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NeSI's Flexible HPC: A programmable infrastructure for advanced research solutions

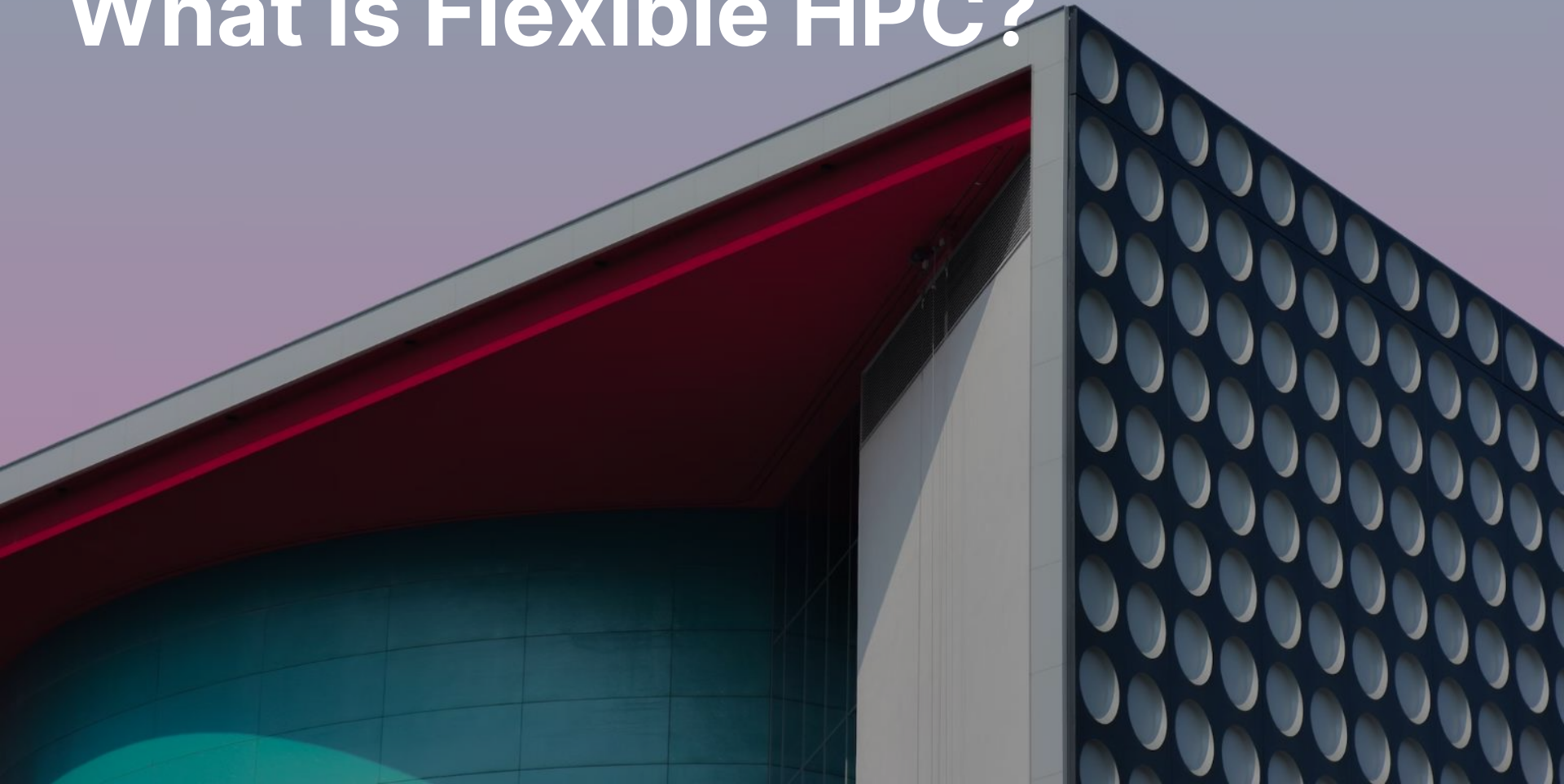
eResearch Australasia 2023



Presentation outline

- What is NeSI's Flexible HPC?
- Where we are now
- Our tenants
- Future pathways

What is Flexible HPC?



Background

NeSI has been providing traditional style HPC in NZ

Flexible HPC:

- Cloud-native eResearch service development and hosting platform
- New styles of access with more interactivity
- Host for BYO kit

Why

- Responding to the demands around diverse needs across the sector
- Equitable access
- On-shore solution for data sovereignty
- Enabling deep collaboration

