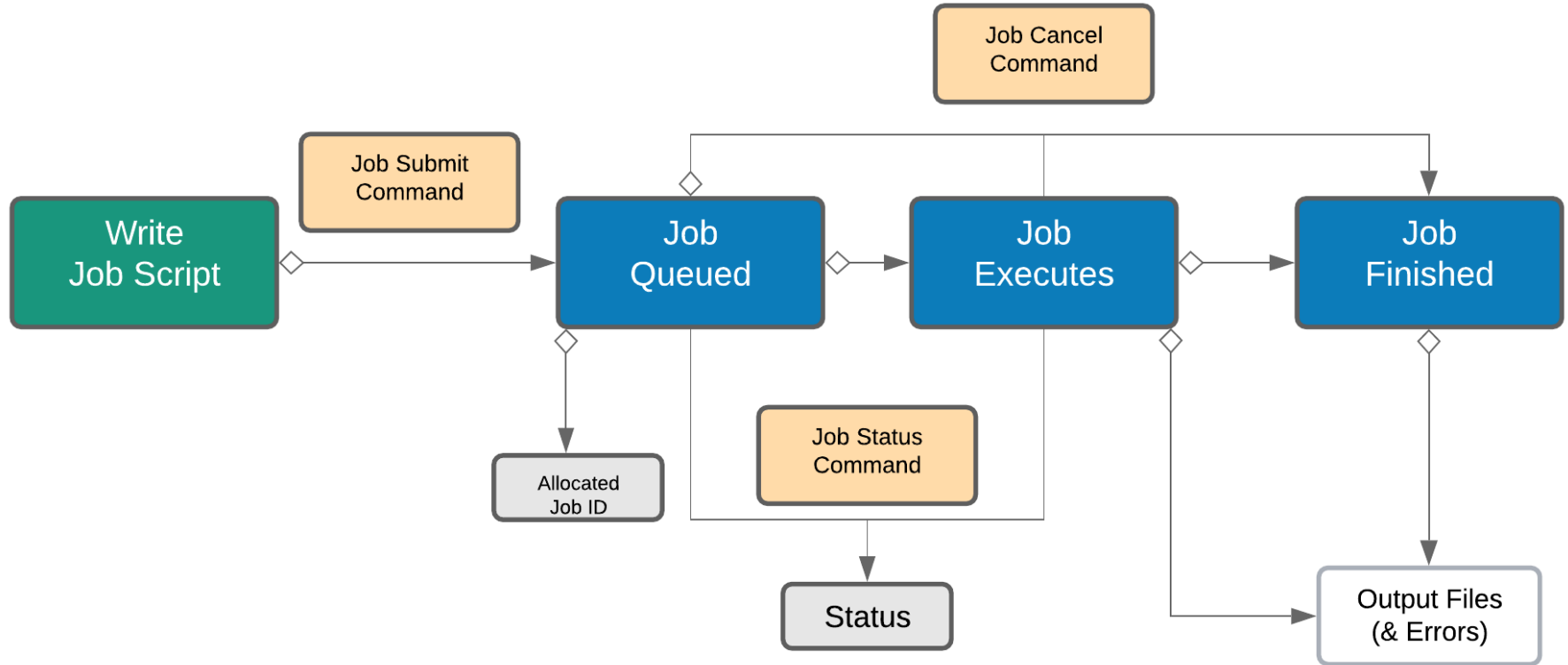


Batch System

What is a batch system?

- Mechanism to control access by many users to shared computing resources
- Queuing / scheduling system for users' jobs
- Manages the reservation of resources and job execution on these resources
- Allows users to “fire and forget” large, long calculations or many jobs (“production runs”)

