MINISTRY OF BUSINESS, INNOVATION & EMPLOYMENT
HĪKINA WHAKATUTUKI

THE UNIVERSITY OF AUCKLAND
NEW ZEALAND

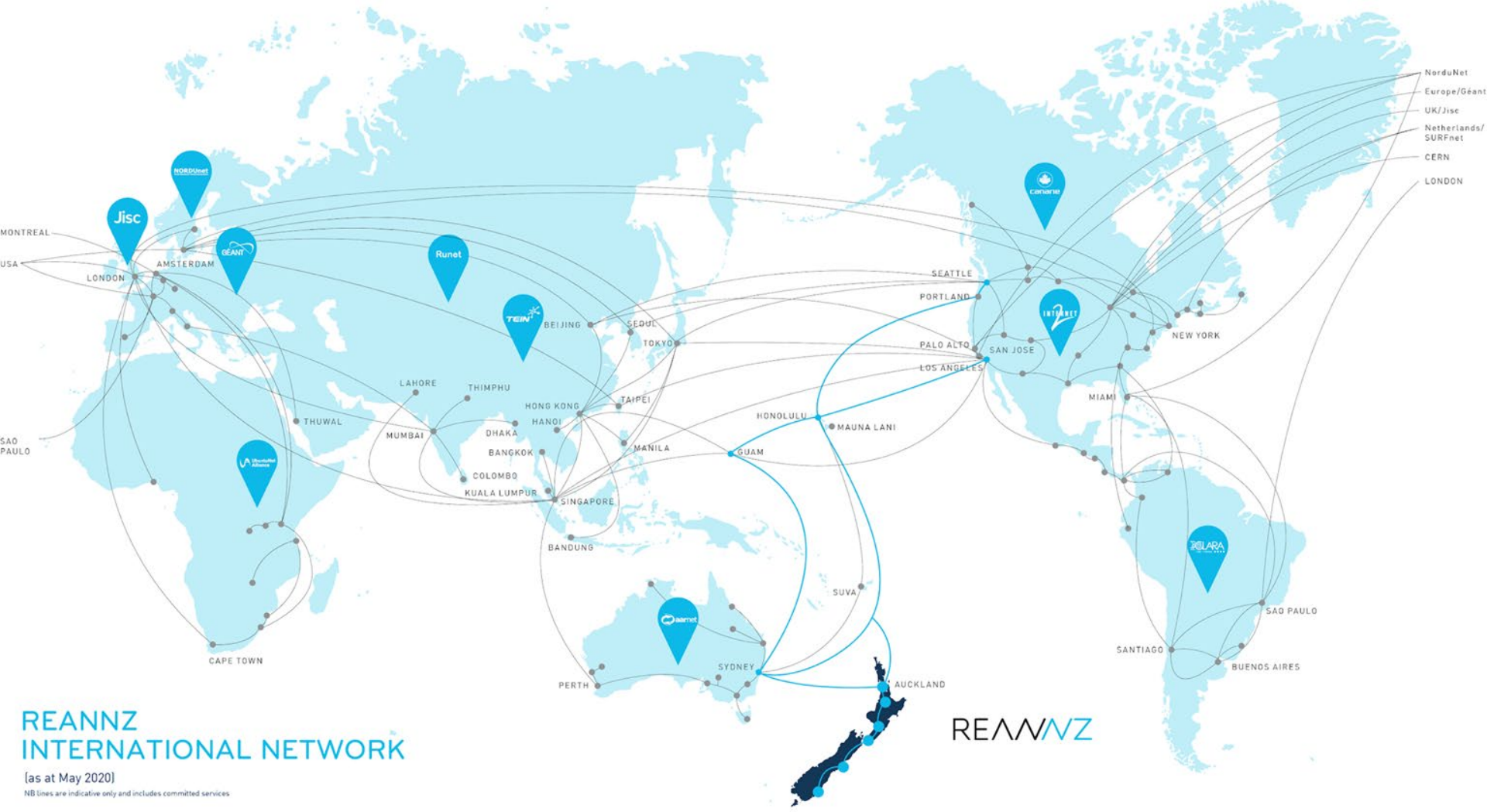
NIWA
Taihoro Nukurangi

UNIVERSITY of OTAGO
Te Whare Wānanga o Otāgo
NEW ZEALAND

Manaaki Whenua
Landcare Research

NeSI: Capability computing & computing capably

Nick Jones, Director, eResearch NZ 2022



REANNZ INTERNATIONAL NETWORK

(as at May 2020)

NB lines are indicative only and includes committed services

REANNZ

NeSI

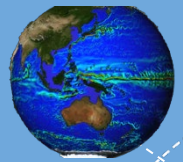
New Zealand eScience Infrastructure

NeSI is a national collaboration of:

- The University of Auckland New Zealand
- NIWA Taihoro Nukurangi
- University of Otago Te Whare Wānanga o Otāgo New Zealand
- Manaaki Whenua Landcare Research
- Ministry of Business, Innovation & Employment Hīkina Whakatutuki

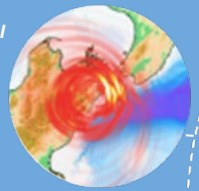
Dr Olaf Morgenstern and Dr Erik Behrens (Earth Science)

Deep South Challenge project using NeSI supercomputers for climate modelling.



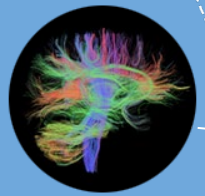
Yoshihiro Kaneko (Seismology)

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)

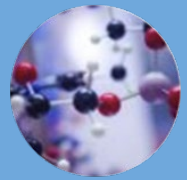
Using NeSI supercomputers for advancing image processing capabilities using computer vision

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.



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NeSI
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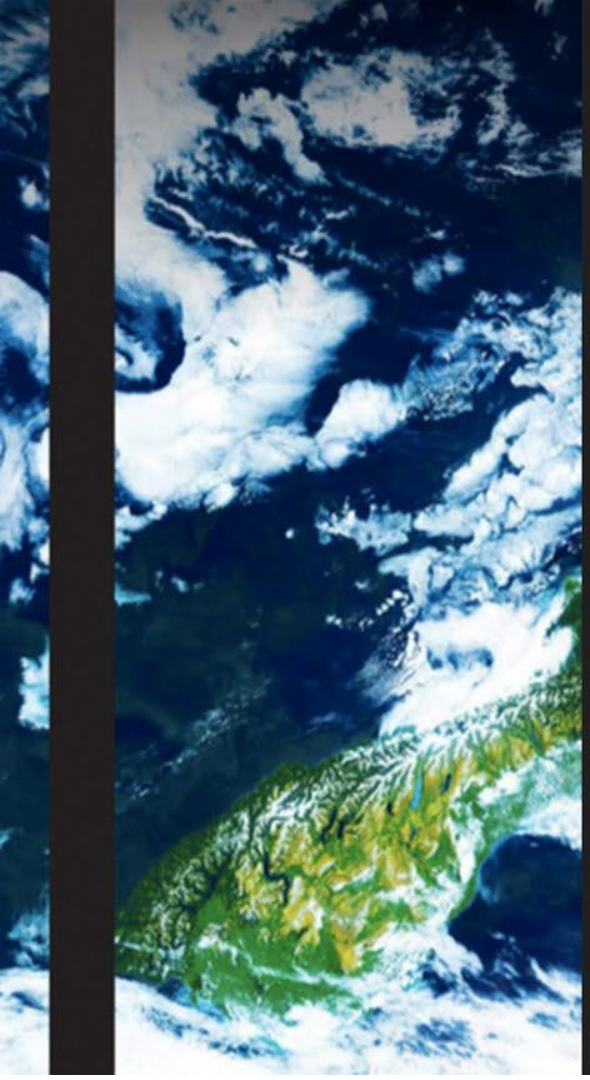

In Māori tradition, the powerful demi-god Māui used a magic hook to haul Te Ika a Māui – the North Island of New Zealand – from depths of the southern oceans.

Today Māui is giving NIWA scientists, and researchers throughout New Zealand, the power to haul in the secrets of science from the depths of the oceans to the atmosphere above.

MĀUI incorporates:

- 464 compute node Cray XC50
- 18 650 x 2.4GHz Skylake cores
- CS500 Virtual labs

MAHUIKA

Mahuika is the Māori goddess of fire. In customary lore, Māui sourced fire for his people by convincing his Grandmother Mahuika to hand over flames burning from her fingers.

Today Mahuika is powering reseachers throughout New Zealand in a range of fields, from genomics research to seismic mapping.

MAHUIKA incorporates:

- 234 compute node Cray CS400
- 8,424 x 2.1GHz Broadwell cores
- CS400 Virtual Labs

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Landcare Research

What is NeSI?

New Zealand eScience Infrastructure (NeSI) designs, builds, and operates a specialised platform of shared high performance computing infrastructure and a range of eResearch services.

All researchers in New Zealand have access to NeSI.

NeSI is a national collaboration of:

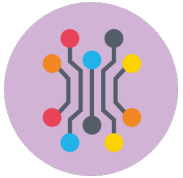
NIWA Taihoro Nukurangi

The University of Auckland New Zealand

Manaaki Whenua Landcare Research

University of Otago Te Whare Wānanga o Otāgo New Zealand

Ministry of Business, Innovation & Employment Hīkina Whakatutuki



High performance computing (HPC) and analytics

- Specialised and fit-for-purpose HPC platform for research
- Data analytics and machine learning platform for research
- Interactive and integrated workflows in/out of NeSI's platforms

Data services & tools

- National Data Transfer Platform providing reliable, high speed, secure data transfer with end-to-end integration
- Hosting of discipline specific actively used research datasets, repositories, and archives

Training and researcher skill development

- Training to grow computational research capabilities in NZ research sector
- Partnership with The Carpentries to teach foundational coding and data science skills to researchers, and Genomics Aotearoa for bioinformatics training

Consultancy

- Experts in computational science, research software & data science engineering
- Lifting computational capabilities of research teams, optimising tools & workflows

Who can access NeSI

- **Collaborators:** University of Auckland, University of Otago, NIWA, Manaaki Whenua Landcare Research

- **Subscribers:** University of Waikato, AUT, Massey University, Genomics Aotearoa, AgResearch, Ministry for Primary Industries, Plant and Food Research, LIC, GNS Science, Pacific Edge, Biotelliga, and others

- **Merit users:** Anyone with competitive external research funding, e.g. Marsden, MBIE, HRC, CoRE, National Science Challenge, etc.

- **Postgraduate students:** Any Masters, PhDs from any institution

NeSI supports digital skills and capability building

‘Intro to NeSI’ sessions | online hacky hours | Carpentries instructor training & skills workshops | code profiling & optimisation workshops | and more…

NeSI and the University of Otago hosted New Zealand’s first Carpentry Connect event in February 2020. →

← NeSI and Genomics Aotearoa co-hosted a Metagenomics Summer School at the University of Auckland in December 2019.

NeSI hosts training webinars sharing tips and tools for computational research and getting started on NeSI platforms. →

Suggest topics / book workshops:
training@nesi.org.nz

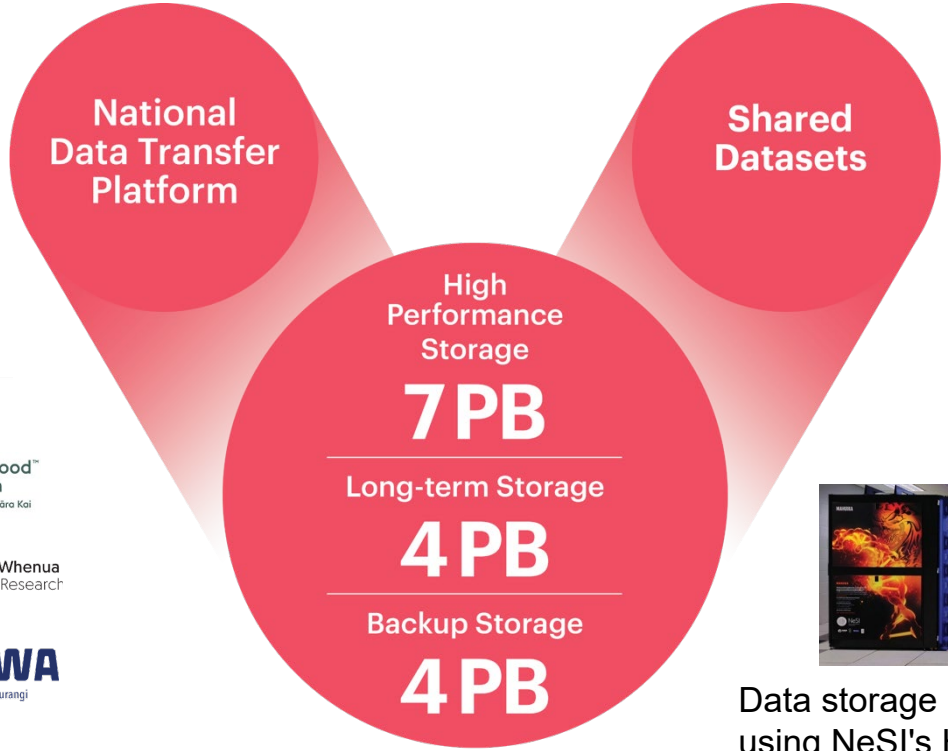
A snapshot of NeSI Data Services:

Secure, high-speed transfer & share capabilities for large research datasets.

