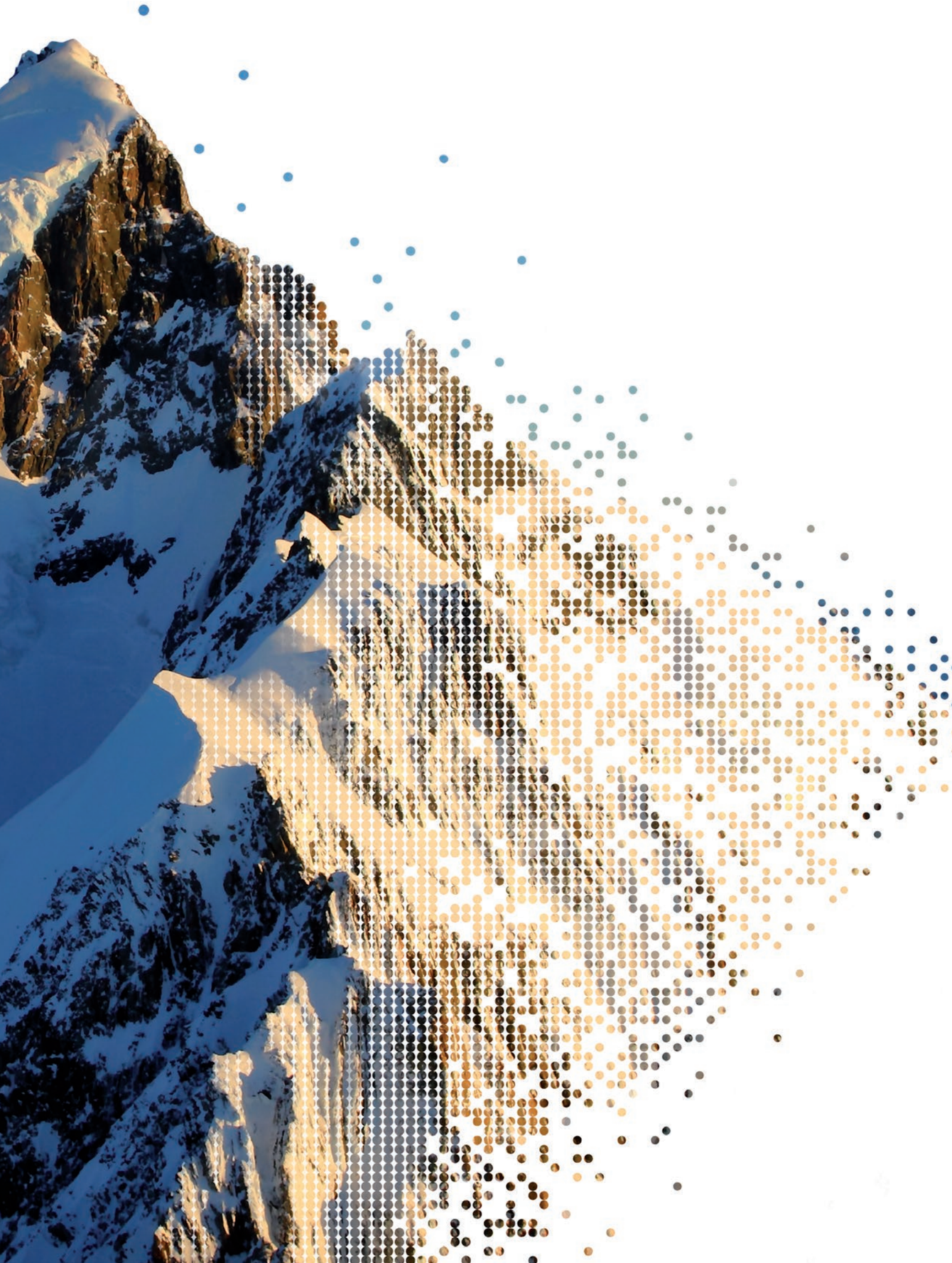
New Zealand
eScience
Infrastructure

2013 Review

Seeking clarity...



from reality

NeSI helps connect researchers to the bigger picture. In 2013 NeSI Supercomputer power ran 3D ice sheet models to analyse changes in the glaciers in New Zealand's Southern Alps. One of many 2013 NeSI projects that brought improved clarity to New Zealand's scientific research.

NeSI
New Zealand eScience Infrastructure

Our purpose is to grow the computing capability of New Zealand researchers to ensure future prosperity

The future prosperity of New Zealand hinges on our ability to accelerate our external competitiveness, and enhance our social wellbeing and environmental sustainability. Finding the right answers to these often-complex challenges demands deeper insights that only astute research can yield.

In today's world of high performance computing (HPC), New Zealand's size means our research capabilities and tools have to be structured to accentuate agility and connectivity. This is where New Zealand eScience Infrastructure (NeSI) plays a pivotal, energising role.

NeSI adds value for New Zealand's researchers by providing the superior computer power and support systems necessary to underpin the integrity of their research. Beyond that, NeSI formulates innovative future strategies to achieve better alignment of institutions and methodologies. The swift evolution of technology and changes to market forces make this pathfinding function essential. New Zealand's size gives us the agility to research, prototype, iterate and improve rapidly. It also prompts the various entities involved in research to pool their ideas and resources for mutual benefit.

Our highlights from 2013

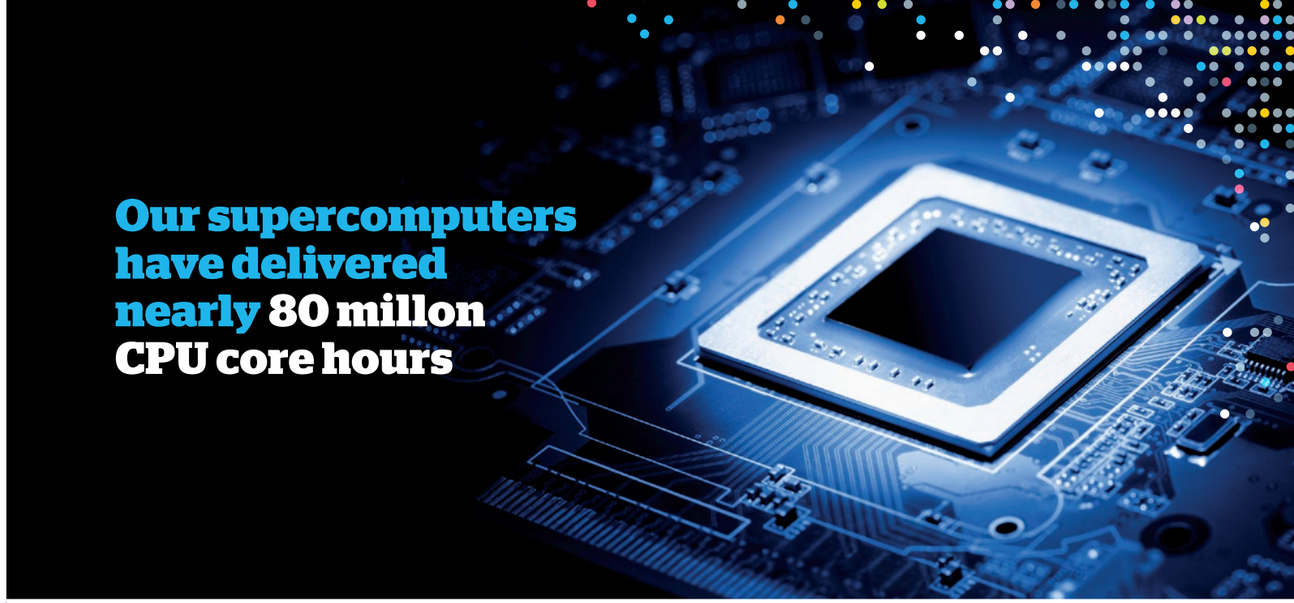
NeSI is a new provider that over the past three years has established an enviable track record of enabling research outcomes. In the words of MBIE's expert review panel, NeSI has provided 'users with a support network second to none across a range of disciplines'.

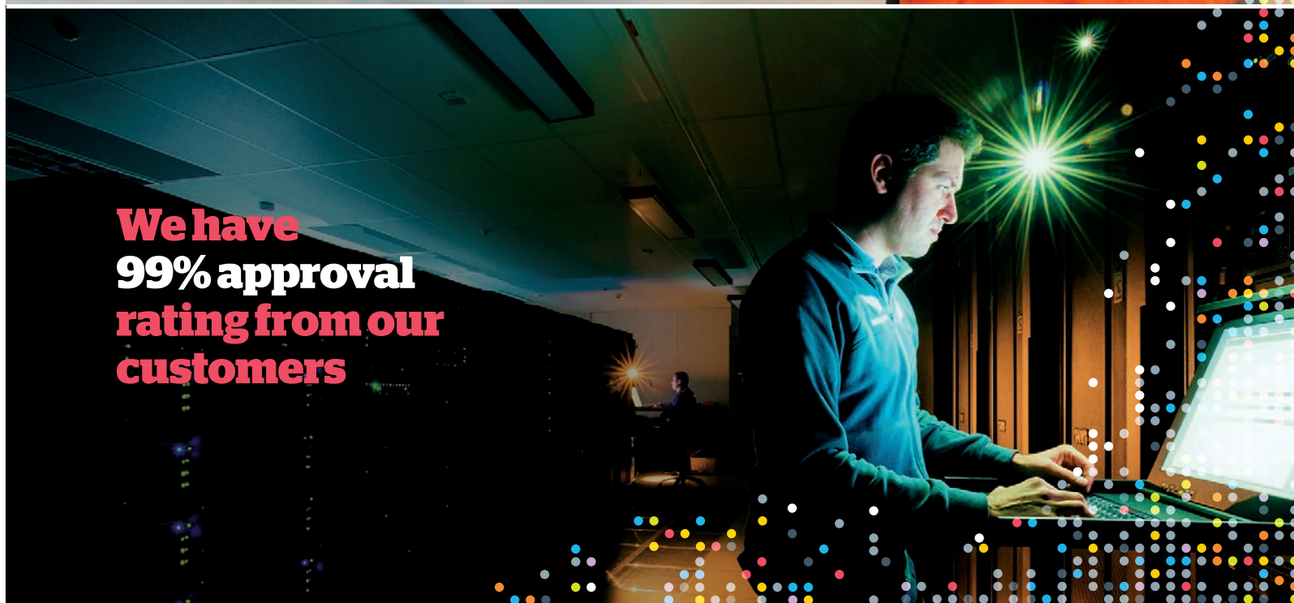
NeSI has shown significant growth in the user base during the last year. The November annual user survey showed 623 researchers accessing NeSI's services during 2013, almost 100% growth from 334 in November 2012. The threshold for postgraduate student access has been lowered by removing the requirement to have a peer-reviewed grant, with students gaining access subject to their supervisor's approval and available funds.

2013 saw an increase in the capacity and reliability of NeSI's HPC platforms, and enhancements to NeSI's computational science capability to deliver on strategic collaborations with the research sector on projects of national significance. A national team of computational science experts was created to work collaboratively within research projects. This team comprises members from across the country and represents a unique national capability.

In 2013 NeSI assumed responsibility for delivering the services of Tuakiri, New Zealand Access Federation Inc. Tuakiri's membership comprises all of New Zealand's eight universities along with six of the country's eight Crown Research Institutes plus one member drawn from the Institutes of Technology and Polytechnics sector.

NeSI is reducing barriers to entry to high performance computing by developing a new service offering for institutions to centrally fund access for their researchers. Called an Institutional Subscription to NeSI services, this new approach is to be launched in 2014.





Strong foundations for growth

Rick Christie
Chairman

Chair's report: NeSI is now an established feature on the landscape of New Zealand's research sector. It's been a challenging five year journey to first propose and then establish NeSI as a fully functioning HPC network collaboration, with its own Board and management, and a commitment to service our research communities throughout New Zealand.

The key to such a journey is the ability of those in governance and management to learn. NeSI has shown strength in this and, overall, progress has been good. As NeSI completes the first three years of life and its first contract, the foundations are strong and the organisation is positioned well for continued growth and sector leadership. We now move into a new phase of renewal of commitments from NeSI's partners, and reinvestment to re-equip the sector with essential infrastructure and skills. The learnings gained have led us to a more refined approach, the aim being to facilitate the involvement of new institutions via a subscription partnership while migrating NeSI to a shared services delivery model to improve support for and access by our research communities.

Strategically the last twelve months have been most formative, seeing the completion of our MBIE review, the launch of eResearch 2020, and the formation of a joint committee between NeSI, NZ Genomics Ltd (NZGL) and REANNZ. NeSI has a track record of thought leadership. From its innovation as a collaborative investment, through its ongoing grass-roots support of the annual community eResearch NZ conference, to the sector-wide strategic foresighting forum eResearch 2020, NeSI has been at the forefront of innovation in bringing the community together.

With continued change anticipated, the mission of our eScience infrastructure is a crucial element in enabling national and international collaboration in research and across institutions. At a time when the sector is going through such dramatic change, we should all take notice of NeSI's commitment to a collaborative culture, with institutions taking a risk and investing together into shared capabilities.

As the sector changes shape, NeSI continues to adapt and bring essential elements together – building on eResearch 2020's early insights into the big data and analytics challenges facing researchers, the opportunities offered by the increased utility of cloud services, and the essential demand for new skills – the year ahead will see a focus on identifying longer term solutions to enable the National Science Challenges and Centres of Research Excellence to achieve their full potential. Underpinning such initiatives there must be a resilient and well-equipped infrastructure system, and here NeSI has strong partnerships forming with REANNZ and NZGL. The joint committee of the Boards of these organisations will be further developed in 2014, with a mandate to identify opportunities for greater value to be realised from joint activities. Within NeSI, the organisation and management will need to develop and adapt, to meet these challenges while continuing to enhance HPC capabilities and eScience services.

The future for NeSI is one of consolidation around current investments, of extension of programmes that deliver these investments into the sector, and of enabling research. Strategic initiatives will shift the organisation to a delivery model aimed at more directly connecting the NeSI team with the science sector, informed by insights from shared services initiatives globally. Significant work will be done through NeSI's renewal process to simplify services delivery, including addressing complexities of a multi-institutional matrix organisation, and to enhance the innovative nature of the organisation. Through these changes the organisation will be well positioned for a new phase of growth and development.

Understanding the research sector, including the needs of researcher, institutional and government customers, is essential, and positions NeSI well to identify infrastructure and skills gaps and related opportunities. As a strategic national investment NeSI will continue to deliver high performance infrastructure with an advanced suite of skills to researchers, and to provide for more efficient coordination of shared investments across government and research sector institutions. I must thank my Board and management for their support for our vision and the outcomes we have achieved, over the last year in particular.

Rick Christie
Chair, Board of Directors

Enabling high performance in research

Nick Jones
Executive Director

Director's report: NeSI is New Zealand's national eScience infrastructure, supporting the innovation sector by contributing to projects in all areas of research, including the origins of the universe, the behaviour of molecules, natural hazards, climate change, the evolution of viruses, blood flow through the brain and nanoscale materials.

NeSI entered into its second year of operations in 2013, continuing to deliver HPC services to researchers nationwide. During 2013, the growth in use of NeSI's platforms was substantial, with just under 80 million CPU core hours delivered. Much of the research that NeSI supports would be unfeasible for New Zealand-based researchers without NeSI's specialised HPC platforms and expert support.

NeSI also provides value to a broader community, showing significant growth in the user base with 623 researchers having accessed NeSI's services during 2013, almost 100% growth from 334 in 2012. Much of this growth comes as a result of the many workshops the NeSI team has delivered across institutions during the year. These engagements allow the team to understand how to map the workflow needs of researchers onto NeSI's platforms while ensuring the reliability of their research in the face of changes to research protocols, methods, and tools. In supporting diverse and geographically widespread research needs, NeSI's team routinely crosses the country, ensuring relationships are in place that facilitate trust and enable change across the research system.

Against this backdrop of complexity it is rewarding for the team to receive the accolades they often do, such as public endorsement by keynote speaker Prof. Richard Easther at the annual national conference for New Zealand's physics community. NeSI's annual survey indicates that more than 90% of researchers report NeSI's staff are helpful and provide attractive national services. This aligns well with the outcomes of NeSI's first MBIE review, wherein an independent panel of experts praised NeSI for providing a support network "second to none".

Several other key successes were highlighted in MBIE's report following their review of NeSI. These include:

- Building a high quality national "virtual" team across five institutions
- Establishing new capabilities in computational science
- Delivering specialist skills collaboratively into research projects of national significance
- Initiating strategic discussions with non-investors on how NeSI can deliver greater value, (e.g. through institutional subscriptions)
- Managing performance across a set of key performance indicators; initiating sector-wide research infrastructure partnerships and strategy formation (e.g. eResearch 2020).