Batch System flow



NeSI Platforms use SLURM

sbatch

submit a batch script

scancel <jobid>

delete one of your jobs from the queue

srun

launch a process across multiple CPUs

sinfo

view information about Slurm nodes and partitions

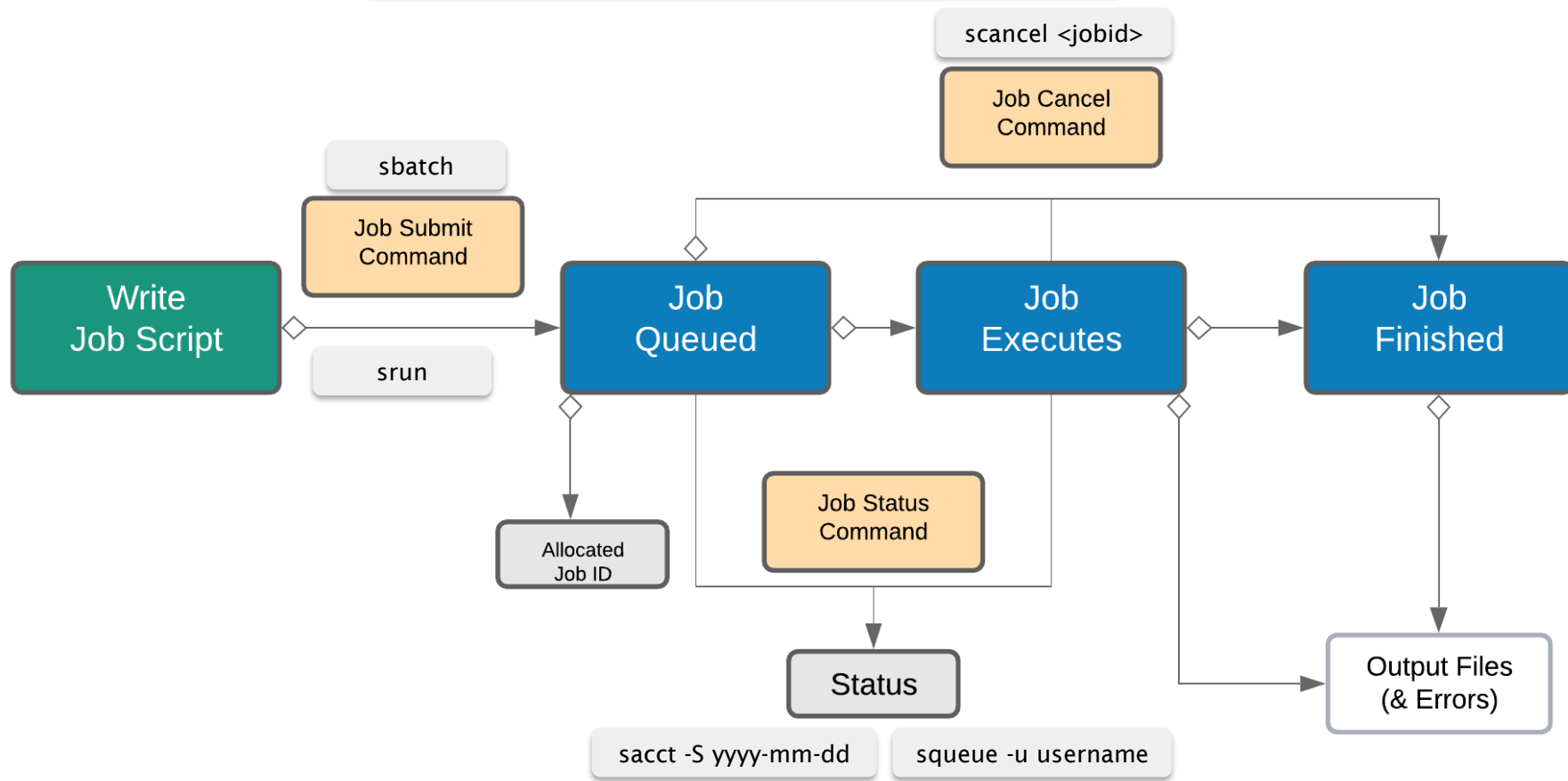
sacct -S yyyy-mm-dd

display accounting data for all jobs and job steps in the Slurm job accounting log or Slurm

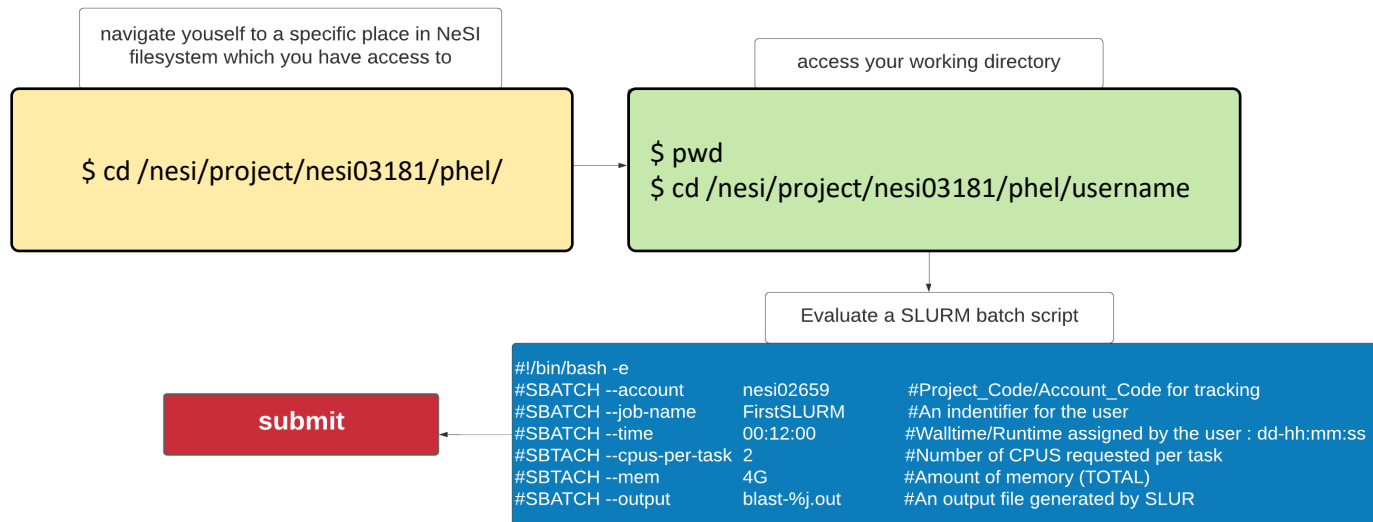
squeue -u username

check the status of jobs on the system

Batch System flow - With the commands



Bringing it altogether



Bringing it altogether – Example 2

Basecalling with GPU



Image courtesy of <https://nanoporetech.com/about-us/news/oxford-nanopore-announces-ps100-million-140m-fundraising-global-investors>

Getting Help :

- Search or submit a request at <http://support.nesi.org.nz>, or email support@nesi.org.nz
- Search through our [support documentation](#)
- If your job failed, please mention:
 - The job ID
 - Your slurm file path
 - What command(s) you used
 - The error message
- [We also have a Consultancy Service \(optimise your code..\)](https://www.nesi.org.nz/services/consultancy) <https://www.nesi.org.nz/services/consultancy>
- Subscribe to updates for systems issues, etc. <https://status.nesi.org.nz/>



New Zealand eScience Infrastructure

NeSI Support: