NeSI

New Zealand eScience Infrastructure

Nick Jones, Director, NeSI
February, 2020


TE RAUHINA


TE RAUHINA


THE PILOT, WAIROA, N.Z. PHOTO BY BURRIDGE


NeSI

MINISTRY OF BUSINESS, INNOVATION & EMPLOYMENT
HĪKINA WHAKATUTUKI

Proposes actions in five main areas:

1. Making New Zealand a magnet for talent
2. Connecting research and innovation
3. Start-up^scale-up
4. Towards an extended ‘Vision Mātauranga’
5. Building firm foundations.

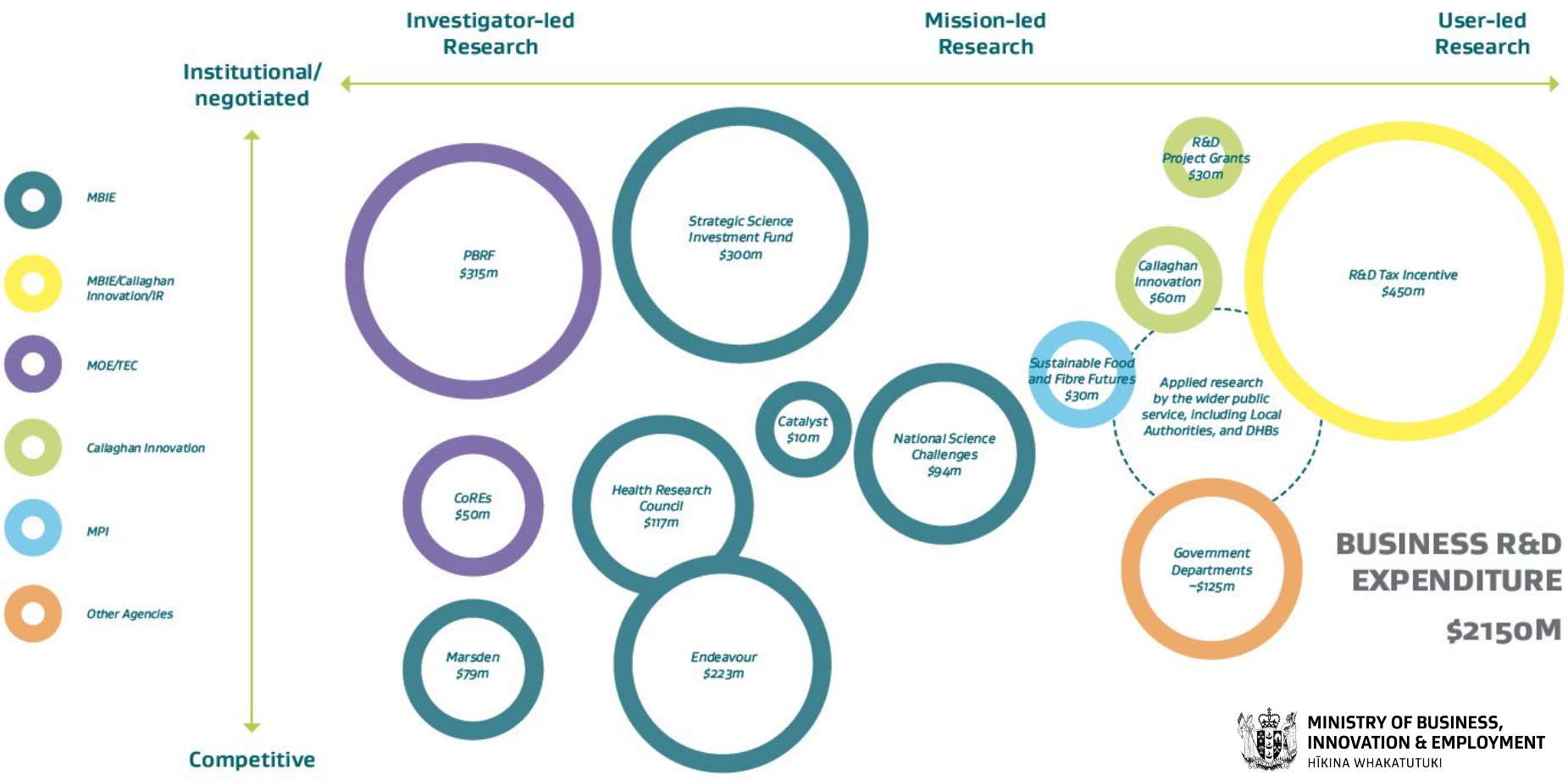
5. Building Firm Foundations

Create a progressive investment programme

Ensure future-focused, fit-for-purpose institutions and infrastructure

Global quality research infrastructure

“Ensure our research infrastructure is placed on a sustainable footing. We will focus on e-research, databases and collections, and international scale infrastructure collaborations.”



MINISTRY OF BUSINESS, INNOVATION & EMPLOYMENT
HĪKINA WHAKATUTUKI

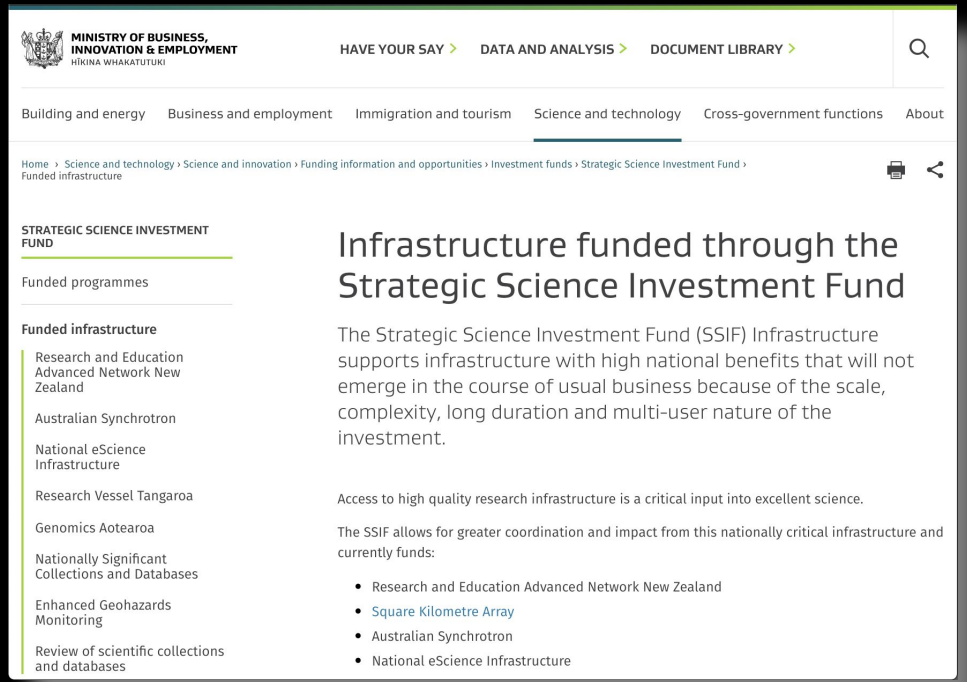
Strategic Science Investment Fund, Infrastructure

“supports infrastructure with high national benefits that will not emerge in the course of usual business because of the investment's scale, complexity, long duration and multi-user nature.”

- REANNZ - advanced research network
- NeSI - advanced research computing
- Genomics Aotearoa
- Nationally Significant Collections & Databases

Related investments

- NZRIS Research Sector Administrative Data
- ORCID Researcher Identity



NeSI
New Zealand eScience Infrastructure

Growing the computing capability of NZ researchers

for our future wellbeing and prosperity

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

NeSI.101

Established in mid-2011

… nearing end of second contract (in year 6 of 7)

Started as a network of separate HPC facilities and services

… providing access to separate facilities to a common standard

Now a nationally managed computing/data platform + team

… enabling a healthy ecosystem: skills, services, infrastructure

MBIE reviewed / evaluated in mid-2017, recommended continued investment with some changes

… draft investment case indicated challenges moving beyond current performance given situation

… key questions around how we built NeSI on a club while also supporting the Rest Of New Zealand

NeSI
New Zealand eScience Infrastructure

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

Disciplines Supported

- Biology
- Engineering
- Astronomy
- Physics
- Computer Science
- Medical Science
- Earth Science
- Social Science
- Mathematics

Core Services

- High Performance Computing & Analytics
- Consultancy
- Training
- Data Transfer & Share

Our Infrastructure

- Māui
- Mahulka

>136 million	>1.7 petaflops	>130 GB/s
CPU core hours available per year	peak performance	IO bandwidth

Making waves in global food production technology

Kendall Clements
(University of Auckland)
Lindsay White
(Auckland University of Technology)

"The molecular work associated with this research generates huge amounts of data, and NeSI's resources provide critical computing infrastructure."

NeSI delivered:

- High performance computing resources — having more than 1 TB of sequence data, Mahuika was used to run their genome assemblies and -omic data analyses.

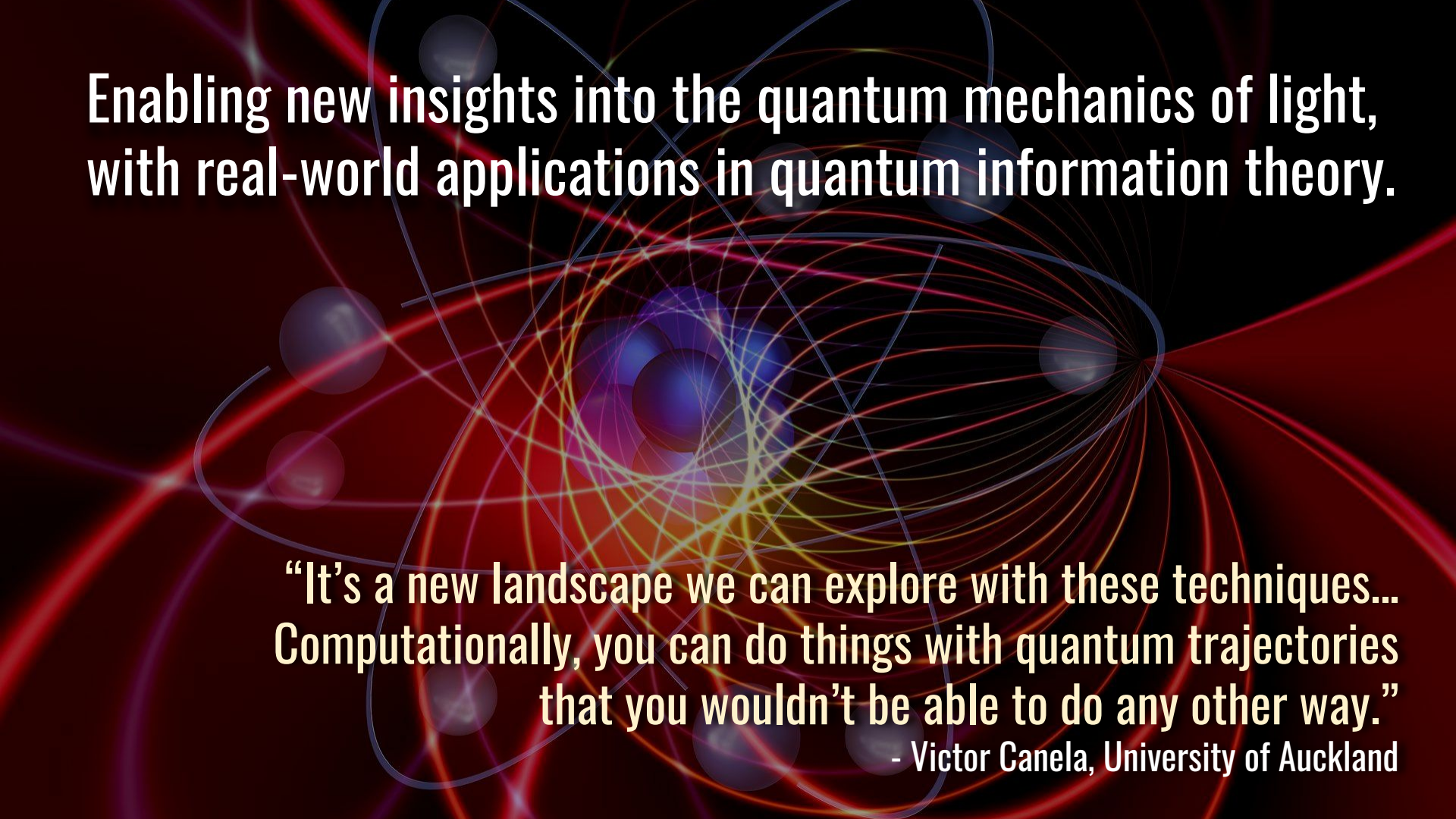
Modelling the careers of cricket players

Oliver Stevenson & Brendon James Brewer
Department of Statistics
University of Auckland

"NeSI allows us to run the model on hundreds of players simultaneously, rather than on one player at a time."

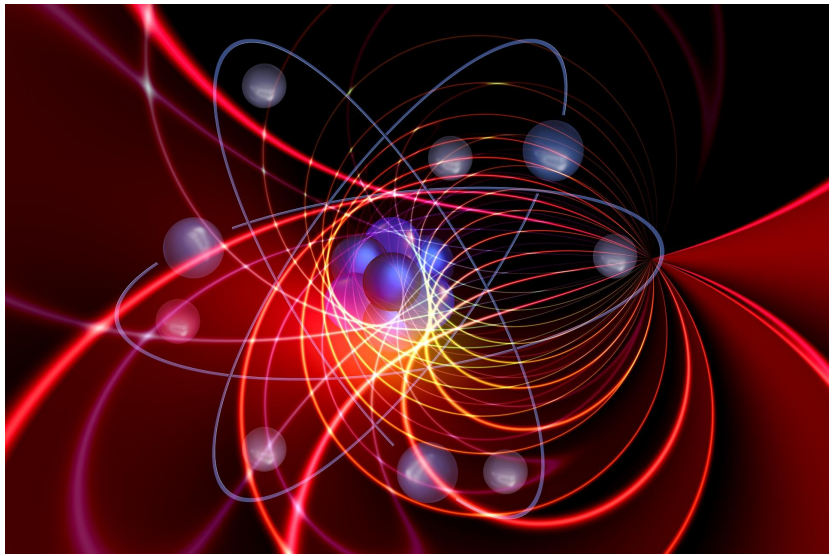
NeSI delivered:

- High performance computing resources


Enabling new insights into the quantum mechanics of light,
with real-world applications in quantum information theory.
“It’s a new landscape we can explore with these techniques...
Computationally, you can do things with quantum trajectories
that you wouldn’t be able to do any other way.”
- Victor Canela, University of Auckland

Understanding the behaviours of light

Victor Canela & Jacob Ngaha
University of Auckland



"We are running close to a hundred jobs at the same time and each job has separate parameters...**NeSI was able to supply a script that keeps track of this automatically.**

NeSI delivered:

- High performance computing resources
- Computational science expertise
- Code optimisation, automation, improved workflow

Using parallel processing to study ocean life

Alexis Marshall
(University of Waikato)

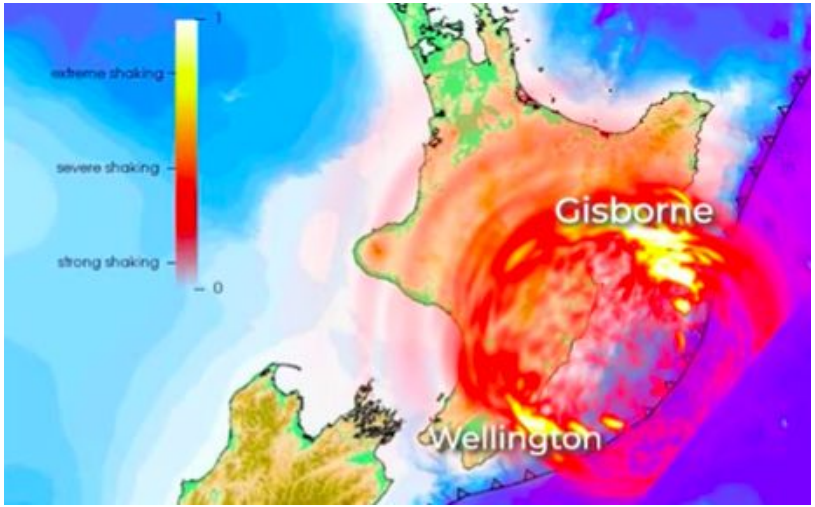
"We contacted NeSI because we were going from trying to assemble 100,000 individual 150 nucleotide base sequences, to trying to assemble 1.4 billion. We were having computational issues with memory, but also time."

NeSI delivered:

- NeSI's Computational Science Team expertise and access to the parallel processing capabilities of NeSI's Mahuika supercomputer helped Alexis reduce her time spent on sample data processing from weeks to 48 hours.

Speeding up seismic simulations to help New Zealand better prepare for massive earthquake events

Yoshihiro Kaneko
(GNS Science)
Bryant Chow
(Victoria University of Wellington)



GNS Science researchers are producing detailed images of the 3D structure and geometry of the Hikurangi mega-thrust region.

NeSI delivered:

- By consulting with NeSI's Computational Science Team, Yoshihiro and Bryant were able to build and run the numerical tools required to simulate seismic wave propagation, creating a model that will help New Zealanders better prepare for future massive earthquake events.

