



HPC For Life Sciences

New Zealand eScience Infrastructure

Dinindu Senanayake

Support

- Expert knowledge in multiple domains



Consultancy

- Analysis, debug and optimization of user applications



NeSI

New Zealand eScience
Infrastructure

Training

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



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





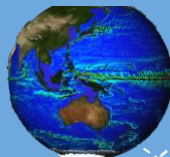
NeSI

New Zealand eScience
Infrastructure

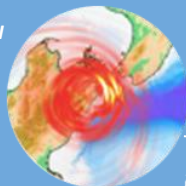
NeSI is a national
collaboration of:



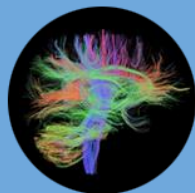
**Dr Olaf Morgenstern
and Dr Erik Behrens
(Earth Science)**
*Deep South Challenge
project using NeSI
supercomputers
for climate modelling.*



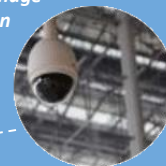
**Yoshihiro Kaneko
(Seismology)**
*GNS Science using NeSI
supercomputers to
recreate earthquake
events to better
understand their
processes and
aftermath effects.*



**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.*



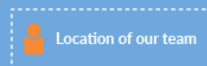
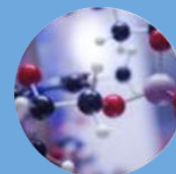
Andrew Chen (Engineering)
*Using NeSI supercomputers for advancing image
processing capabilities using computer vision*



**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.*





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 Higinio
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

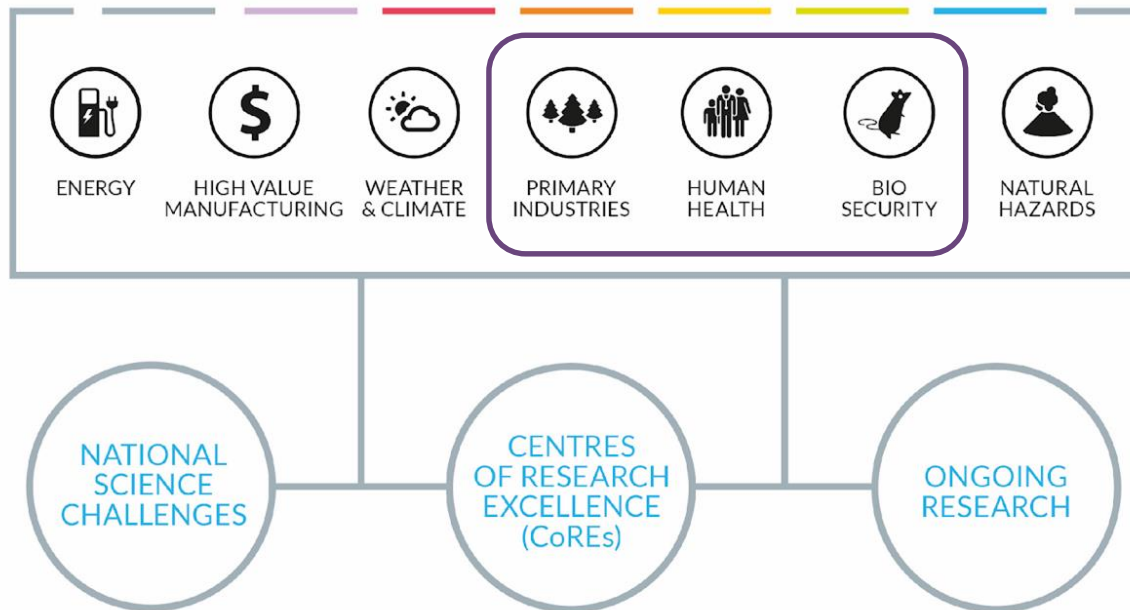


Damian Wheeler
Site Manager,
University of Otago



Jeff Zais
Senior Science Advisor &
Platforms Architect,
NIWA

Computing capability for future prosperity



Life Sciences in Mahuika: Project holders



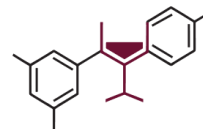
**genomics
aotearoa**



**MASSEY
UNIVERSITY**



**UNIVERSITY
of
OTAGO**
Te Whare Wānanga o Ōtago
NEW ZEALAND



**BRAGATO
RESEARCH INSTITUTE**
NEW ZEALAND GRAPE AND WINE RESEARCH
RANGAHAU KAREPE, WĀINA O AOTEAROA



**THE UNIVERSITY OF
WAIKATO**
Te Whare Wānanga o Waikato



Plant & Food
RESEARCH
RANGAHAU AHUMARA KAI



**Manaaki
Whenua**
Landcare
Research

agresearch
āta mātai, mātai whetū



Ministry for Primary Industries
Manatū Ahu Matua

Mahuika: 9216 cores

Maui: 19,940 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)

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.