REANNZ globus

Six NZ endpoints:

The University of Auckland New Zealand
Plant & Food Research Rangahau Ahumāra Kai
agresearch āta mātai, mātai whetū
Manaaki Whenua Landcare Research
University of Otago Te Whare Wānanga o Otāgo New Zealand
NIWA Taihoro Nukurangi



Virtual labs and portals.
Support of FAIR principles.

genomics aotearoa

Co-designing longer-term data management solutions:

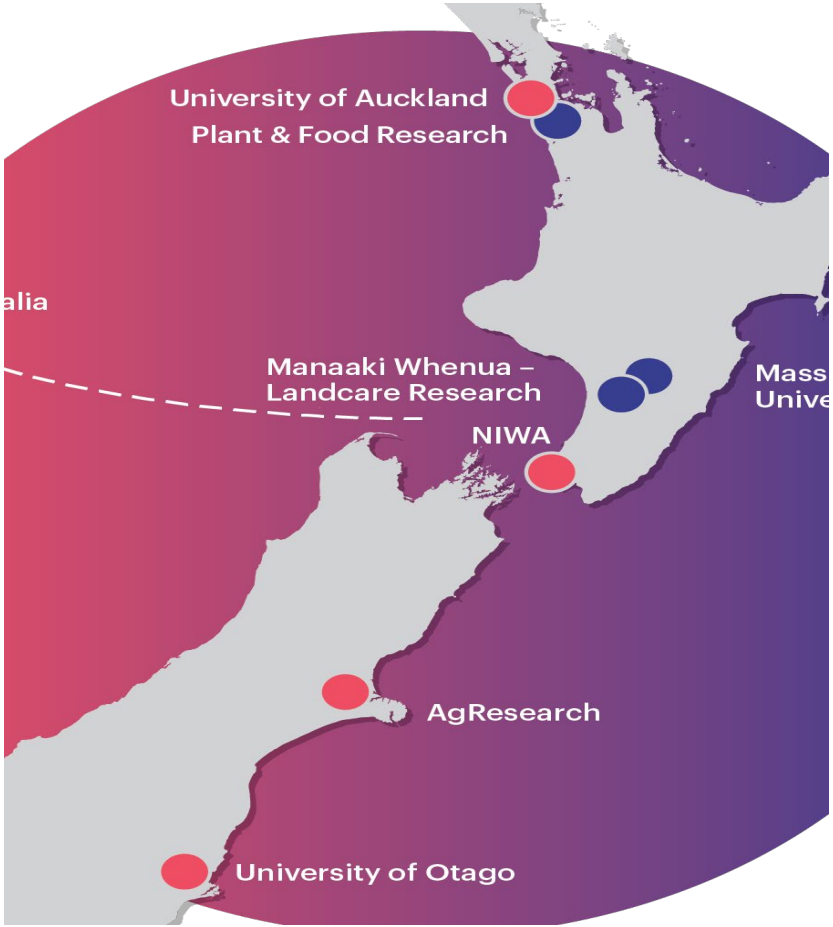
- Aotearoa Genomic Data Repository
- Rakeiora project

Data storage resources for projects using NeSI's HPC platform.

National Data Transfer Platform

activities in 2020

870 TB	72 million	5,107
Amount of data transferred	Number of files transferred	Number of transfers made



Computational & Data Science engineering

- A consultancy service offered to NeSI platform users, generally at no cost to the researcher
- NeSI **Research Software Engineers** and **Data Science Engineer** work directly with research group members to **raise the capability** of the research group

Our team can assist with:

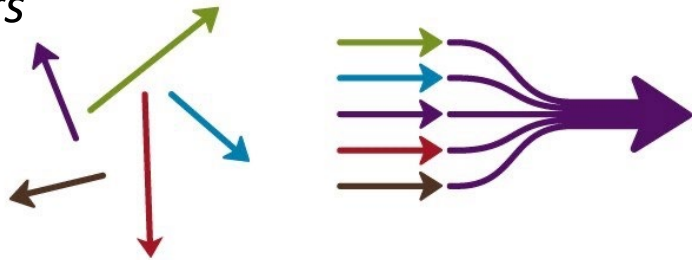
- **Workflow parallelisation** – allowing more inputs to be processed simultaneously
- **Software parallelisation** – use of technologies such as OpenMP or MPI to process one single input more quickly
- **Code optimisation** – redesign of algorithms to improve overall speed or efficiency of resource use
- **Improving I/O performance** – speed up reading from or writing to the disk, or to reduce the amount of data that must be read or written
- **Porting to GPU** – accelerate code by offloading computations to a coprocessor
- **Improving software sustainability** – introducing best practices such as version control and unit testing

Contact support@nesi.org.nz

Partnerships seeking collective impact

- Work **with** communities and institutions
- **Collectively** commiting to **common** goals and objectives
- Solved by **coordinated** and **complementary** activities

“rallying various stakeholders to collectively deliver on a shared goal of growing the computational capability of researchers”