Using machine learning to study marine mammals

Giacomo Giorli
National Institute of Water and Atmospheric Research (NIWA)

"By understanding the abundance and distribution of different marine mammals in New Zealand, we can inform conservation policy, management of marine resources, licensing for offshore activity and create better environmental impact assessments."

NeSI delivered:

- Working with NeSI's Computational Science Team, Giacomo was able to use machine learning techniques to categorise the sounds from three whale species. Information about these species will be used to inform regulation on marine activity, as well as conservation efforts.

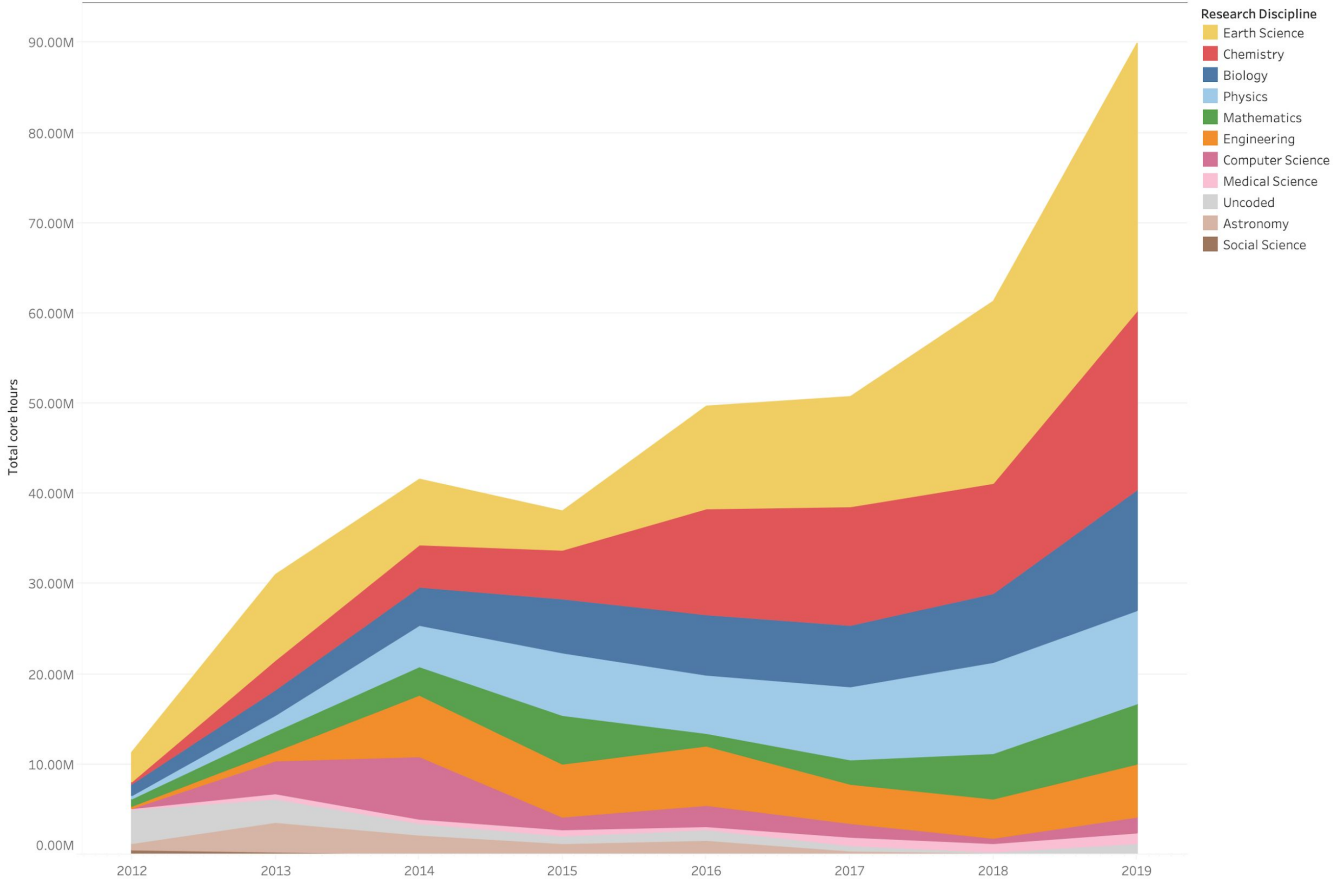
A partnership approach to building skills in NZ's genomics research sector

Together, NeSI and Genomics Aotearoa have the domain knowledge, technical skills, and motivation to address the skills gap facing New Zealand's genomics and bioinformatics sector.

The Outcome:

- In order to address skills gaps in scripting and workflow management, as well as access gaps to high performance computers and data sharing tools, NeSI and Genomics Aotearoa are collaboratively delivering highly-relevant genomics skills training that facilitates capability growth among New Zealand researchers.

Core Hours Used (grouped by Research Discipline)



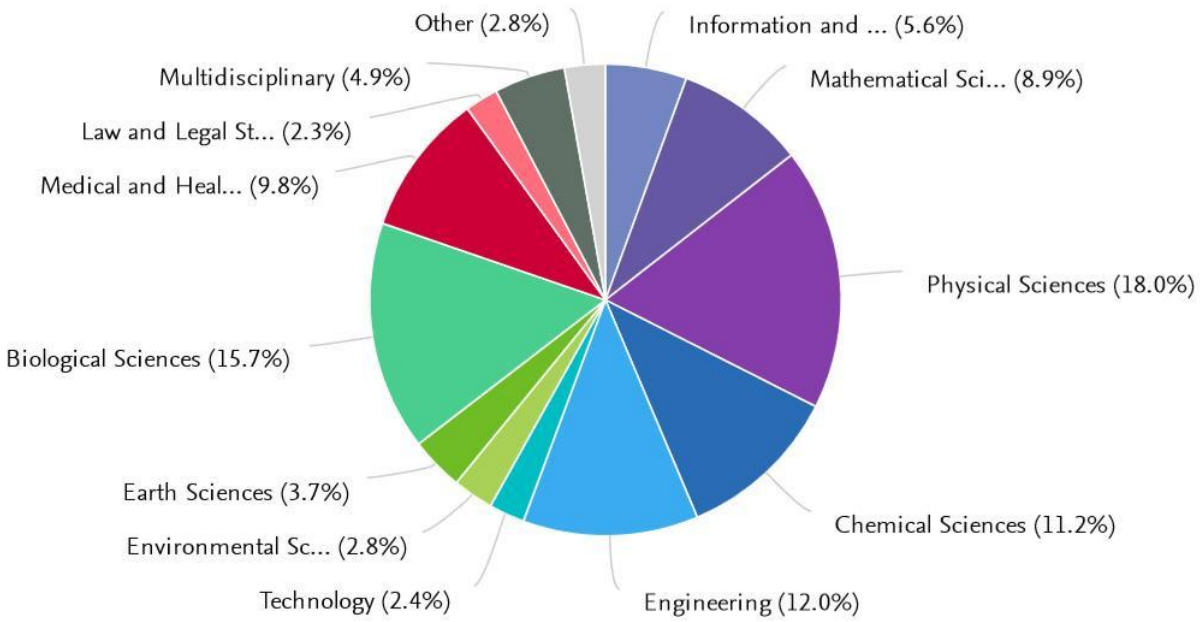
NeSI Research Impact

Year range: 2013 to 2019 /Q1.