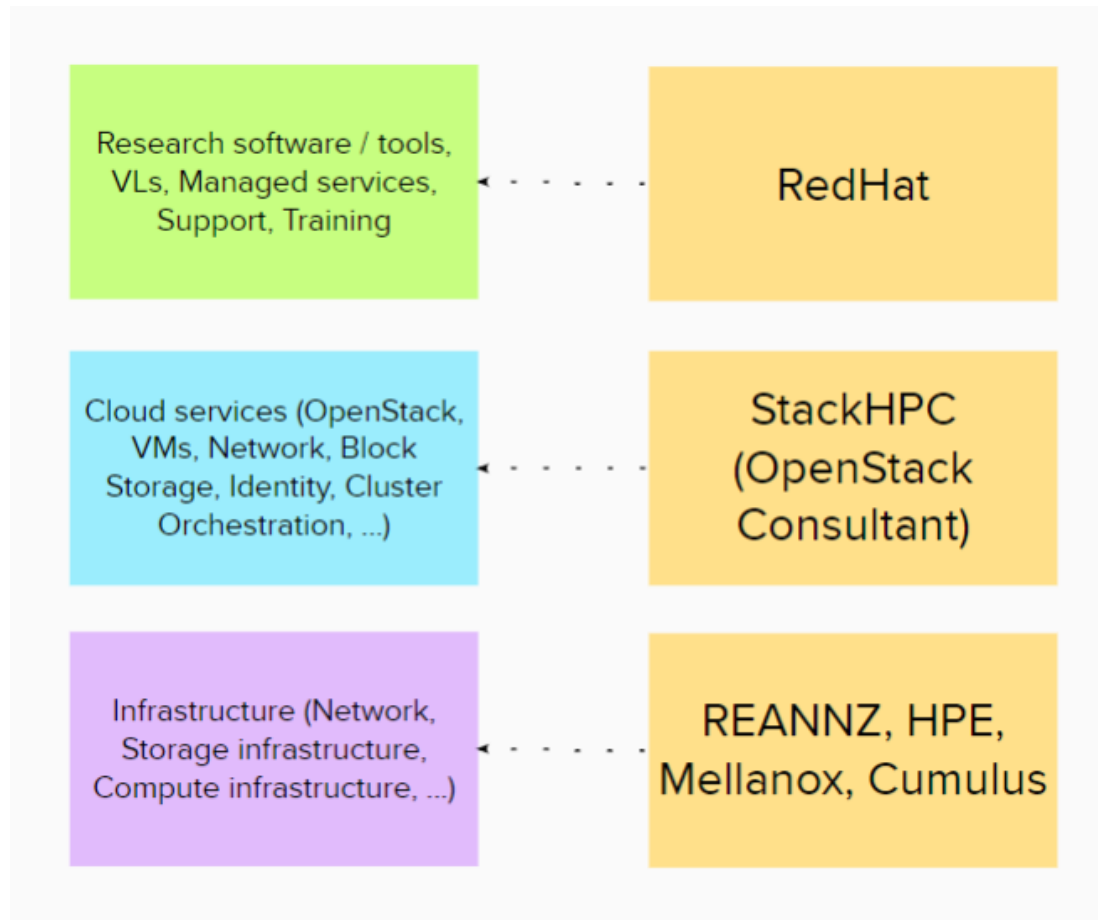
Infrastructure solution

Research software / tools,
VLs, Managed services,
Support, Training

Cloud services

Infrastructure

Infrastructure solution - partnerships and collaborations



Where we are now



Research Developer Cloud



Research Developer Cloud

Infrastructure -as-a-Service

Our platform's cloud building blocks include:

<https://www.nesi.org.nz/developercloud>



Compute

Virtual machines optimised for high-performance computational needs. Multiple flavours of CPU and GPU resources to support a range of compute and memory requirements.



Images

Tailored operating systems to meet your research computing and data needs. Ready-to-use options available, as well as capability to create custom images and contribute to a pool of community-developed images.



Storage

Scalable storage space that can be dynamically mounted to your Compute instances. Options to encrypt storage volumes for added security.



Networks

Fast, reliable, and secure connectivity built on the [REANNZ national network](#). Options for network customisation and security groups.



Identity

Identity management services to create application credentials and control access to your projects.

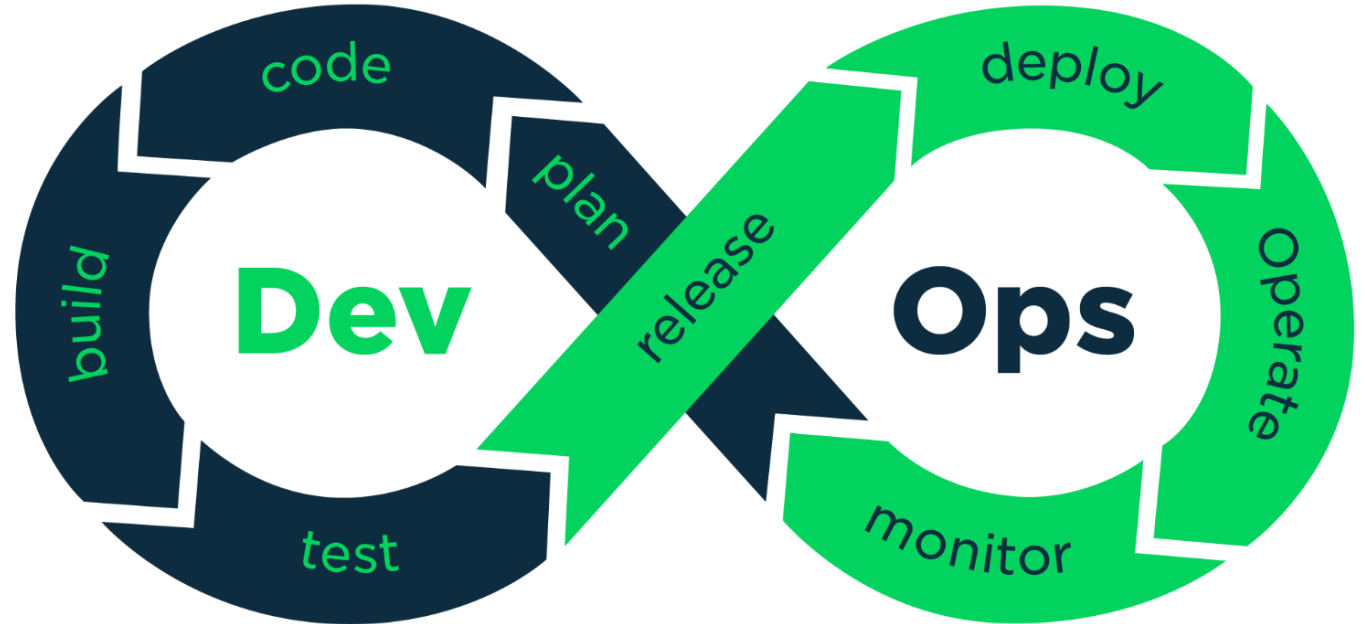


Application Programming Interface (API)

All services are programmable via a public API to enable repeatable definition of infrastructure through software code.