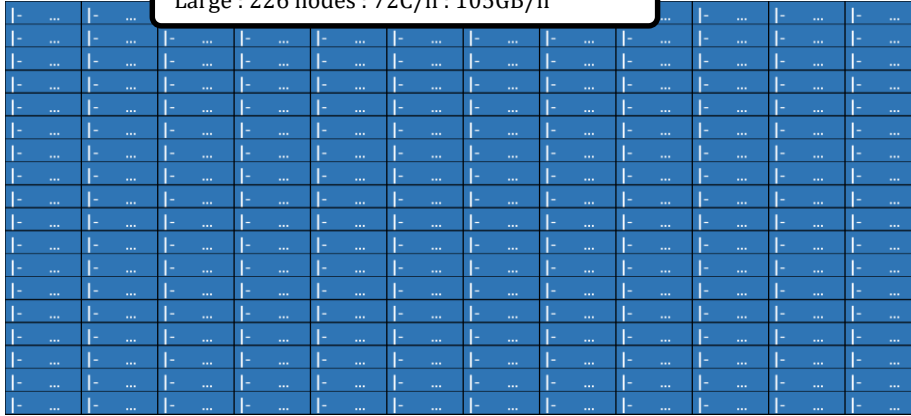
Today Mahuika is powering researchers throughout New Zealand in a range of fields, from genomics research to seismic mapping.

MAHUIKA incorporates:

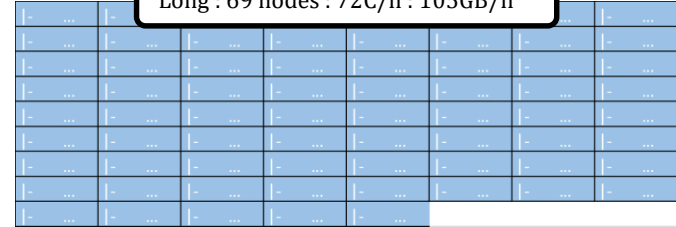
- 234 compute node Cray CS400
- 8,424 x 2.1GHz Broadwell cores
- CS400 Virtual Labs