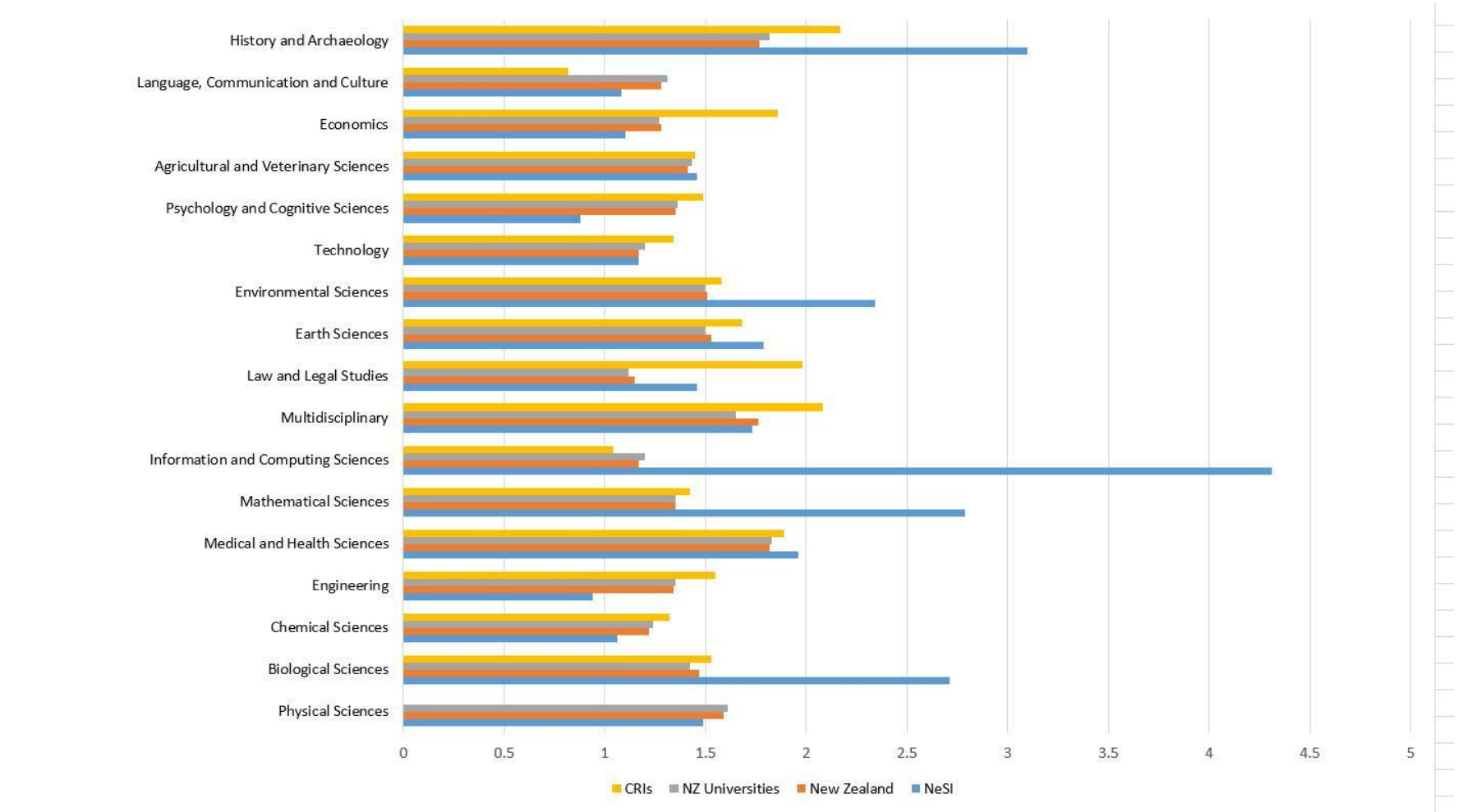
Journal articles **343**	Authors **1,334**	Field-Weighted Citation Impact **1.80**
Citation Count **5,456**	Citations per Publication **15.9**	

Data source: Scopus
Citation analysis: SciVal

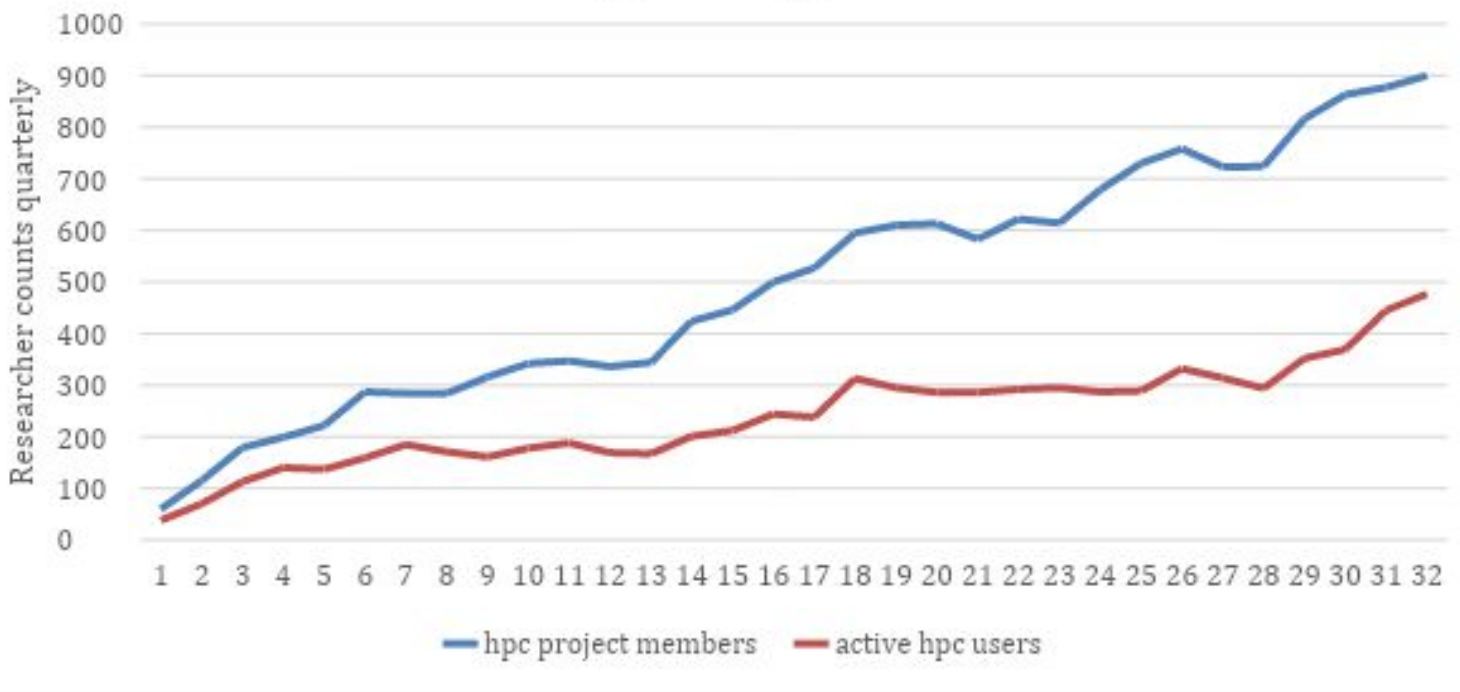
Publications by Subject



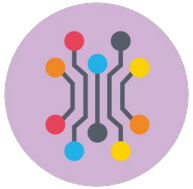
Field Weighted Citation Impact 2013-18



Researchers actively using NeSI vs project team members



Services



High performance computing (HPC) and analytics

- High performance computing & data platform for research
- Data analytics, modelling, and simulation software applications
- Virtual labs, visualisation, pre/post processing, cloud integration

Data transfer and share

- High speed, secure data transfer using Globus (global data management platform)
- End-points nationally and internationally to support end-to-end collaboration

Training and researcher skill development

- In-person and online training to grow skills in NZ research sector
- Partnership with The Carpentries - global programme teaching foundational coding and data science skills to researchers

Consultancy

- Computational science experts available to lift computational capabilities of research teams, as well as optimise tools & workflows

Mahuika and Māui are housed inside the purpose-built NIWA High Performance Computing Facility in Wellington

Robin Bensley
Business Operations Manager,
University of Auckland

Blair Bethwaite
Solutions Manager,
University of Auckland

Thomas Berger
Product Manager,
University of Auckland

Fabrice Cantos
HPC Operations Manager,
NIWA

Laura Casimiro
Operations Coordinator,
University of Auckland

Brian Flaherty
Data Services Product Manager,
University of Auckland

Kim Frew
Science Engagement Manager,
University of Auckland

Megan Guidry
Research Communities Advisor,
University of Auckland

Greg Hall
Systems Engineer,
University of Auckland

Yuriy Halytskyy
Systems Engineer,
University of Auckland

Wolfgang Hayek
Scientific Programmer,
NIWA

Matt Healey
Application Support Specialist,
University of Otago

Aaron Hicks
Systems Engineer,
NIWA

Jose Higino
Systems Engineer,
NIWA

Jun Huh
Business Innovation
and Growth Manager,
University of Auckland

Nick Jones
Director,
University of Auckland

Marko Laban
Software Product
Engineering Lead,
University of Auckland

Nancy Lin
Data Analyst,
University of Auckland

Nooriyah Lohani
Research Communities Advisor,
University of Auckland

Jana Makar
Communications Manager,
University of Auckland

Peter Maxwell
Application Support Specialist,
University of Auckland

Alexander Pletzer
Scientific Programmer,
NIWA

Nitharsan Puwanendran
Analyst Programmer,
University of Auckland

Georgina Rae
Engagement Manager,
University of Auckland

Kumaresh Rajalingam
Analyst Programmer,
University of Auckland

Ben Roberts
Application Support Specialist,
Manaaki Whenua –
Landcare Research

Albert Savary
Application Support Specialist,
University of Otago

Chris Scott
Scientific Programmer,
University of Auckland

Dinindu Senanayake
Genomics Support Specialist,
University of Auckland

Anthony Shaw
Application Support Analyst,
University of Auckland

Nick Spencer
Site Manager
Manaaki Whenua –
Landcare Research

Callum Walley
Application Support Analyst,
University of Auckland

Damian Wheeler
Site Manager,
University of Otago

Jeff Zais
Senior Science Advisor &
Platforms Architect,
NIWA

Wednesday 12 Feb

1:30 - 1:50 pm - **Megan Guidry -** Training: It's better together

1:30 - 5:30 pm - **Chris Scott -** First steps in machine learning with NeSI

1:50 - 2:10 pm - **Callum Walley -** Engineering HPC: What's going on?