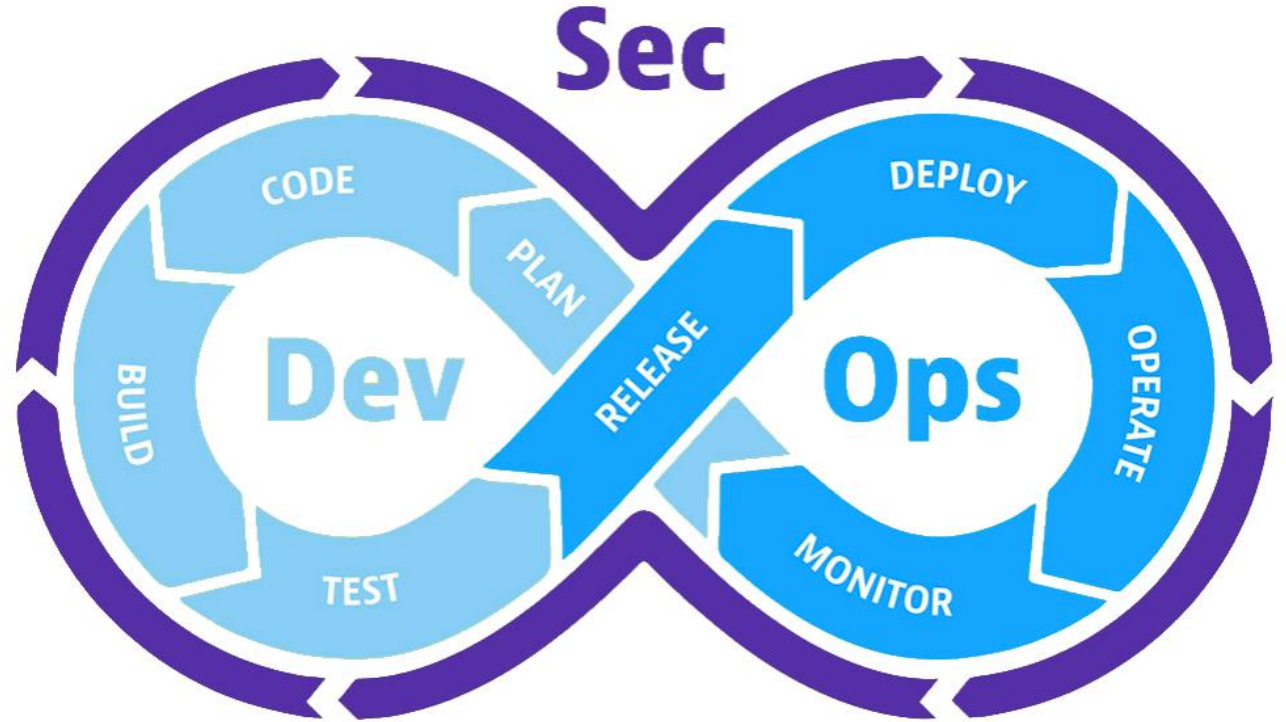
DevOps

Focused on delivering a great developer experience

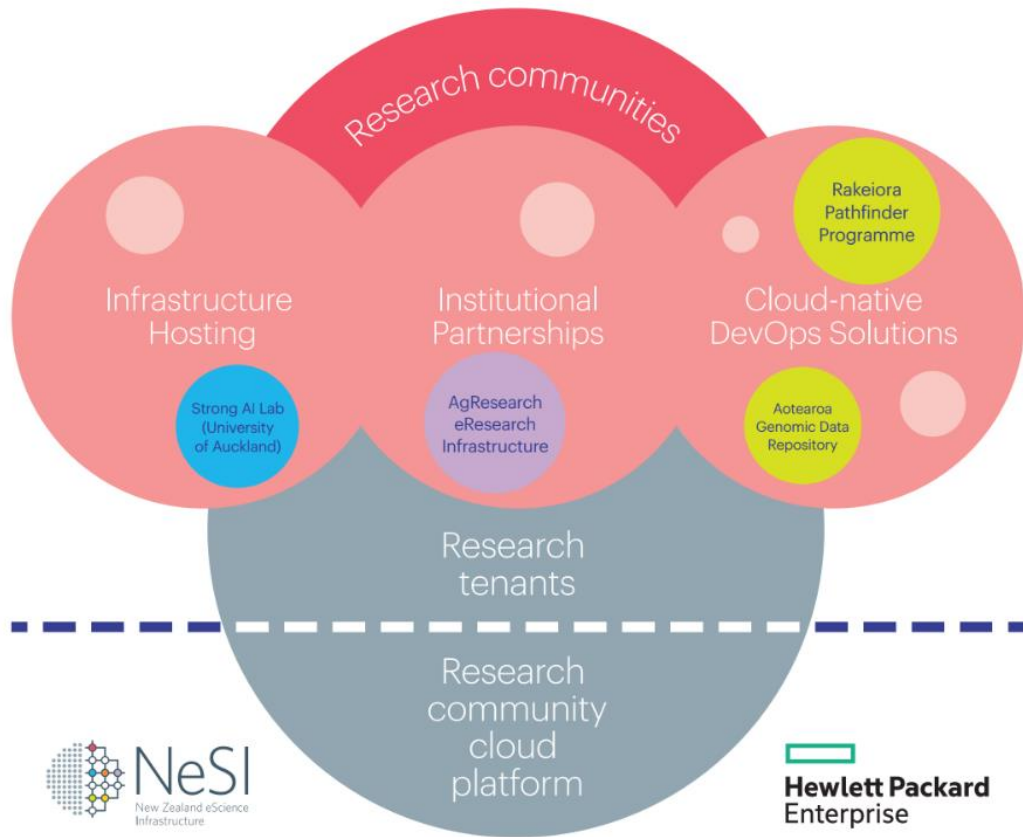


The DevOps workflow. Source: Pease, 2017.