Mahuika Partitions

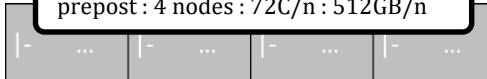
Large : 226 nodes : 72C/n : 105GB/n



Long : 69 nodes : 72C/n : 105GB/n



prepost : 4 nodes : 72C/n : 512GB/n



bigmem : 9 nodes : 72C/n : 512GB/n



GPU : 4 nodes



ga_hugemem
128C : 4TB

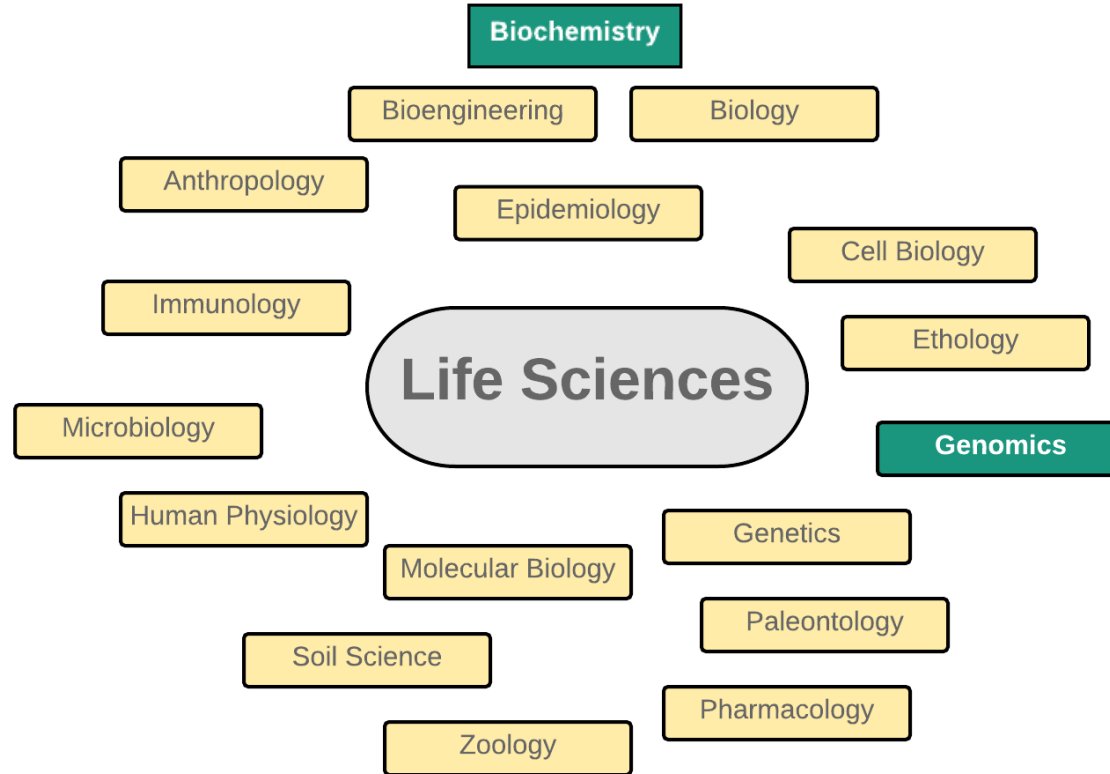
ga_bigmem
72C : 512 GB

hugemem
176C(s) : 6TB

hugemem : 2 nodes : 80C (s)/n : 1.5 TB/n

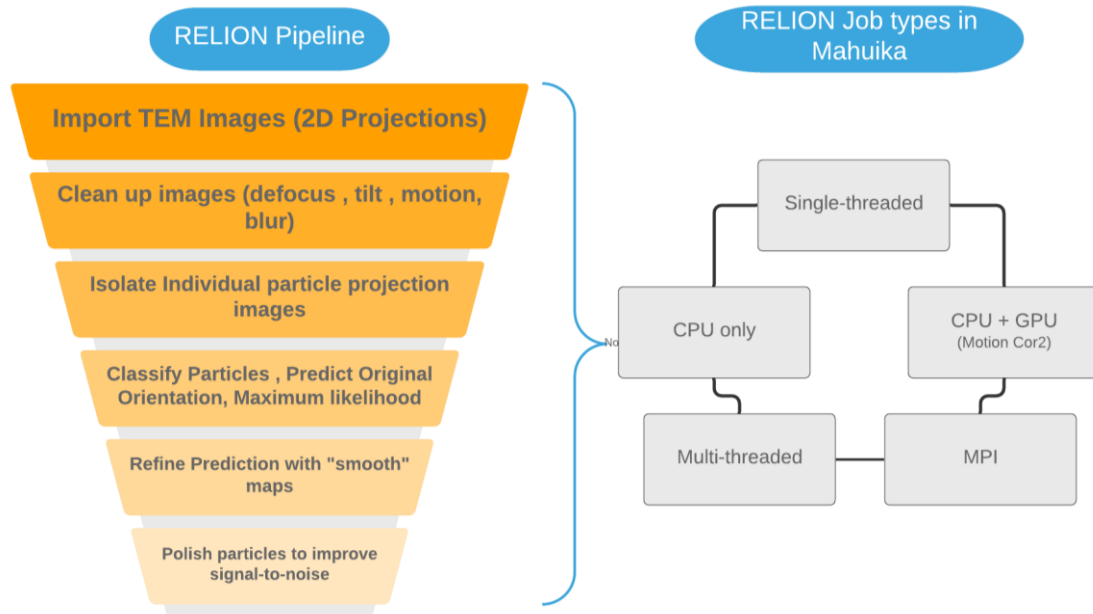