2:10 - 2:30 pm - **Marko Laban -** Cloud-native technologies in eResearch: Benefits & challenges

2:50 - 3:00 pm - **Jun Huh -** Learning how to learn

3:30 - 4:30 pm - **Megan Guidry** - Building and supporting a NZ digital literacy training community

3:30 - 4:30 pm - **Blair Bethwaite** - Research Cloud NZ

Thursday 13 Feb

11:00 - 11:20 am - **Wolfgang Hayek -** Singularity containers on HPC

11:00 am - 12:20 pm - **Brian Flaherty -** Building a national/regional data transfer platform: Globus BoF

1:30 - 1:50 pm - **Nick Jones -** Advancing New Zealand's computational research capabilities and skills

1:30 - 1:50 pm - **Jun Huh -** User journey-driven product management

1:30 - 5:30 pm - **Blair Bethwaite** - Containers in HPC tutorial

1:50 - 2:10 pm - **Brian Flaherty** - Where Data Lives: NeSI, taonga and growing repository services

Thursday 13 Feb (cont.)

1:50 - 2:10 pm - **Jeff Zais** - Worldwide trends in computer architectures for data science

2:10 - 2:30 pm - **Dinindu Senanayake** - HPC for life sciences: Handling the challenges posed by a domain that relies on big data

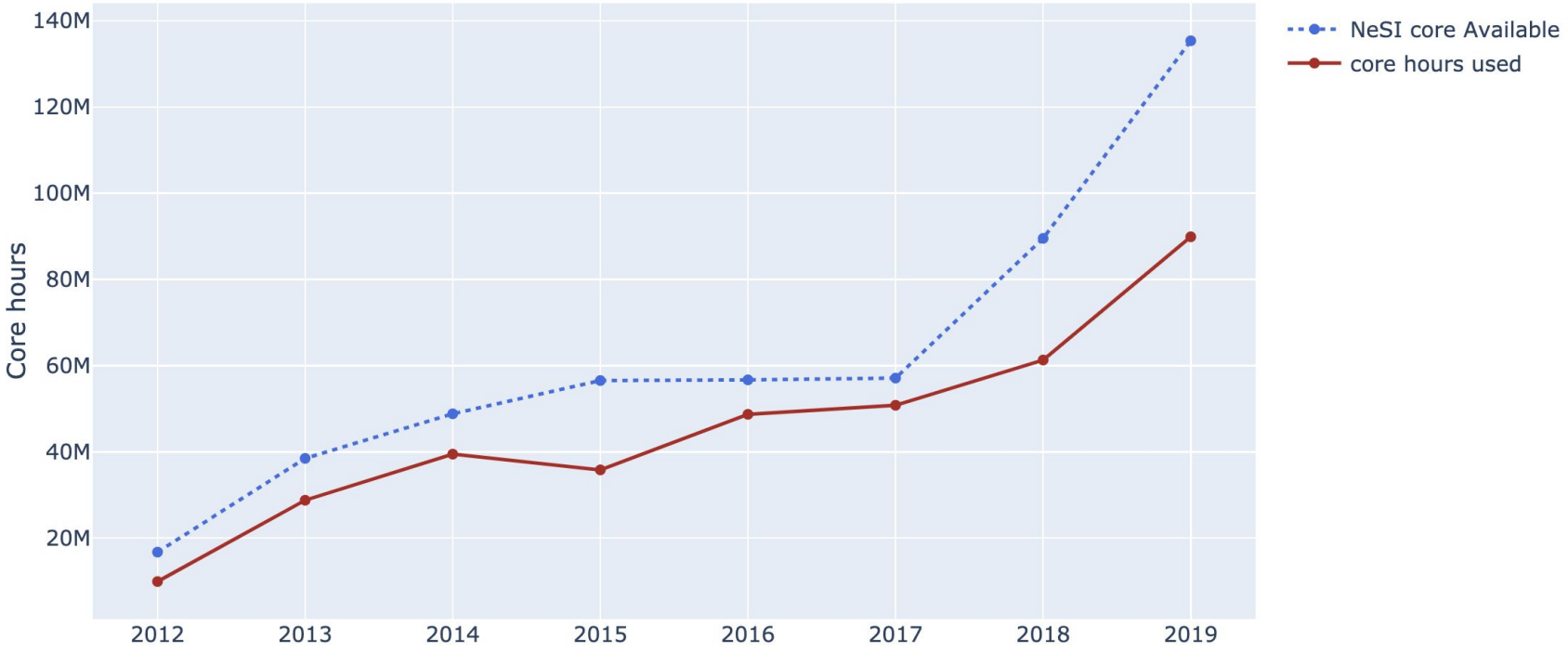
3:30 - 5:30 pm - **Jana Makar** - Growing the eResearch workforce in an inclusive way

Friday 14 Feb

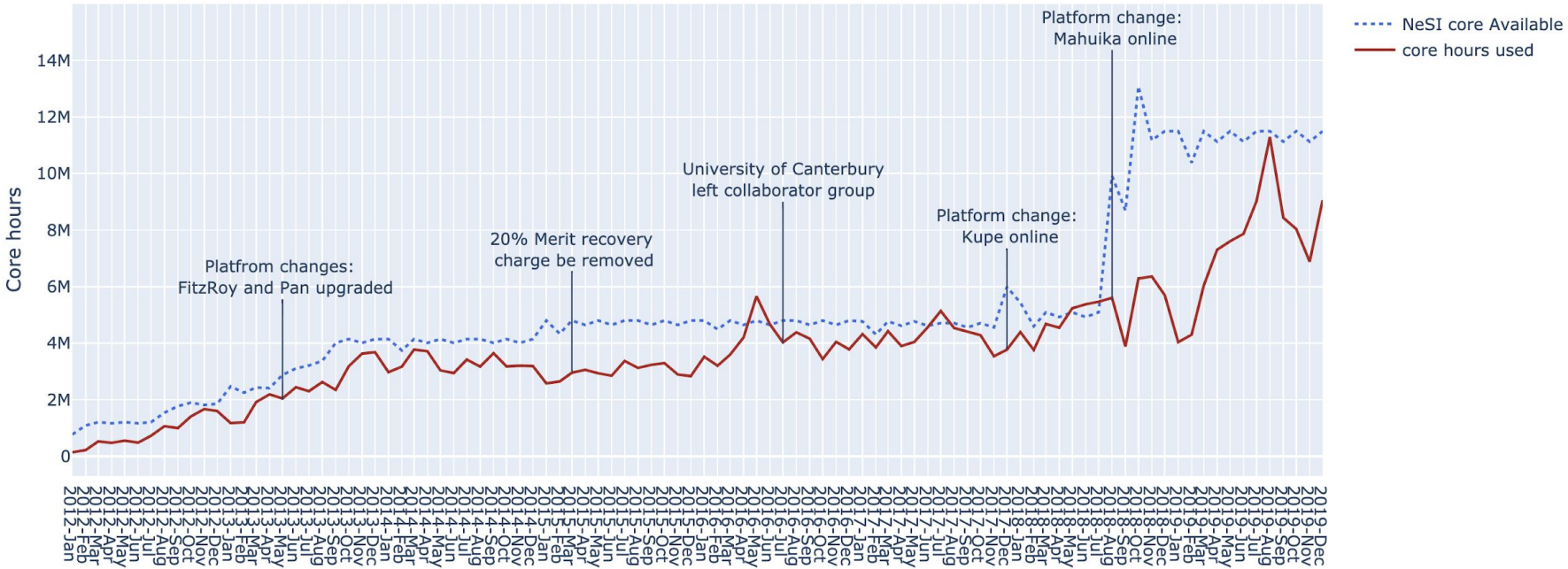
11:20 - 11:40 am - **Alexander Pletzer** - Enhancing eResearch productivity with NeSI's consultancy service

1:30 - 3:40 pm - **Nooriyah Lohani -** Research Software Engineering (RSE) community update and next steps in New Zealand