DevOps and DevSecOps



Delivering impact towards research communities through collaboration



REANZ

A team of global experts driving innovation

StackHPC



Our tenants



Our tenants

Early tenants with varying styles:

- Rakeiora project: Prototyping a walled garden solution for Māori communities to have full control and consent
- SAIL group (Strong AI Lab, University of Auckland): Bare metal hosting of special kits for machine learning
- AGDR (Aotearoa Genomic Data Repository): Building and deploying a data repository as a cloud based solution
- AgResearch: Extensive partnership that includes dedicated hardware, custom services, and service management
- (Internal) Training environment for ML101

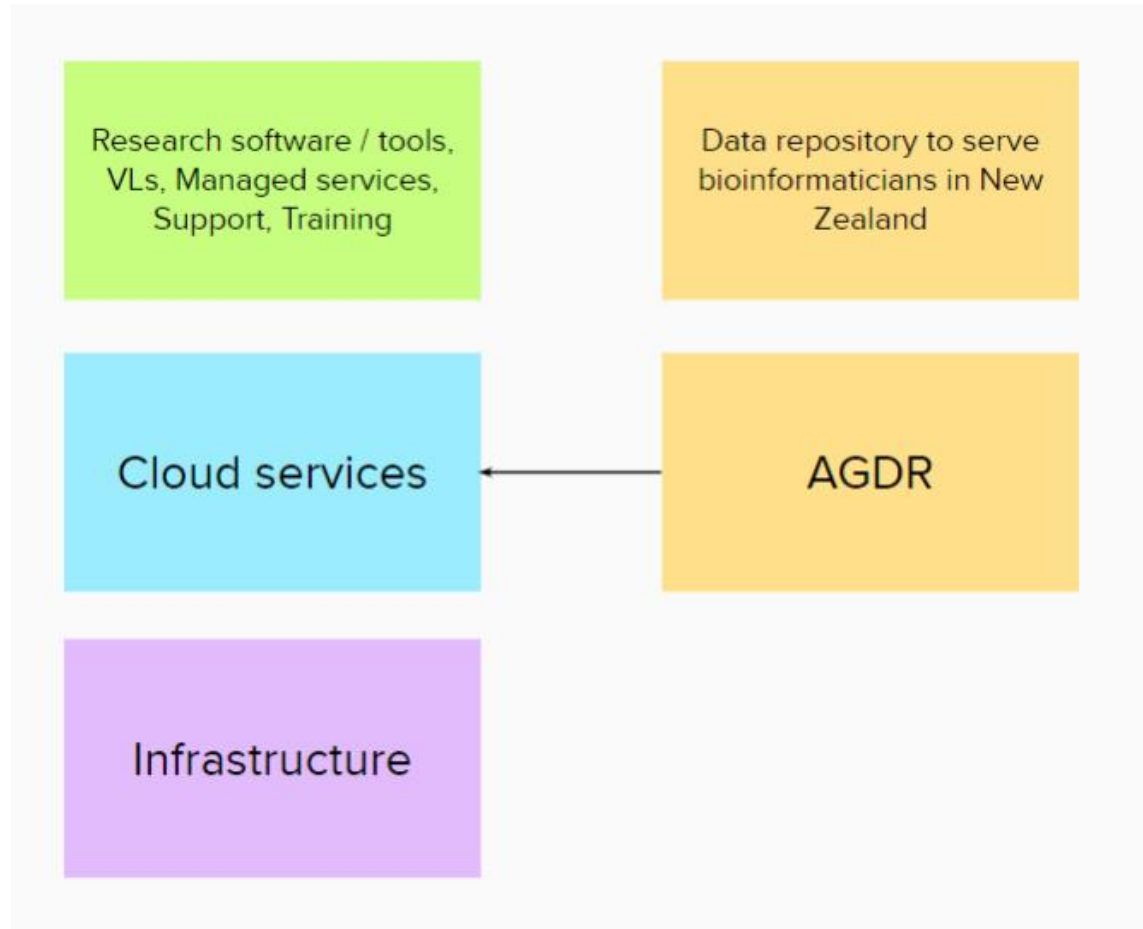
AGDR (Aotearoa Genomic Data Repository)

Collaboration with Genomics Aotearoa. Repository for genome sequencing data for taonga species

Challenges: data and platform onshore, kaitiakitanga, FAIR

Technology used: Gen3 (Open source genomic domain data repository solution, University of Chicago), Kubernetes (for platform management, health and scaling), Google Forms / Zendesk (for application process)

AGDR





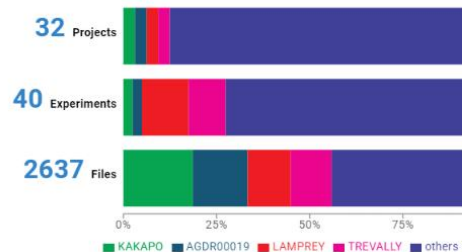
kākāpō chick photo by Dianne Mason, 2009 CC2.0

Aotearoa Genomic Data Repository

The Aotearoa Genomic Data Repository has been jointly developed by Genomics Aotearoa and NeSI to provide a secure place for the New Zealand research community to store and share genomic data. Version 1.0 of the repository is up and running, but we are still adding functionality, so you will see ongoing improvements as we implement new features.

Projects

Submit Data



AGDR:

Publication

Aotearoa genomic data repository: An āhuru mōwai for taonga species sequencing data

DOI: [10.1111/1755-0998.13866](https://doi.org/10.1111/1755-0998.13866)

“This resource has been developed to follow the principles of Māori Data Sovereignty, and to enable the right of kaitiakitanga (guardianship), so that iwi, hapū and whānau (tribes, kinship groups and families) can effectively exercise their responsibilities as guardians over biological entities that they regard as taonga (precious or treasured).” - from the abstract

Keywords: CARE principles; Māori; benefit-sharing; data repository; indigenous data sovereignty.