Life Sciences in Mahuika: branches and sub-disciplines

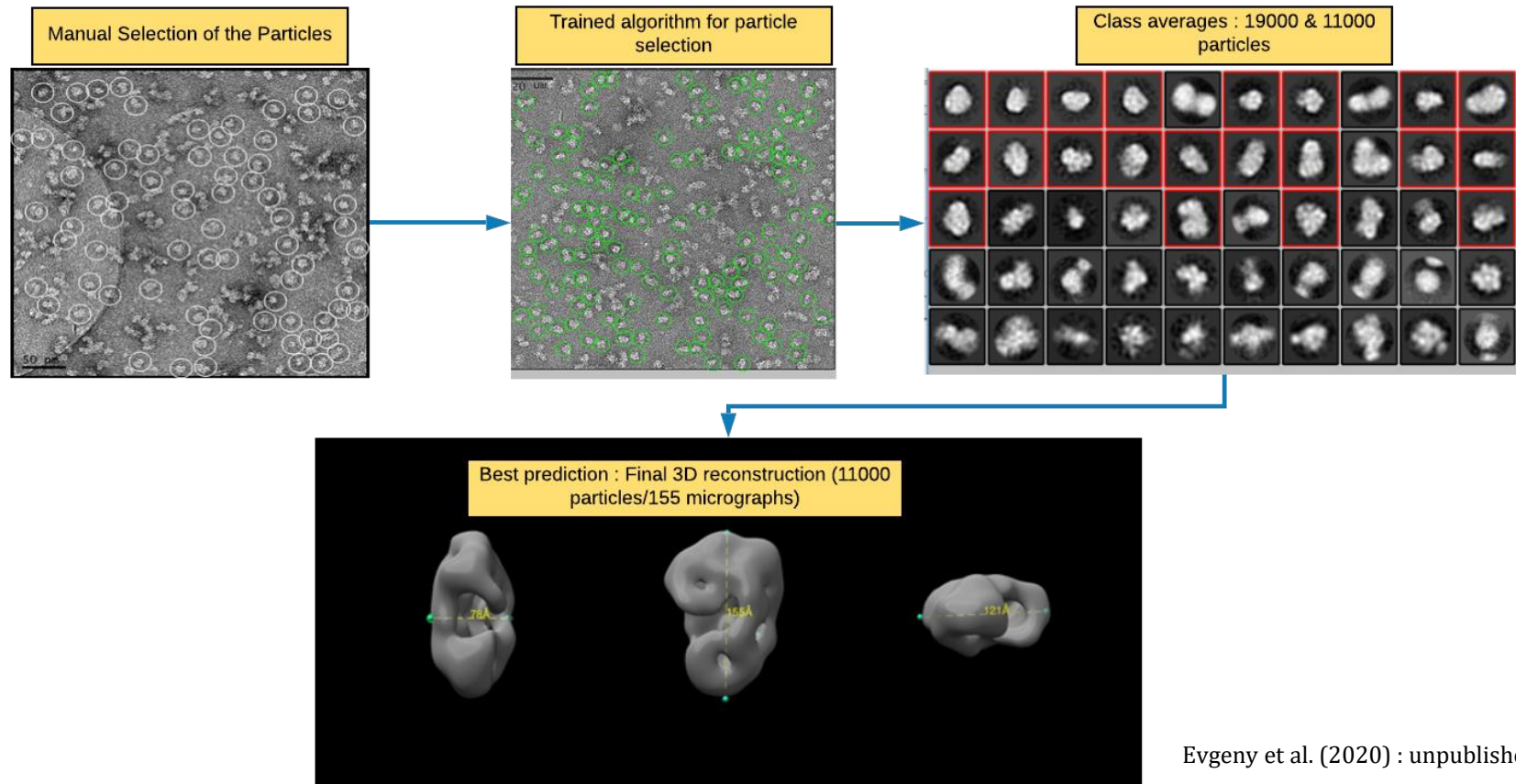


Cryo-EM Image processing in Mahuika

Objective : RELION (for REGularised Likelihood Optimisation, pronounce rely-on) is a stand-alone computer program that employs an empirical Bayesian approach to refinement of (multiple) 3D reconstructions or 2D class averages in electron cryo-microscopy (Cryo-EM).