Total core hours 2012 - current



Total core hours 2012 - current

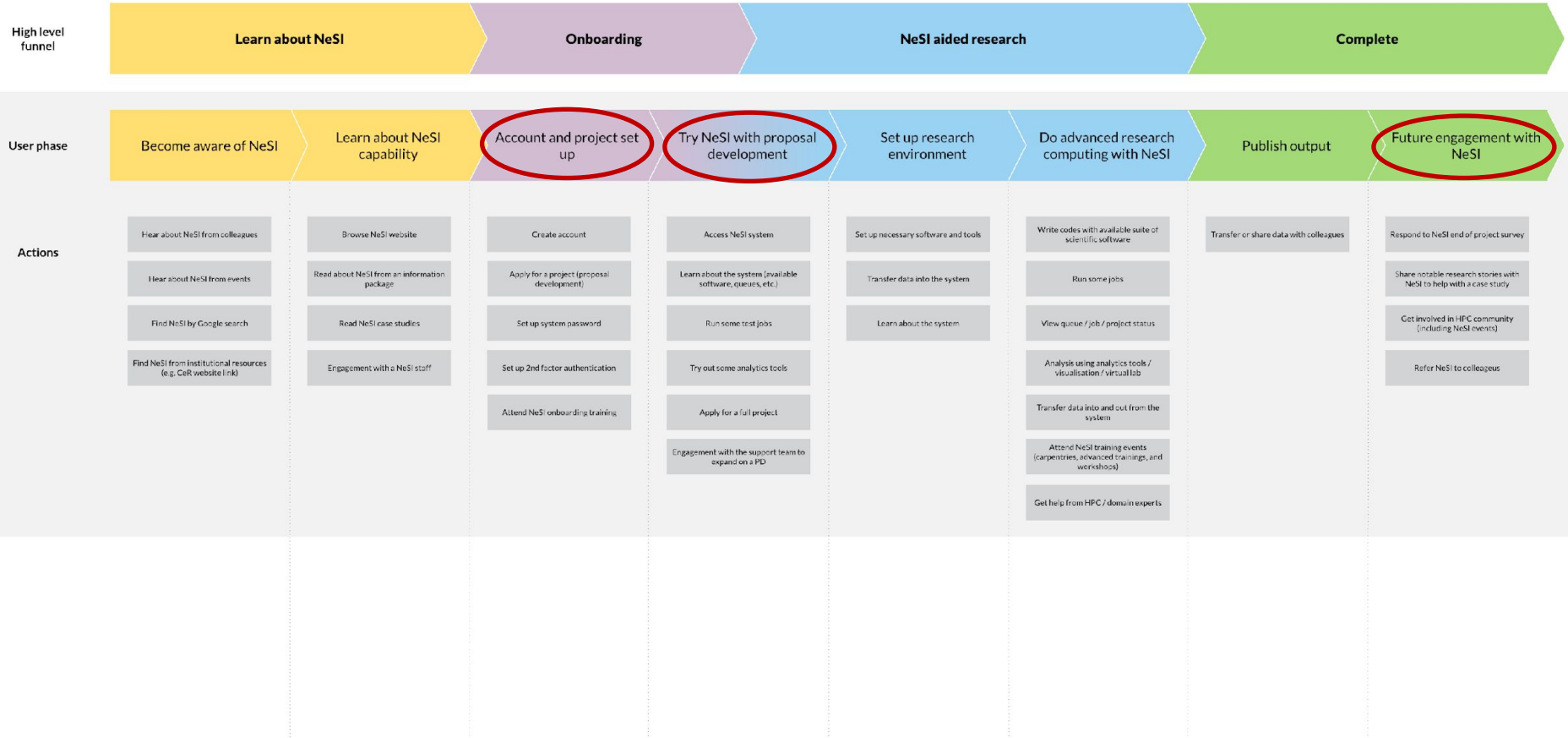


NeSI user journey

Actor: a researcher using NeSI for the first time (not an HPC expert)

Scenario: They want to use advanced research computing resources to do better research (a resource can be hardware, tools, knowledge, expert support, training, and more)

Expectations:
* clear online information of resources
* domain experts to provide best practices, tools, and knowledge to do best research
* options to upskill along the way as needed
* friendly and helpful support



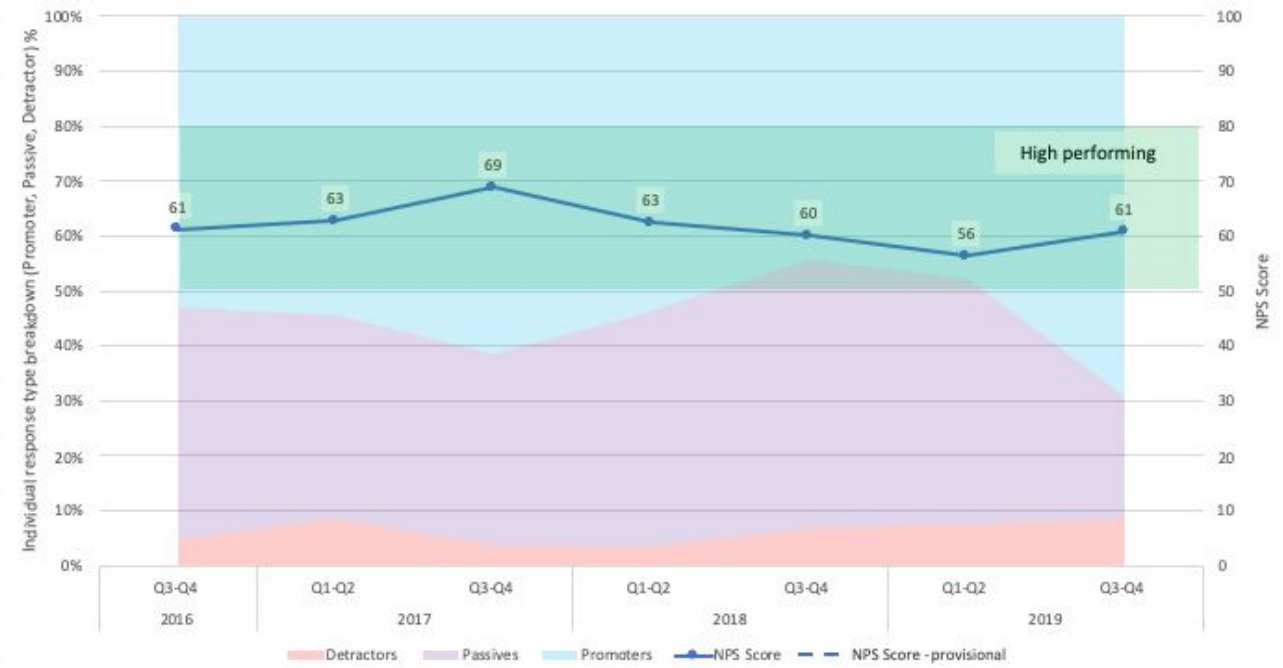
Getting started ...

HPC Compute & Data Analytics

Achievements & successes

- Scale up in usage and users across the infrastructure
- Maintain high quality support service - 3.1k requests, 99%+ satisfaction @ 43% response rate
- Reduced complexity to log in
- Rolling upgrade and maintenance of the systems.
- National fit-for-purpose review and allocations
- Enhancements to internal data-models to enable richer allocation management and reporting
- Entitlement controls to improve dynamics of use and ROI
- Purchase to increase national availability of high memory nodes
- Building-up data analytics: AI/ML frameworks directly available, container support, documentation, workshops
- Piloted new services - Globus, data archive, Jupyter notebooks

NeSI Net Promoter Score from end of project surveys



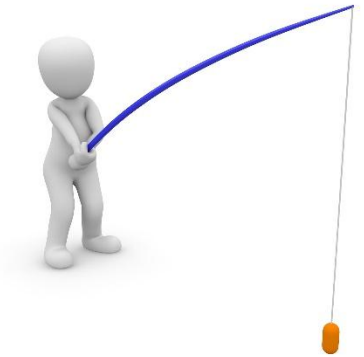
HPC Compute & Data Analytics

Insights & learnings

- Capacity growth driven by code scale up as well as user growth
- Memory per CPU is more highly demanded than envisaged
- Storage is a scarce resource:
  - Currently implementing retention policy + data management software between different tiering storage (nobackup, persistent, nearline)
- Proactively identify inefficient use of resources in user workflows
- More Collaborator-hosted projects are moving to Maui style MPI machine than has been seen in the past
  - Opportunity to dynamically rebalance institutional entitlements between machines
- Changes in senior leadership team - retirment, maternity = 3 new senior members
  - New expertise and perspectives coming in