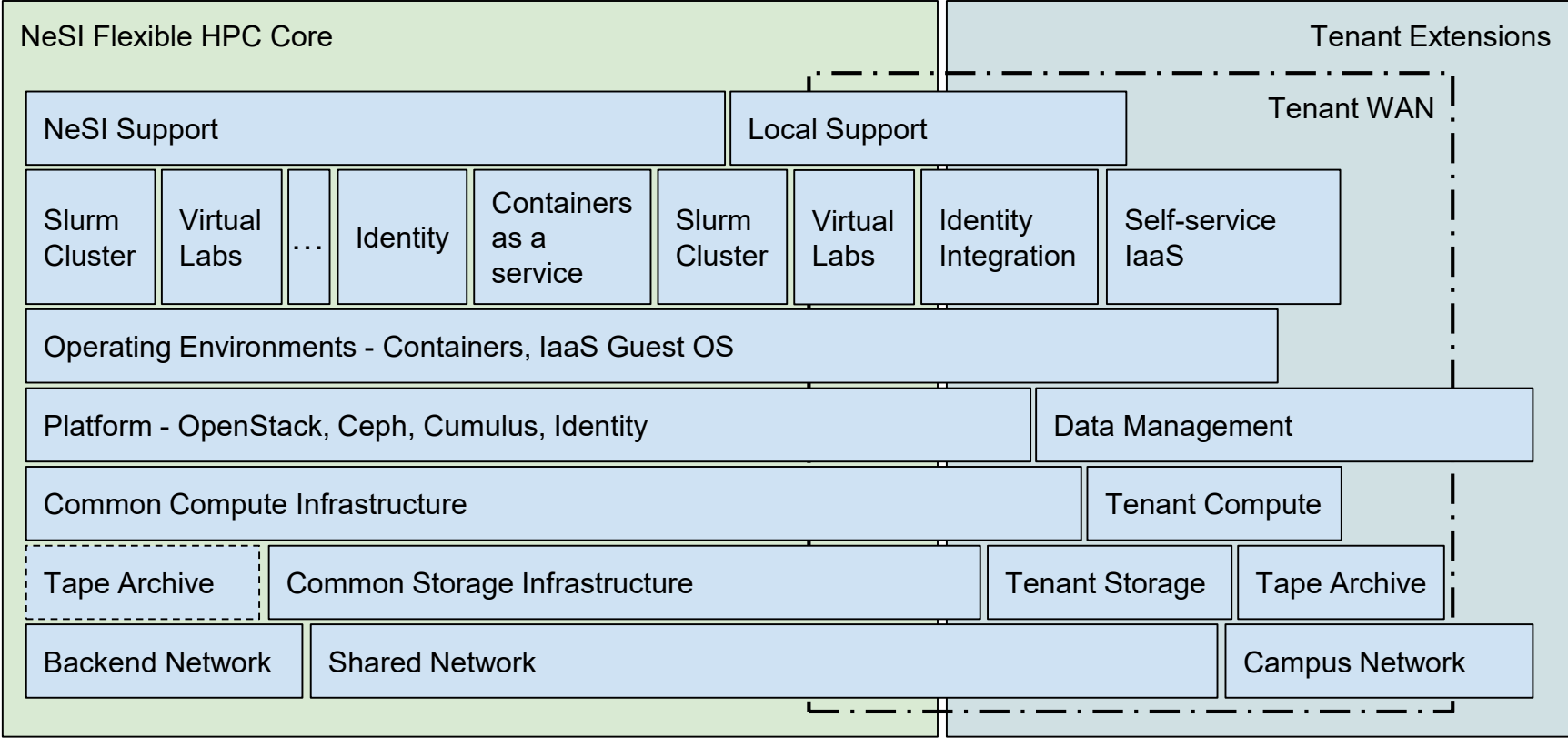
AgResearch

Institutional level collaboration to develop a full eRI (eResearch Infrastructure) for the researchers at AgResearch. Full suite of tools and services and ongoing development and support.

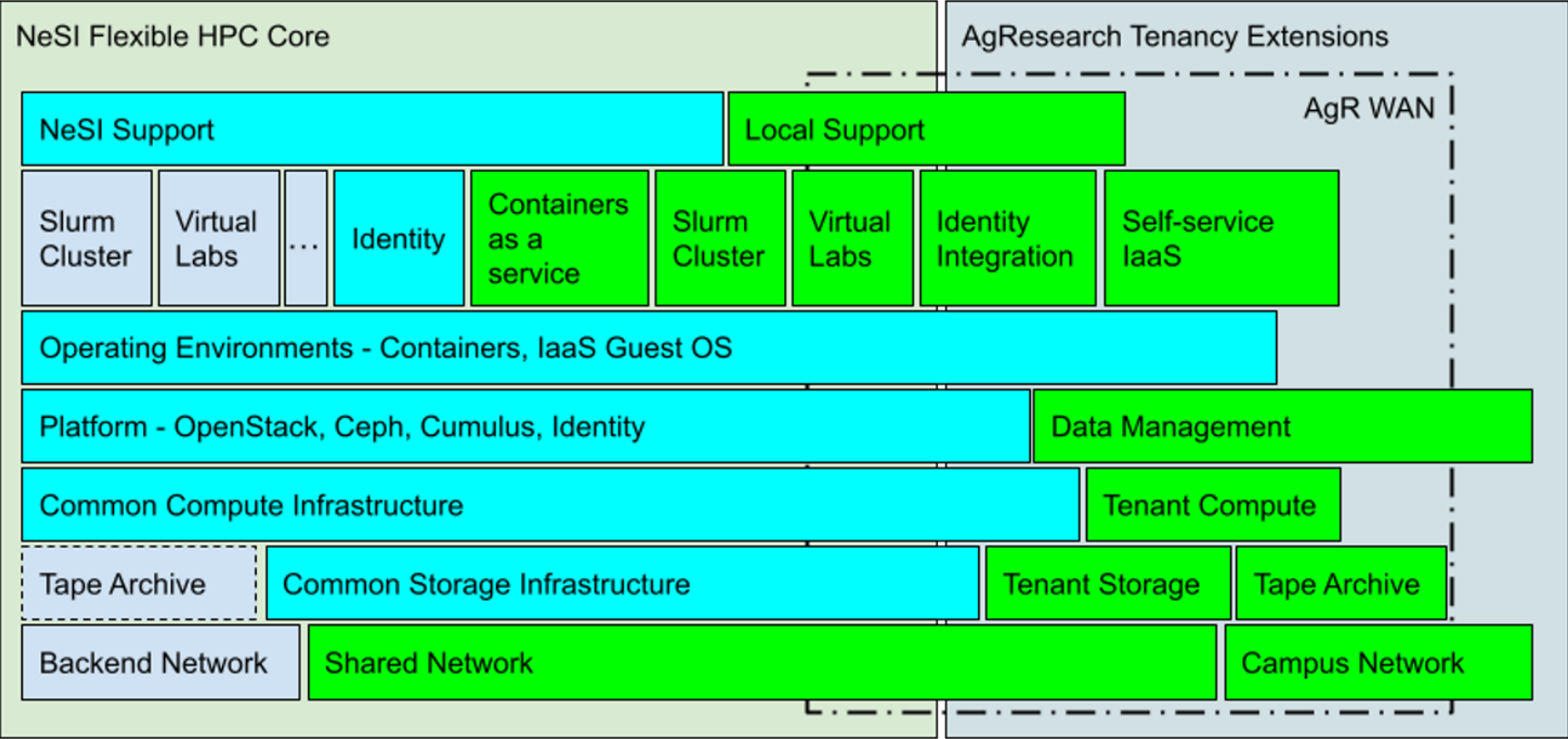
Challenges: Data migration, identity management, developing and supporting a growing list of tools and services.