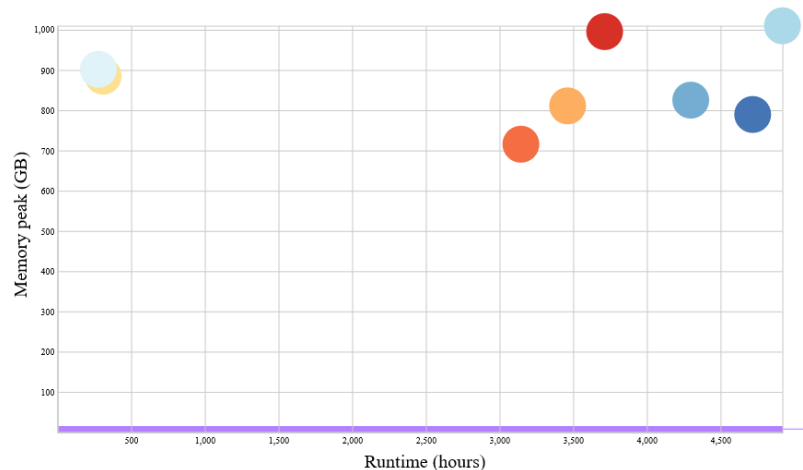
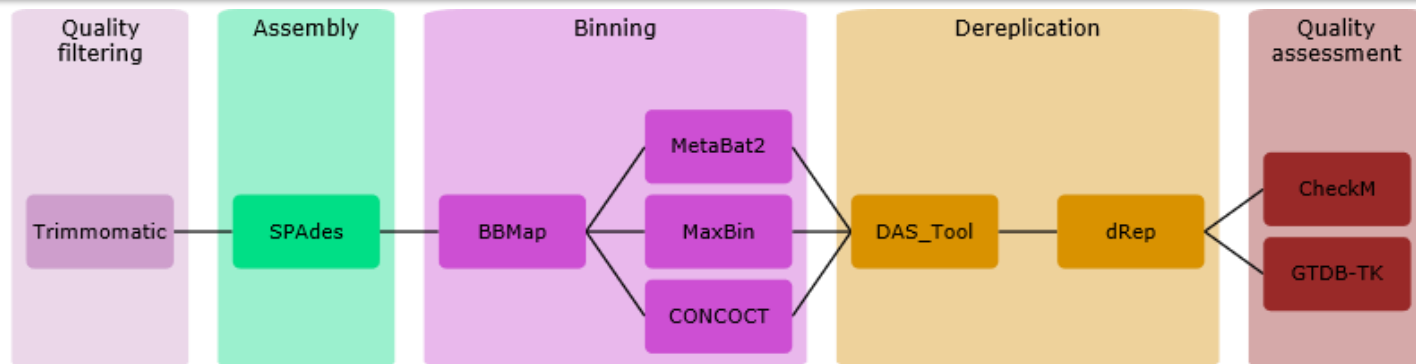