Source: http://www.northfieldpromise.org/about/collective-impact/

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Antarctic Science Platform
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NATURAL HAZARDS RESEARCH PLATFORM
AUT
RSE
RSE-AUNZ
globus
Department of Conservation
Te Papa Atawhai
CallaghanInnovation
New Zealand's Innovation Agency
Plant & Food Research
Rangahau Ahumāra Kai
THE UNIVERSITY OF WAIKATO
Te Whare Wānanga o Waikato
Science New Zealand
QuakeCoRE
NZ Centre for Earthquake Resilience
Te Hiranga Rū
hrc nz
Health Research Council of New Zealand
Te Kaunihera Rangahau Hauora o Aotearoa
BRAGATO RESEARCH INSTITUTE
NEW ZEALAND GRAPE AND WINE RESEARCH
RANGAHAU KAREPE, WĀINA O AOTEAROA
PACIFIC EDGE LTD
Hewlett Packard Enterprise
BIOTELLIGA
Harnessing nature's genius
RUTHERFORD DISCOVERY FELLOWSHIPS
ROYAL SOCIETY TE APĀRANGI
PlantTech
Livestock Improvement
VICTORIA UNIVERSITY OF WELLINGTON
TE HERENGA WAKA
REANNZ
MARSDEN FUND
TE PŪTEA RANGAHAU A MARSDEN
Ministry for Primary Industries
Manatū Ahu Matua
MOANA PROJECT
PAWSEY supercomputing centre
aarnet
Australia's Academic and Research Network
MASSEY UNIVERSITY
TE KUNENGA KI PŪREHUROA
UNIVERSITY OF NEW ZEALAND
UC UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND
THE DEEP SOUTH
Te Kōmata o Te Tonga
National SCIENCE Challenges
MetService
TE RATONGA TIRORANGI
AeRO
Australasian eResearch Organisations
NCI AUSTRALIA
MetOcean SOLUTIONS
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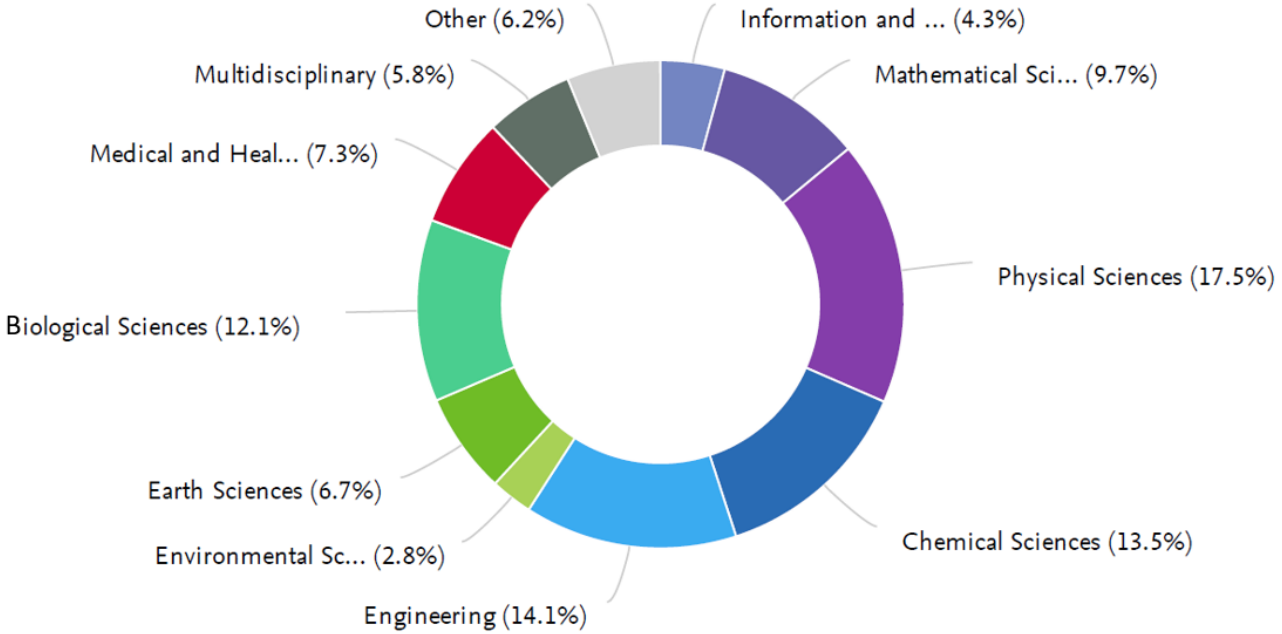
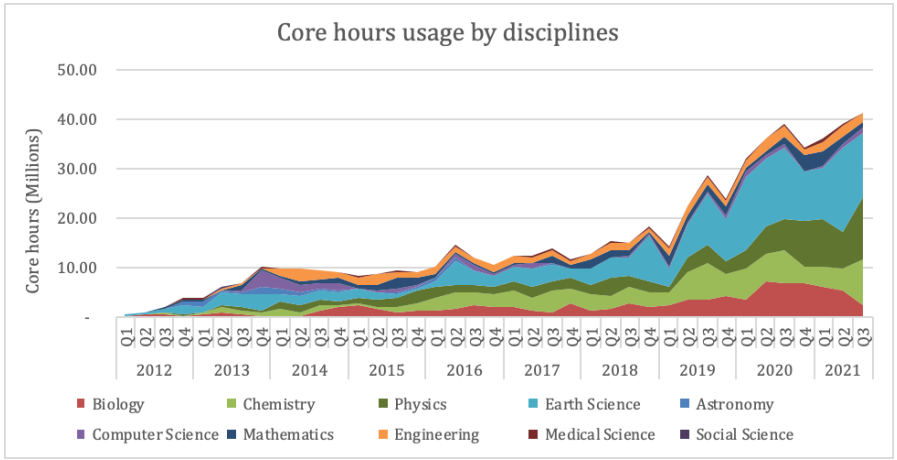
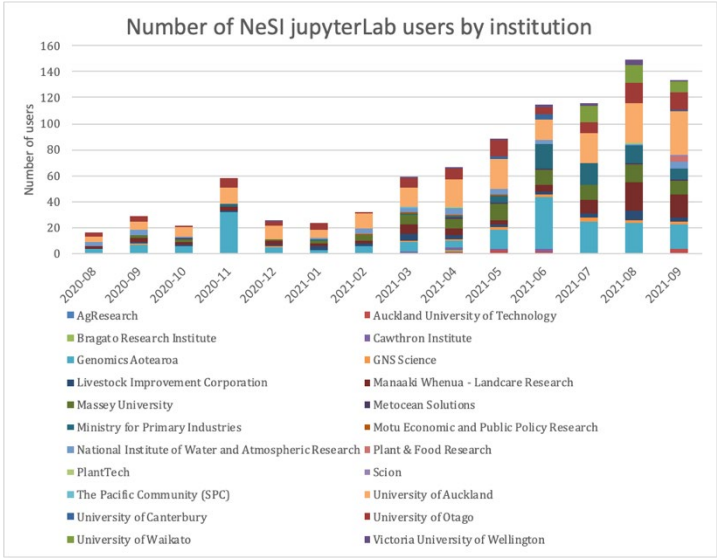
Landcare Research

Publications by Subject: Year Range 2013-19



Researcher use and satisfaction





Research Impact

Benchmarks 2011-2020 - Field-Weighted Citation Impact

- NeSI supported publications from 2011 to date: 748
    - **NeSI**: 654 publications; **FWCI 1.66**; 28.8 citations per publication
    - **CRIs**: 16,374 publications 2011-2020; **FWCI 1.55**; 21.5 citations per publication
    - **NZ Universities**: 131,53 publications; **FWCI 1.55**; 17.5 citations per publication