Technology used: Keycloak (identity management), Open OnDemand (interface layer for end users to access various services), Slurm appliance (Slurm based cluster back-end to provide compute)

FlexiHPC tenancy cake - detailed view



AgResearch tenancy




eRI OnDemand Apps Files Jobs Clusters Interactive Apps Monitoring My Interactive Sessions Help Logged in as bergert@agresearch.co.nz Log Out


OPEN
OnDemand

OnDemand provides an integrated, single access point for all of your HPC resources.

Recently Used Apps



Jupyter Lab
System Installed App




Remote Desktop
System Installed App

Message of the Day


This server is the property of AgResearch Ltd. Unauthorised access strictly prohibited. All access may be monitored.

Pinned Apps A featured subset of all available apps


Interactive Apps



Remote Desktop
System Installed App




IGV
Integrative Genomics Viewer



Jupyter Lab
System Installed App

Monitoring



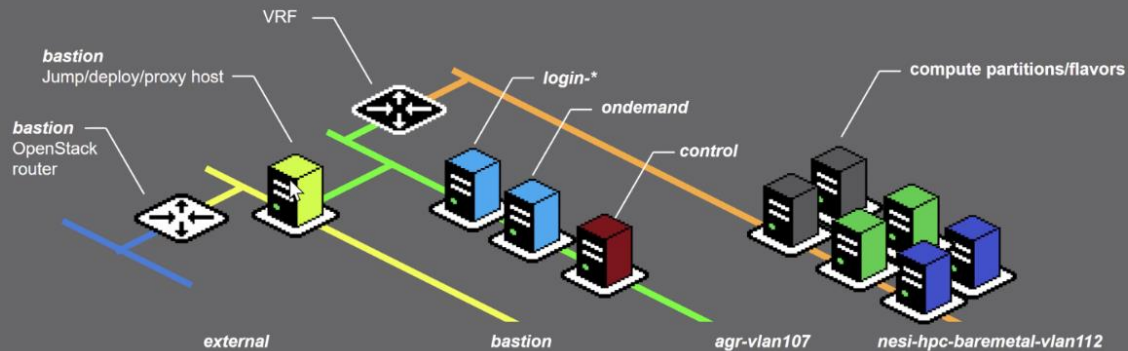
Grafana
System Installed App

powered by **OPEN OnDemand**

OnDemand version: 3.0.1

Architecture diagram

Overview



NeSI's training environment

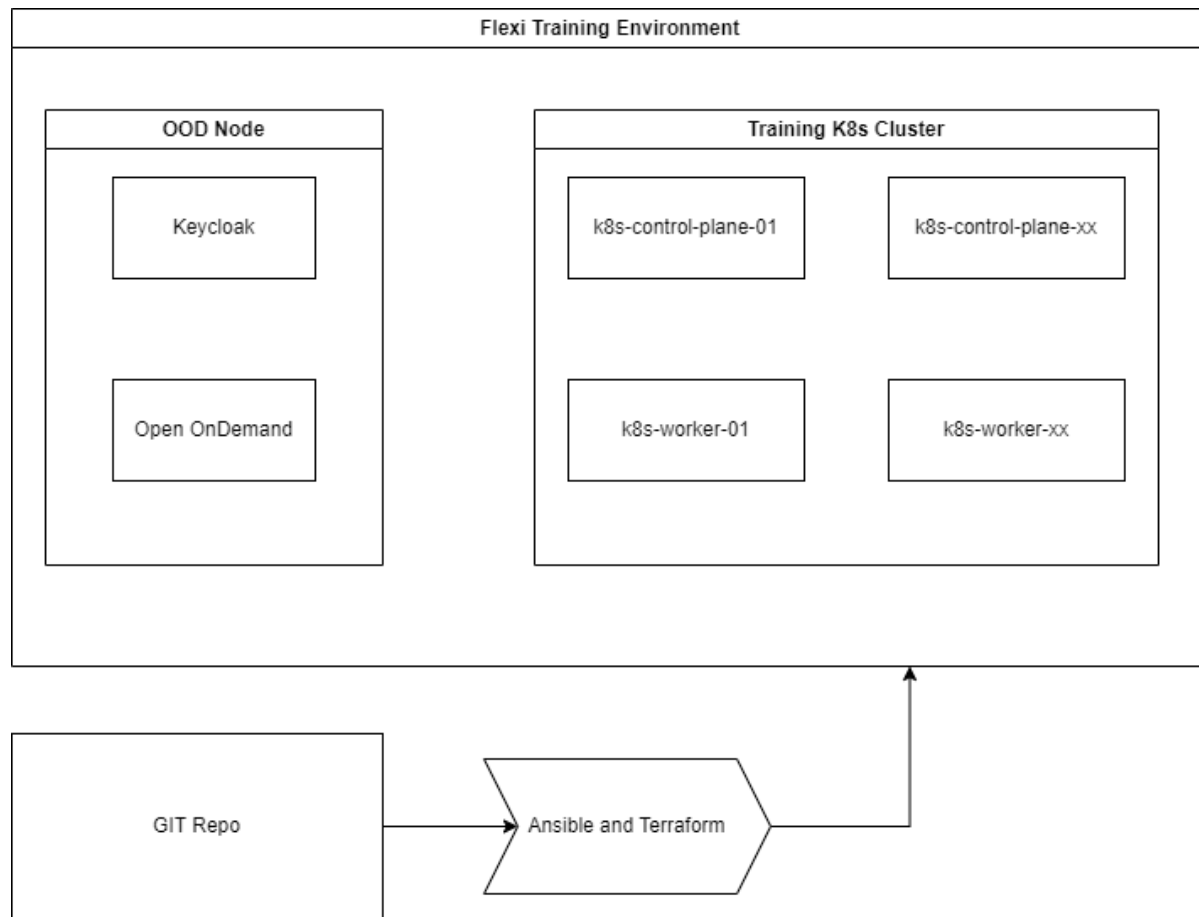
Internal prototyping project for long term training goals. An environment where a non-NeSI trainer can self organise training events as needed.