Selection, Prediction and 3D Reconstruction



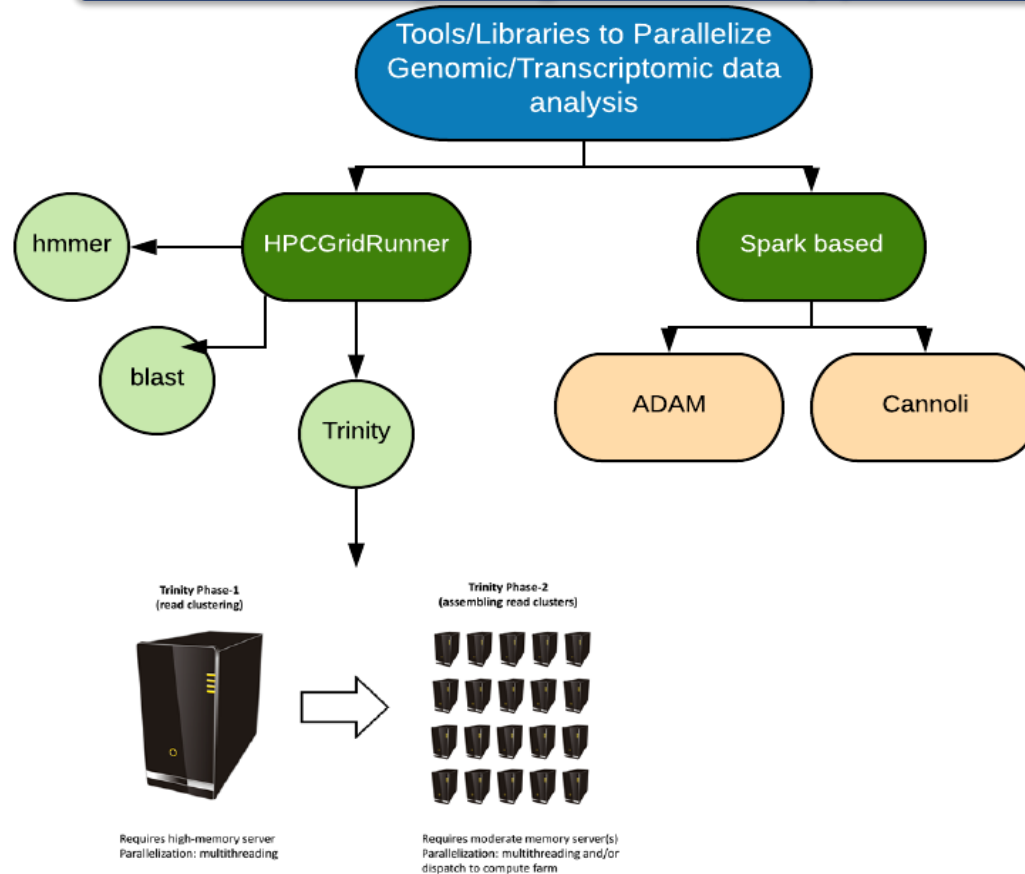
Evgeny et al. (2020) : unpublished

Environmental Metagenomics Pipeline: Developed and Optimised in Mahuika

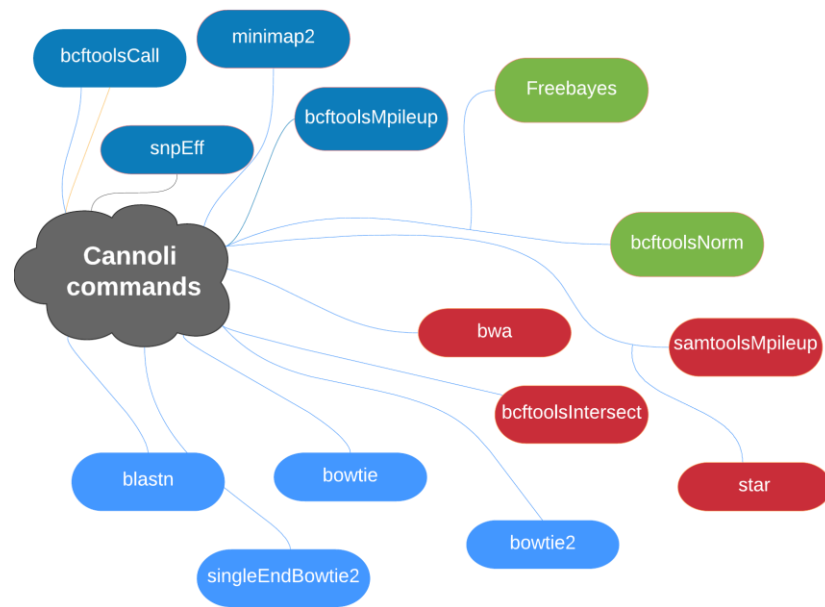
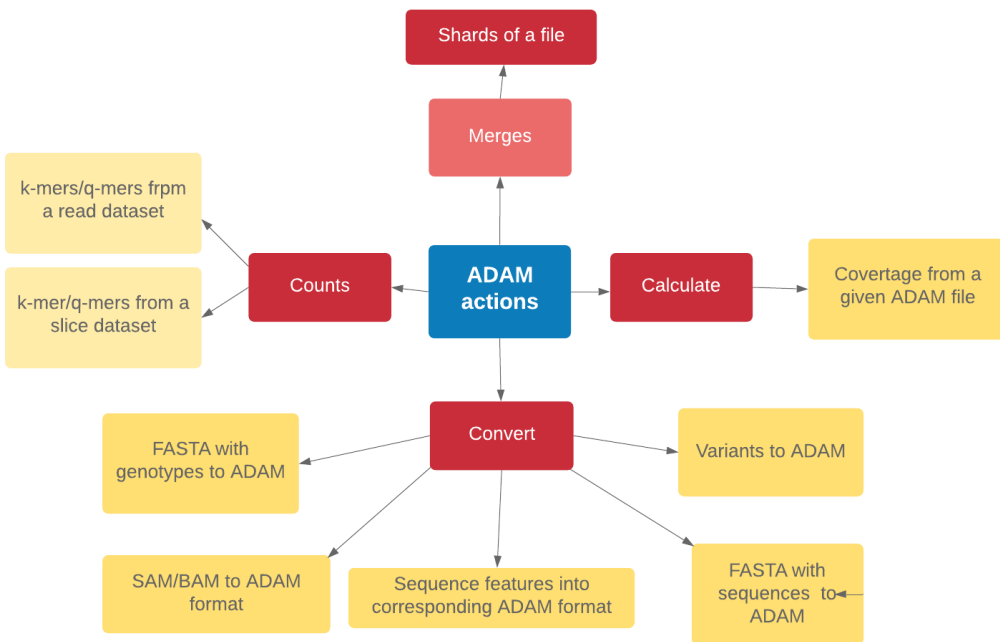