Source: Scival

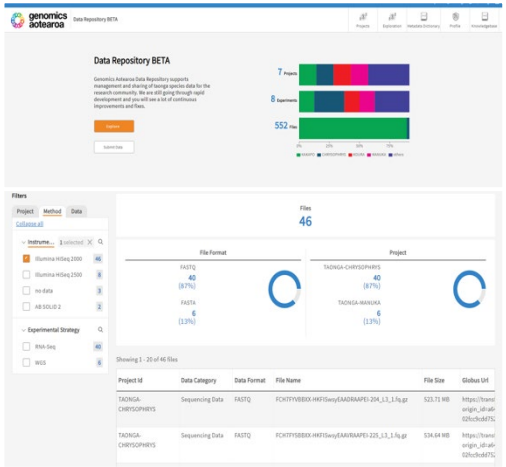
genomic

GA/NeSI Training Summary (11.06.2019-30.11.2020)

Number of Events	Number of Attendees	Number of Host Institutes (unique)
24	491	8

Access to NeSI's specialised high performance computing (HPC) platform, including tailored software environments and data management services, and skills training in computational research tools and approaches.

Rakeiora: A pathfinder for genomic medicine in Aotearoa/New Zealand

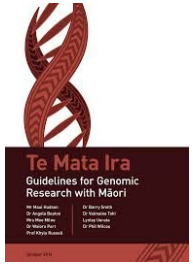


Gen3
Data Repository

A solution designed as a genomic data repository by University of Chicago and The National Cancer Institute

20+ instances live or being developed around the world with active community.

Inheriting a lot of domain specific knowledge designed by others.



- Genome sequences from hundreds of individuals co-led and co-governed with Māori and stored securely but accessible for ethically approved and consented research
- Data linkable and protected with careful governance and approval to primary and secondary care health data and National Health Datasets
- Recommendations for process scale up
- Knowledge on how to apply research for health benefits

Antarctic Science Platform

“This partnership is critical for our future projections work. By having access to this world class supercomputing resource, our modellers are enabled to create ever improving forecasts that increase the resilience of New Zealanders and can guide how we best respond to climate change challenges"
- Nancy Bertler, Director of Antarctic Science Platform

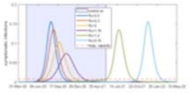
A whole ecosystem response to Covid-19

Te Pūnaha Matatini
Complexity is at our heart

Evolution

Early March

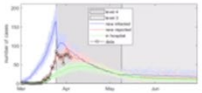
Deterministic SEIR model



- OK for long term scenarios but not elimination or single-seed outbreaks
- Run on laptop in < 1 minute

Early April

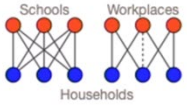
Stochastic model



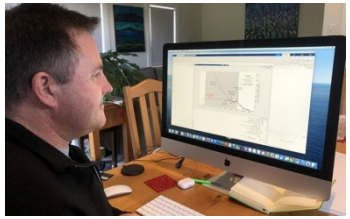
- Good for short and long term scenarios
- Can look at elimination and single-seed outbreaks
- Run on laptop in ~ 1hr

Mid July

Network model



- Good for short term scenarios
- Can look at single interventions (e.g. university closure)
- Run on NeSI in ~ 1day



It takes a #teamof5million

Te Pūnaha Matatini
Data ▪ Knowledge ▪ Insight

NeSI
New Zealand eScience Infrastructure

E/S/R
Science for Communities

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Te Whare Wānanga o Tāmaki Makaurau
NEW ZEALAND