Challenges: Self provisioning, identity, user experience for trainers and trainees

Technology used: Open OnDemand, KeyCloak, JupyterLab, Kubernetes



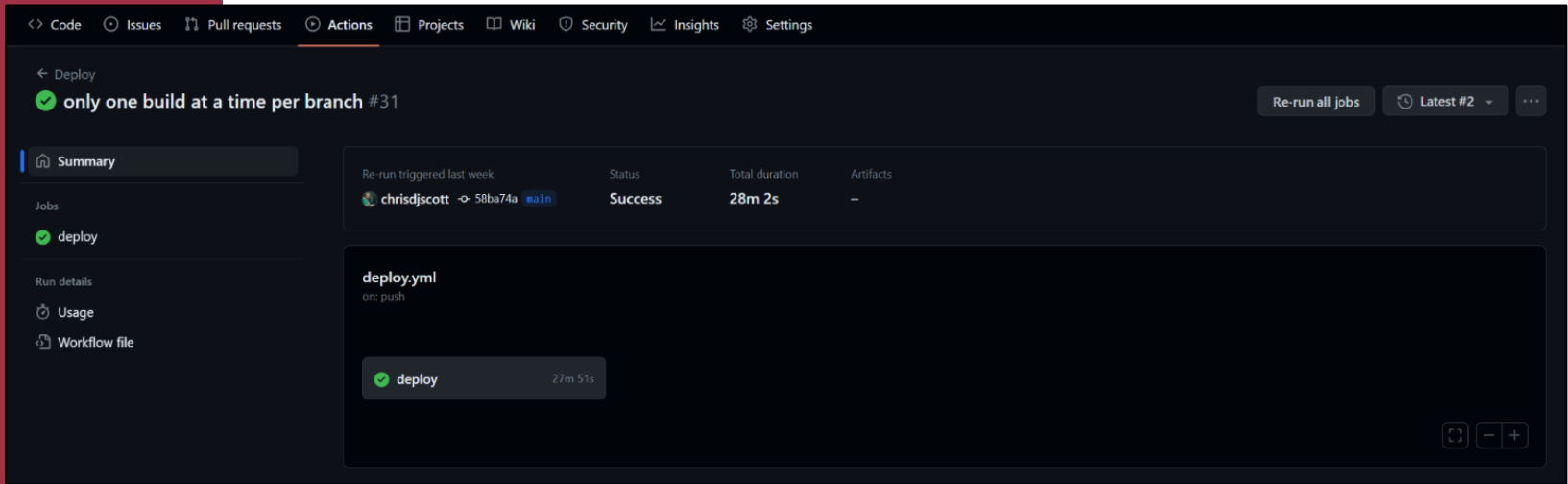
Training environment: Architecture



**Training
environment:**

**Developer
experience**

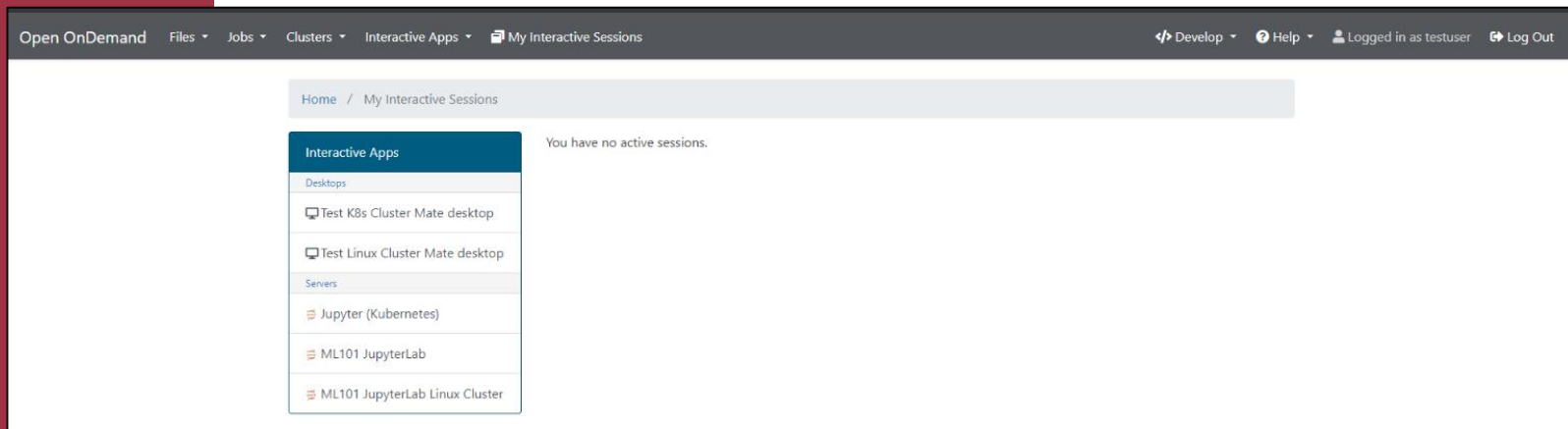
- Git Repo showing terraform against FlexiHPC
- <https://github.com/nesi/FlexiHPC.Terraform.ComputeSetup.Example>
- Code is reusable with other OpenStack providers
- Can be integrated with DevOps pipelines/actions