Waite et al. (2019)

Abandoning single node approach

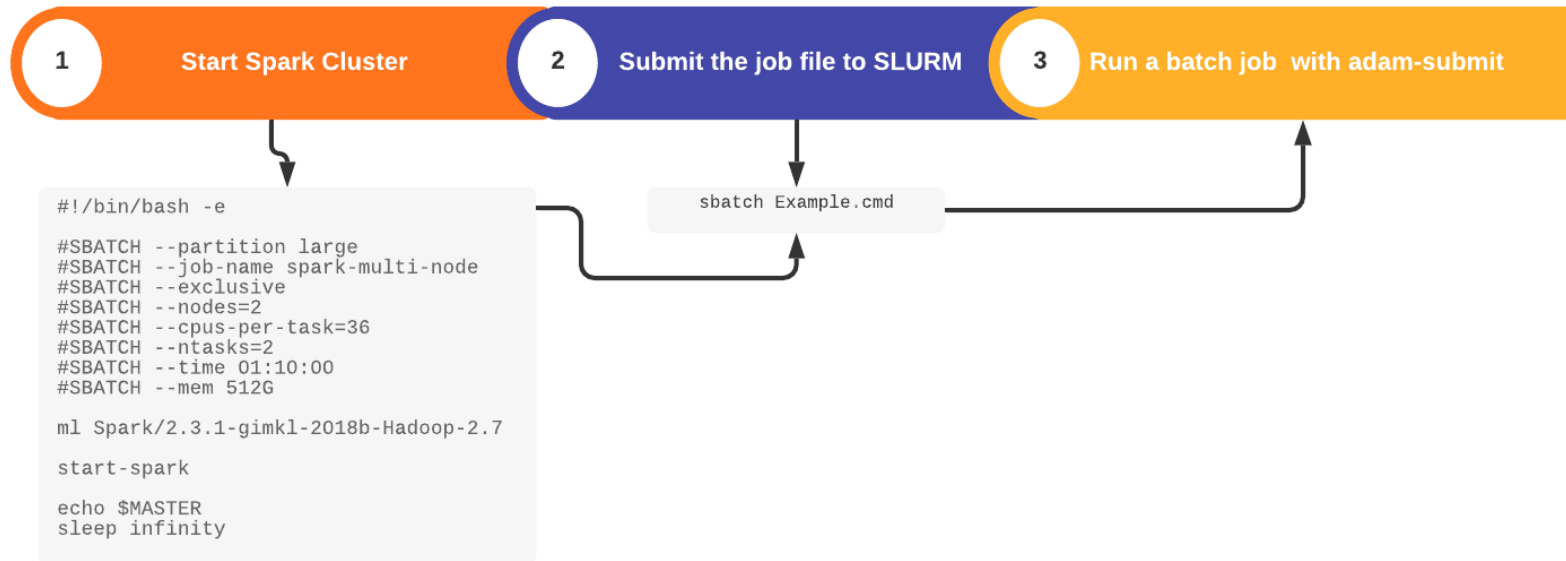


ADAM and Cannoli commands

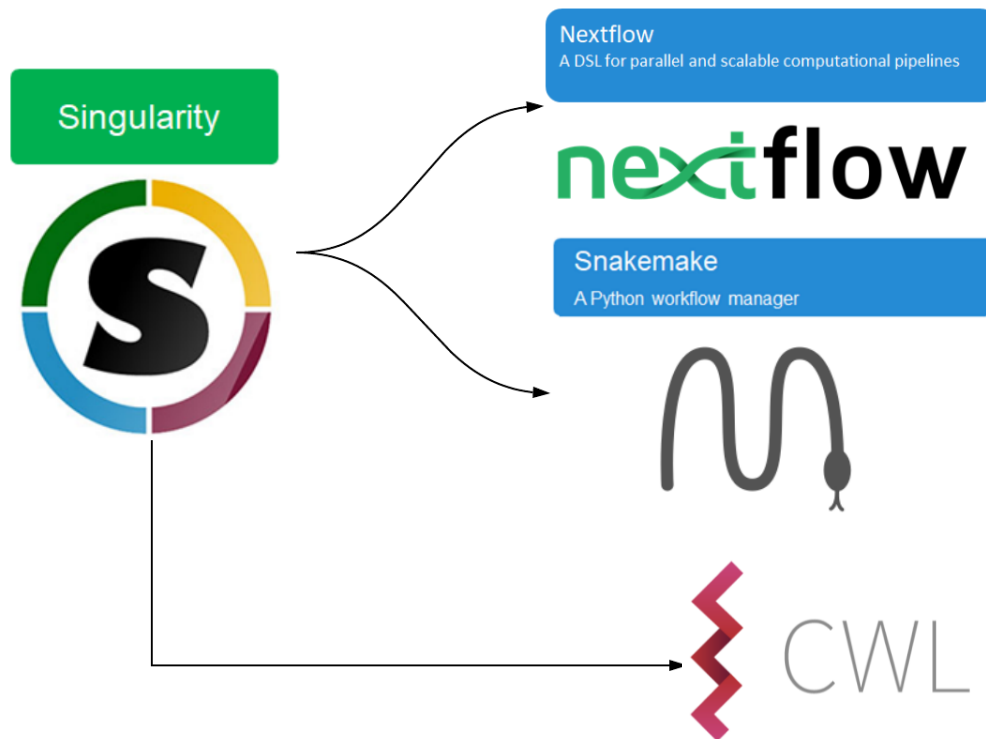


Reference : <http://bdgenomics.org/>

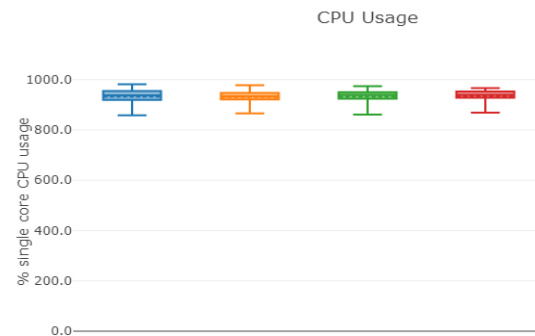
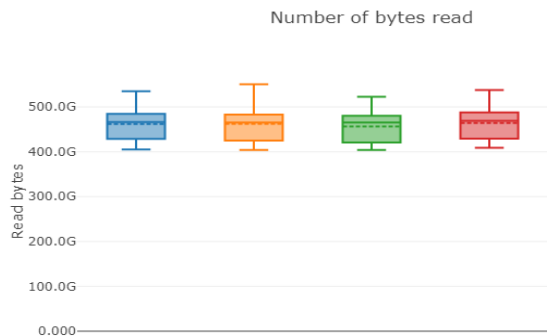
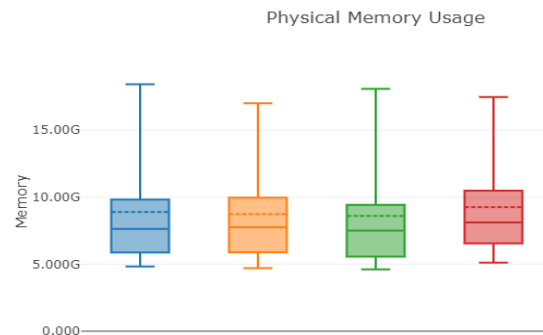
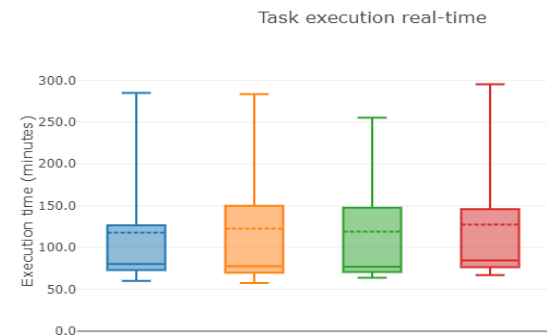
Launching ADAM via SLURM



Reproducibility: Containers & Workflows



Beyond Reproducibility: Using Workflows to get the best out of available resources (convenient profiling)



Guhlin, J. (2019)

NeSI @ eResearch NZ - Talks & Workshops:



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