Everyone doing their part

UNIVERSITY of OTAGO
Te Whare Wānanga o Otāgo
NEW ZEALAND

TE HERENGA WAKA WELLINGTON
VICTORIA UNIVERSITY OF WELLINGTON

MASSEY UNIVERSITY
TE KUNENGA KI PŪREHUROA
UNIVERSITY OF NEW ZEALAND

UC UNIVERSITY OF CANTERBURY

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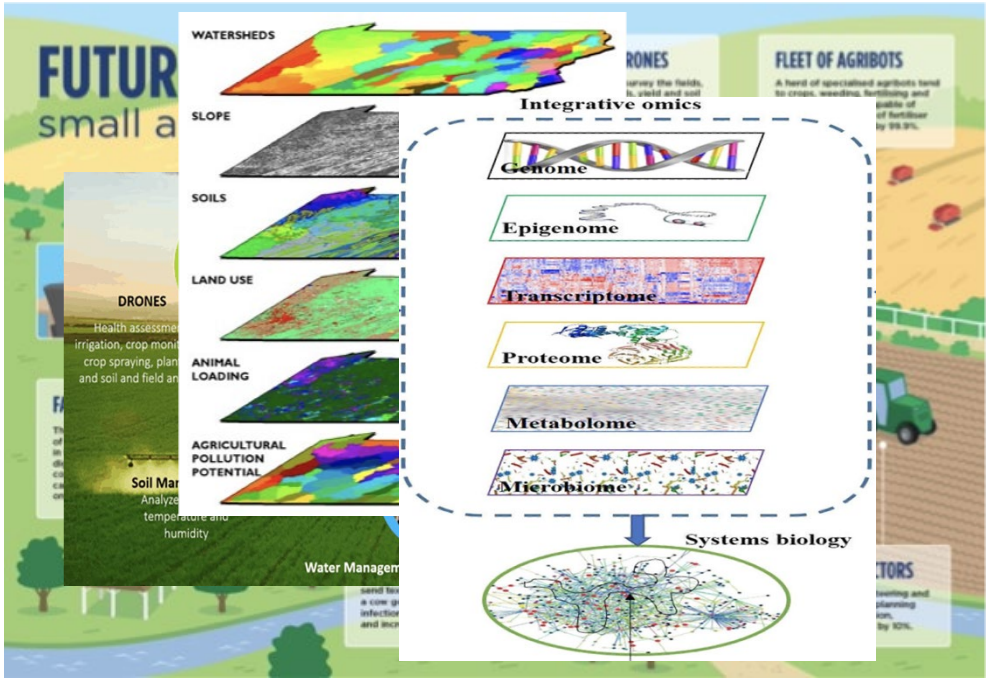
MANATŪ HAUORA

genomics aotearoa

hrc Health Research Council of New Zealand

AgResearch eResearch Platform



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Current State

Infrastructure	Aged HPC No longer fit for purpose
Capability	Fragmented and siloed
Support Model	Disjointed
Data Management	No clear Framework
Digital Tools & Services	Lack of clear understanding

Strategic Objectives

- eResearch Infrastructure
- Growing Capability
- Digital Services
- eResearch Sector Leader

Future State

- Fit for purpose Infrastructure
- Progress made towards Data and digitally savvy workforce
- Structured Advice, Consultancy and Training
- Data Catalogue RDM Framework Data Lifecycle
- Domain Specific Tools & Services

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A Flexible eResearch Infrastructure

- Key dependency for the successful delivery of Platform services
- Collaboration with New Zealand eScience Infrastructure (NeSI)
- Central data store and HPC
- AgResearch owned infrastructure but can burst into NeSI Cloud!

agresearch
āta mātai, mātai whetū

NeSI
New Zealand eScience Infrastructure

eResearch NZ 2021

- co-hosted by NeSI, REANNZ, and Genomics Aotearoa
- 160+ attendees
- virtual & in-person
- opened by Hon. Dr Ayesha Verrall, Associate Minister of Research, Science and Innovation
- presentations, panels, training, workshops, Birds-of-a-Feather (BoFs)

RSE-AUNZ

NeSI New Zealand eScience Infrastructure

NZ Research Software Engineers Conference 2022

Check for details
https://www.rseconference.nz

Who attends:

- Researchers and academics who code
- Software engineers & system admins working in the research domain
- Generalists who bring together the research and technical domains
- Crown Research Institutes, universities, and other public sector organisations

ENERGY
HIGH VALUE MANUFACTURING
WEATHER & CLIMATE
PRIMARY INDUSTRIES
HUMAN HEALTH
BIO SECURITY
NATURAL HAZARDS
NATIONAL SCIENCE CHALLENGES
CENTRES OF RESEARCH EXCELLENCE
ONGOING RESEARCH

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Join our mailing list at https://www.nesi.org.nz/
(training alerts, newsletters, event announcements, etc.)

Follow us on social channels

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New Zealand eScience Infrastructure

Technical questions ...

Email our Team: support@nesi.org.nz

Visit our Support site: https://support.nesi.org.nz/

Ready to get started ...

Apply for access: https://www.nesi.org.nz/apply