Training environment:

Developer experience

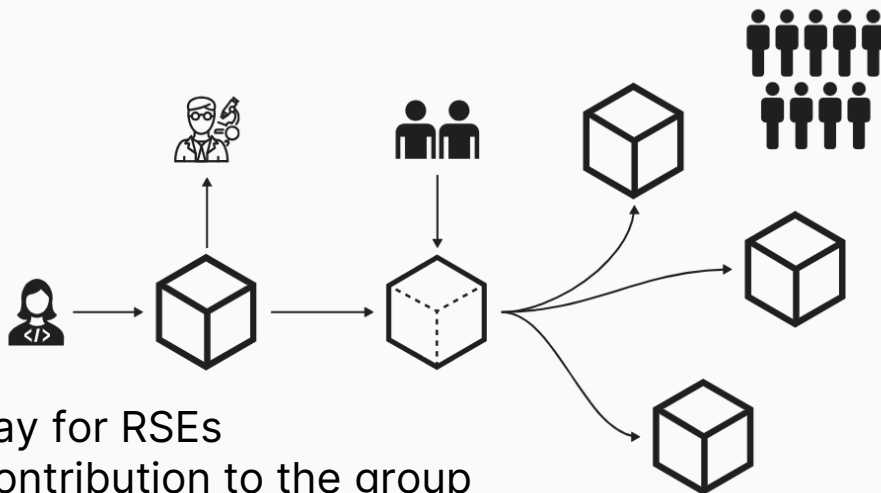
- Training Environment Git Repo
- <https://github.com/nesi/training-environment>
- Based off the Terraform Repo but also includes Ansible



Future pathways



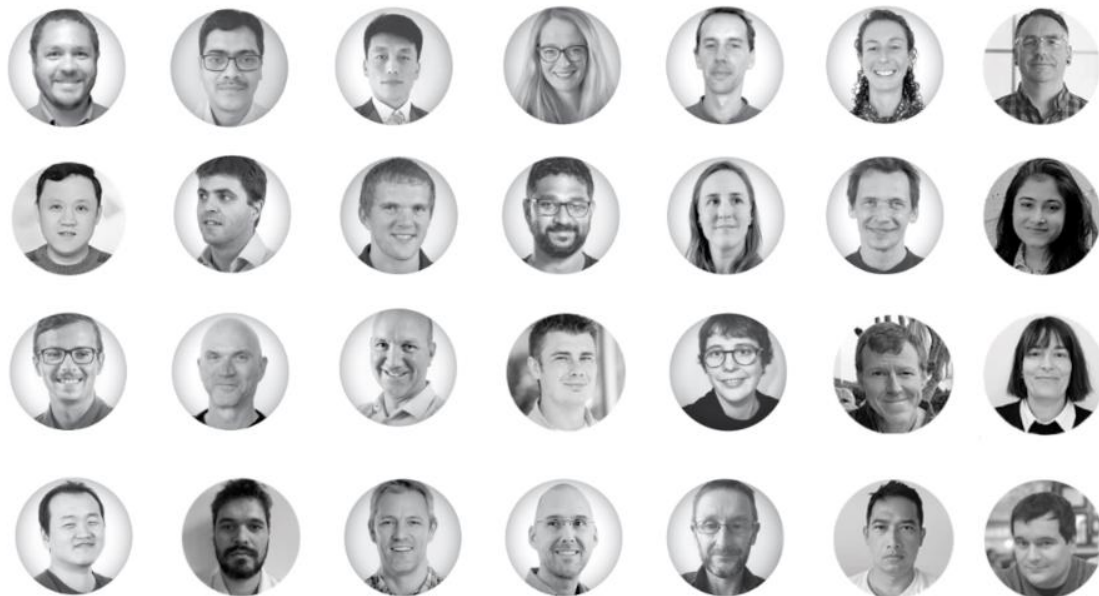
Future vision



- Pathway for RSEs
 - Contribution to the group
 - To the organisation
 - Wider communities, the sector as a whole, domain, international
- How?
 - DevOps, open standards, community building tools
 - GitLab, Terraform/Ansible, K8s...
 - Learn from Australian WorkflowHub, ARCOS, etc.
- Blueprints / patterns / expertise

Reflections

- Tenancy onboarding has been gradual and deliberate, with collaboration in mind
- Needs that we are seeing:
 - Data: repositories, sensitive data
 - DevOps skills
 - Infrastructure needs
- Working towards building key differentiators that can address the gap areas
 - Working alongside and enabling RSEs
 - DevOps focus
 - Blueprints / patterns / expertise
 - Open standards
 - Building relationships



Connect with us

We want to learn about

- How are the different areas of needs handled across organisations in Australia?
- What are some of your major challenges?

Let us get connected and continue sharing our learnings and ideas.

You can read more about Flexible HPC at:

<https://www.nesi.org.nz/flexi/>

Please feel free to reach out to us at support@cloud.nesi.org.nz or jun.huh@nesi.org.nz

Related presentations

Tuesday

- 12:05 - *An update on the NeSI AgResearch Partnership as the rubber hits the road* - Georgina Rae, Ben Taylor
- 12:45 - *Building custom web portals for HPC and mid-tier computing* - Thomas Berger
- 16:05 - *Rakeiora Genomics Platform: building a prototype for genomic medicine in Aotearoa* - Claire Rye

Thursday

- 13:00 - *Building Effective and Efficient Research Security Practices* - Michael Karich (Lightning talk)

We'd love to connect with you

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<https://www.nesi.org.nz/>

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NeSI

New Zealand eScience
Infrastructure