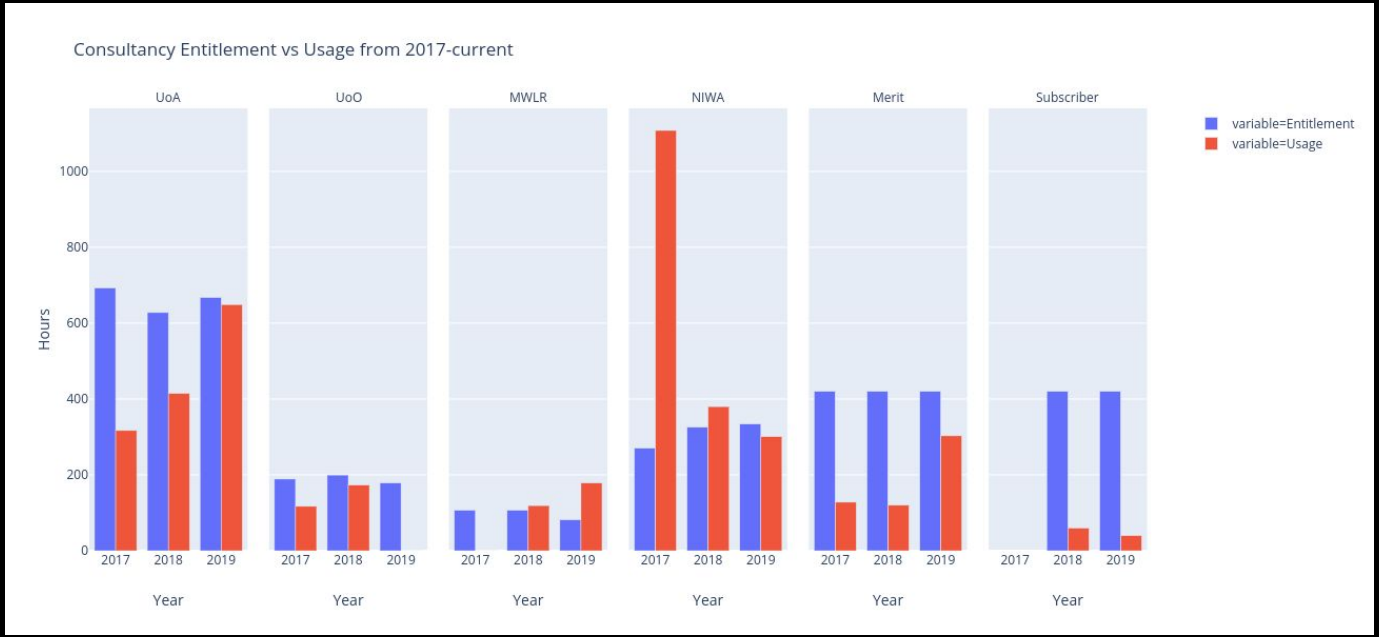
Computational Science consultancy

- A service offered to NeSI platform users, generally at no cost to the researcher
- A research group granted access to one or more of NeSI's Scientific Programmers
- Projects offered ~90h over 3 months
- Goal is **raise the capability** of the research group so emphasis is on **transferring skills**



Challenge: identifying projects which would benefit

Computational Science Consultancy



Computational Science Consultancy

Achievements & successes

- 25 projects underway during 2019 (up from 13 in 2018)
- Researchers reporting benefits in new survey
  - 82 % improved time to solution
  - 73 % upskilled or improved knowledge
  - 55 % enabled or enhanced research capability
  - 27 % improved software sustainability
- Lots of good feedback
  - “The Consultancy service was excellent. It was exactly what I was looking for. In addition to streamlining my research, I've also upskilled...”
  - “We have hugely benefitted from this project. NeSI staff has been absolutely terrific helping us solving visualization problems and optimizing our use of resources. It has been a huge help for the project.”
- Pipeline of new projects filling up

Computational Science Consultancy

Insights & learnings

- Good pipeline of new projects
  - Working with App Support to identify projects and turn more tickets into consultancies has worked really well
  - Regularly presenting at conferences
- Great to have members of other teams contributing to consultancy projects
- Still some work to do
  - Spending more time on consultancy projects (may have to spend less on other tasks?)
  - Balancing our time between institutions/classes (work closer with representatives from institutions to create a prioritised queue of projects?)
- Looking forward to the new Data Science Engineer

Training

Enabling researchers to do better research…

by supporting communities: digital skills and capability building

Plant and Food: Software Carpentry

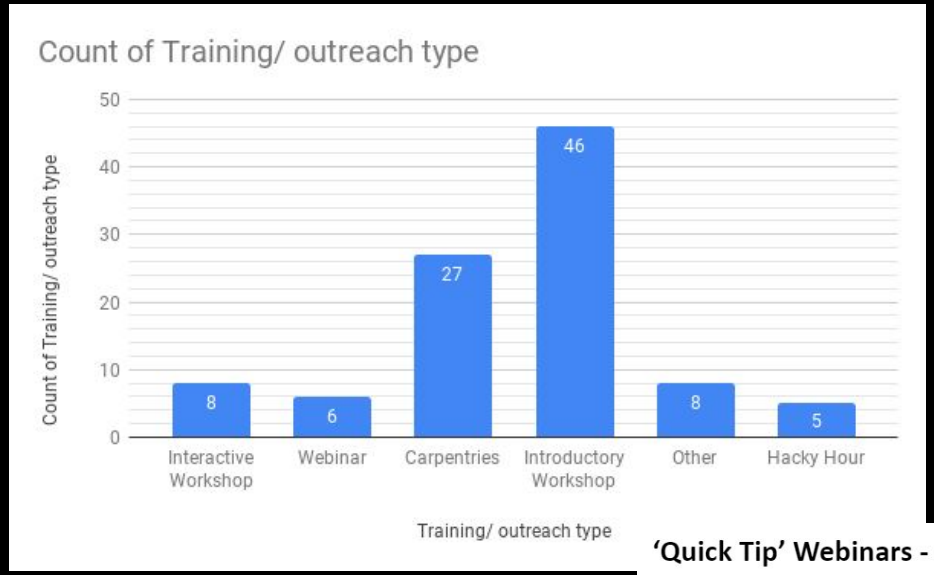
CRI Coding Conference 2016

NeSI at University of Otago Day

Winter bootcamp: University of Auckland Software Carpentry workshop

Scion: Software Carpentry

Training



'Quick Tip' Webinars - Aug - Nov 2019

NeSI

New short webinars on tools & skills to help you use NeSI

- 30 - 45 min sessions, delivered by NeSI team members
- Interactive - questions encouraged!
- Will be recorded & posted to NeSI YouTube

Requests for topics?? Email: training@nesi.org.nz

Date / Time	Topic
Tues 20 Aug @ 1 - 1:45 pm	NeSI HPC 101: Tips for job scaling & running tests
Wed 11 Sept @ 2:30 - 1 pm	NeSI Data Transfer Platform: How to share data & set up groups using Globus
Wed 9 Oct @ 1 - 1:45 pm	Getting Started with NeSI: How to move your data on and off the NeSI platforms
Wed 6 Nov @ 12:30 - 1:15 pm	Need help? How to access and use NeSI support and consultancy

Training

Achievements & successes

- Just under 100 training events for 2019
- 70% of NZ instructor trainees have checked out
- Supported 26 Carpentries workshops throughout NZ
  - Our partnership with GA resulted in the delivery of 6 Genomics Data Carpentry courses in 6 months
- NeSI's first training webinar series
  - 4 webinars
  - Recordings available on youtube
- Online Hacky Hours were trialed

Training

Insights & learnings

- Training is a team effort! Thanks to everyone who has contributed
- Raising community awareness re:training is key
- We can still improve the processes around preparing for and running online events
- We love having researchers speak at our webinars!
- Demand for courses continues to grow

Data Transfer & Share

National Data Transfer Platform Launch

Data Transfer & Share

Achievements & successes

- May relaunch
- May & September NeSI hosted training Webinar of the 'Quick Tips' webinar series.
- Presentations at eResearch NZ, Figshare Fest & eResearch Australasia
- Genomics Aotearoa Data Repository: Group-based membership & access controls
- Increased usage

2019

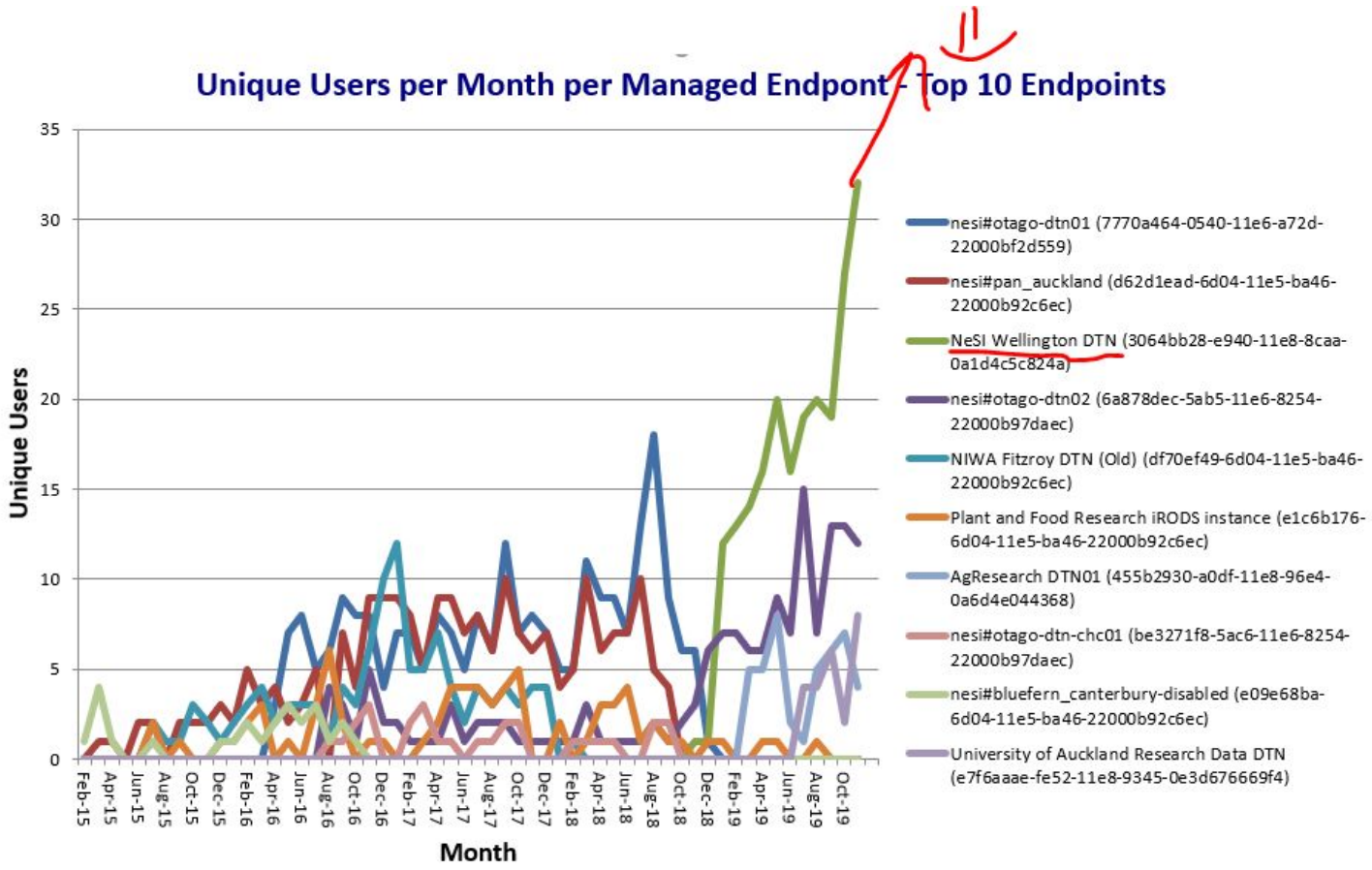
76.5TB	166.2 million	3991
Amount of data transferred	Number of files transferred	Number of transfers made

Data Transfer & Share

Insights & learnings

- Opportunities to grow the platform:
  NZ: CRIs, Universities, Catalyst Cloud
  AU: Aarnet, Synchrotron, Garvan Sequencing Lab…
- Globus automated workflows
- Need to resolve myproxy/authentication issues (EduGain as possible solution)

Data Transfer & Share



Partnerships

AUT UNIVERSITY
NEW ZEALAND

genomics aotearoa

REANNZ

agresearch
āta mātai, mātai whetū

Partnerships

Achievements & successes

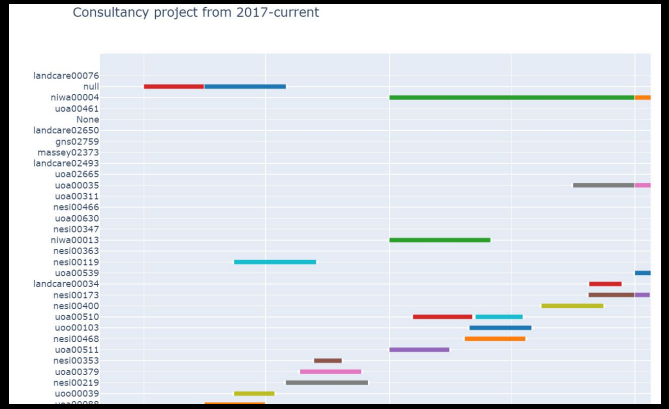
- Engagement at research domain level
  - Genomics Aotearoa and Genomics Community
  - Engineering Community
  - RSE Community
  - Women in HPC
- Broader set of Subscriptions
  - AUT, AgResearch, GNS, Canterbury (through QuakeCore)
- Quarterly Service Governance with partners
  - Ongoing set of actions
    - Training and engagement in CRIs
    - All partners have varied needs

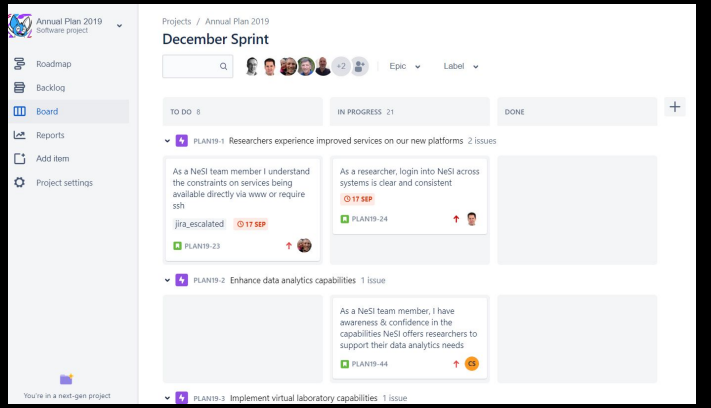
Partnerships

Insights & learnings

- Takes time and energy to maintain partnerships
  - Number of relationships is broadening
  - Set of needs and points of interest is broadening
- Genomics Aotearoa is an energiser to make us consider our services and engagement approach
  - Joint training plans
  - How to evolve our Data services
    - Long term storage
    - Publication of data

Services Innovation (changes to NeSI the “Platform”)





Services Innovation (changes to NeSI the “Platform”)

Achievements & successes

- How we work: Agile at the leadership and team level
- Work on our infrastructure
  - New large and huge memory nodes are first to be procured from our Platform Acquisition Fund
  - Piloting our incremental investment processes
- Recruitment ongoing
  - New Leaders
  - Auckland, NIWA, Otago increases in staffing
- Supporting our Stakeholders
  - Improvements to administrative data and reporting on impact and return on investment

Services Innovation (changes to NeSI the “Platform”)

Insights & learnings

- Getting incremental procurement to change capacity/capability was difficult (process, alignment of stakeholders)
- Transitioning from NeSI 2.1 to NeSI 2.2 was not part of the plan, we have the chance to get better aligned on sector needs to drive NeSI 3
- NeSI services and set of stakeholders is becoming broader; we need better tools (automation, new metrics) to show value

Robin Bensley
Business Operations Manager,
University of Auckland

Blair Bethwaite
Solutions Manager,
University of Auckland

Thomas Berger
Product Manager,
University of Auckland

Fabrice Cantos
HPC Operations Manager,
NIWA

Laura Casimiro
Operations Coordinator,
University of Auckland

Brian Flaherty
Data Services Product Manager,
University of Auckland

Kim Frew
Science Engagement Manager,
University of Auckland

Megan Guidry
Research Communities Advisor,
University of Auckland

Greg Hall
Systems Engineer,
University of Auckland

Yuriy Halytskyy
Systems Engineer,
University of Auckland

Wolfgang Hayek
Scientific Programmer,
NIWA

Matt Healey
Application Support Specialist,
University of Otago

Aaron Hicks
Systems Engineer,
NIWA

Jose Higino
Systems Engineer,
NIWA

Jun Huh
Business Innovation
and Growth Manager,
University of Auckland

Nick Jones
Director,
University of Auckland

Marko Laban
Software Product
Engineering Lead,
University of Auckland

Nancy Lin
Data Analyst,
University of Auckland

Nooriyah Lohani
Research Communities Advisor,
University of Auckland

Jana Makar
Communications Manager,
University of Auckland

Peter Maxwell
Application Support Specialist,
University of Auckland

Alexander Pletzer
Scientific Programmer,
NIWA

Nitharsan Puwanendran
Analyst Programmer,
University of Auckland

Georgina Rae
Engagement Manager,
University of Auckland

Kumaresh Rajalingam
Analyst Programmer,
University of Auckland

Ben Roberts
Application Support Specialist,
Manaaki Whenua –
Landcare Research

Albert Savary
Application Support Specialist,
University of Otago

Chris Scott
Scientific Programmer,
University of Auckland

Dinindu Senanayake
Genomics Support Specialist,
University of Auckland

Anthony Shaw
Application Support Analyst,
University of Auckland

Nick Spencer
Site Manager
Manaaki Whenua –
Landcare Research

Callum Walley
Application Support Analyst,
University of Auckland

Damian Wheeler
Site Manager,
University of Otago

Jeff Zais
Senior Science Advisor &
Platforms Architect,
NIWA

support@nesi.org.nz

https://www.nesi.org.nz/apply

www.nesi.org.nz

@NeSI_NZ