These significant achievements come down to the people that make up NeSI, and the opportunities presented to them by researchers to deliver value within research programmes.

These clear signs of success within two years of establishment show the foundations are in place and NeSI is well positioned to deliver further value as it grows and evolves.

With 2014 underway, sights are firmly set on continuing with this strong track record. The demand for support and collaboration continues to grow – researchers and institutions increasingly seek advice on how best to support their research needs for advanced computation, and aim to acquire the skills to do so. In 2014 NeSI's growth plans will ramp up as NeSI's first institutional subscribers come on board, opening up the potential for greater value to be realised across the sector.

NeSI's future is coming into focus. The organisation is well positioned to provide critical infrastructure and capabilities to enable New Zealand research, and anticipates ongoing growth and development to support new priorities.

While growth and continued "second to none" support remains the focus, the case has been made for NeSI's renewal and continuation. To facilitate sector input into the future shape and performance of NeSI the highly strategic eResearch 2020 vision forming programme has supported discussions with National Science Challenges and Centres of Research Excellence, and will report back on this first phase analysing future research sector e-infrastructure needs.

NeSI's collaborators have all indicated their commitment to continue as investors, and other institutions in the sector have also indicated their desire to play a stronger role. With HPC now established nationally, NeSI's new horizon is taking shape, with emerging challenges of big data and increasing degrees of collaboration both nationally and internationally framing the direction.

Nick Jones
Executive Director

Our Board of Directors

Governance and management responsibilities for NeSI are carried out by a Board responsible for strategy, policy, and approval of major initiatives and investments, and a management team led by a Director, responsible for executive management, planning and overseeing day-to-day operations.

Rick Christie

Chair, Independent Director, Professional Director
NeSI

Stephen Whiteside

Director, Organisational Performance & CIO
University of Auckland

Prof. Andrew Rohl

Independent Director & Professor of Computational Science
Curtin University

Dr Murray Poulter

Chief Scientist, Atmosphere, Hazards & Energy
NIWA

Prof. Steve Weaver

Deputy Vice-Chancellor (Research)
University of Canterbury

Anne Berryman

Observer Manager National Science Development Team
Ministry of Business, Innovation & Employment (MBIE)

As the Crown is a key partner supporting NeSI, the Crown appoints an observer.

Our management team

Executive management is the responsibility of the Director and management team. The role of the Director is to design, develop, and implement strategic plans in a cost-effective and timely manner, ensuring services agreements are adhered to, and to prioritise development projects.

Nick Jones

Executive Director

Nick's research sector experience has been complemented by commercial directorships in start-up ventures. In 2013 he established a national consultation, eResearch 2020, to build vision and guiding principles for future investments into research computing infrastructures.

Kirsten Brown

Team Administrator & Executive Assistant to the Director

Background includes academic publishing with Elsevier's Social Science and Medicine Journal, and as the Administrator for the Centre of Methods and Policy Application in the Social Sciences (COMPASS).

Kieron Mottley

Business Manager

Formerly Business Analyst at New Zealand Ministry of Health in charge of developing databases and systems holding national datasets.

Dan Sun

Service Delivery Manager, NeSI Canterbury

Background in software development, professional services and service management.

Michael Uddstrom

Service Delivery Manager for HPCF, NIWA

Principal scientist at NIWA for environmental forecasting, meteorology and remote sensing.

Marcus Gustafsson

Service Delivery Manager, NeSI Auckland

Background includes theoretical physics, materials science, industry engineering consultancy and computer modelling.

Ella Rokotyan

Project Coordinator & Reporting Analyst

Career includes work as a telecommunications sales support engineer and project coordinator in Russia.

Sat Mandri

Service Manager for Tuakiri, New Zealand Access Federation Inc

Background in service development, managing start-ups, C-level engagement, execution of design, and delivery of innovative solutions, establishment and development of cohesive teams and governing bodies. Industry experience in telco, banking and retail, aviation, supply chain and logistics and higher education.

Andrew Farrell

Technical Programme Manager

Background includes experience in commercially-focused R&D labs, MPEG-4 video standardisation, contributing to the implementation of reference software, research in Cloud Computing and building platforms for cloud services at HP Labs in Bristol.

Tim McNamara

Communities & Communications Programme Lead

Background includes experience in the science and innovation sector, humanitarian affairs as well as emergency management.

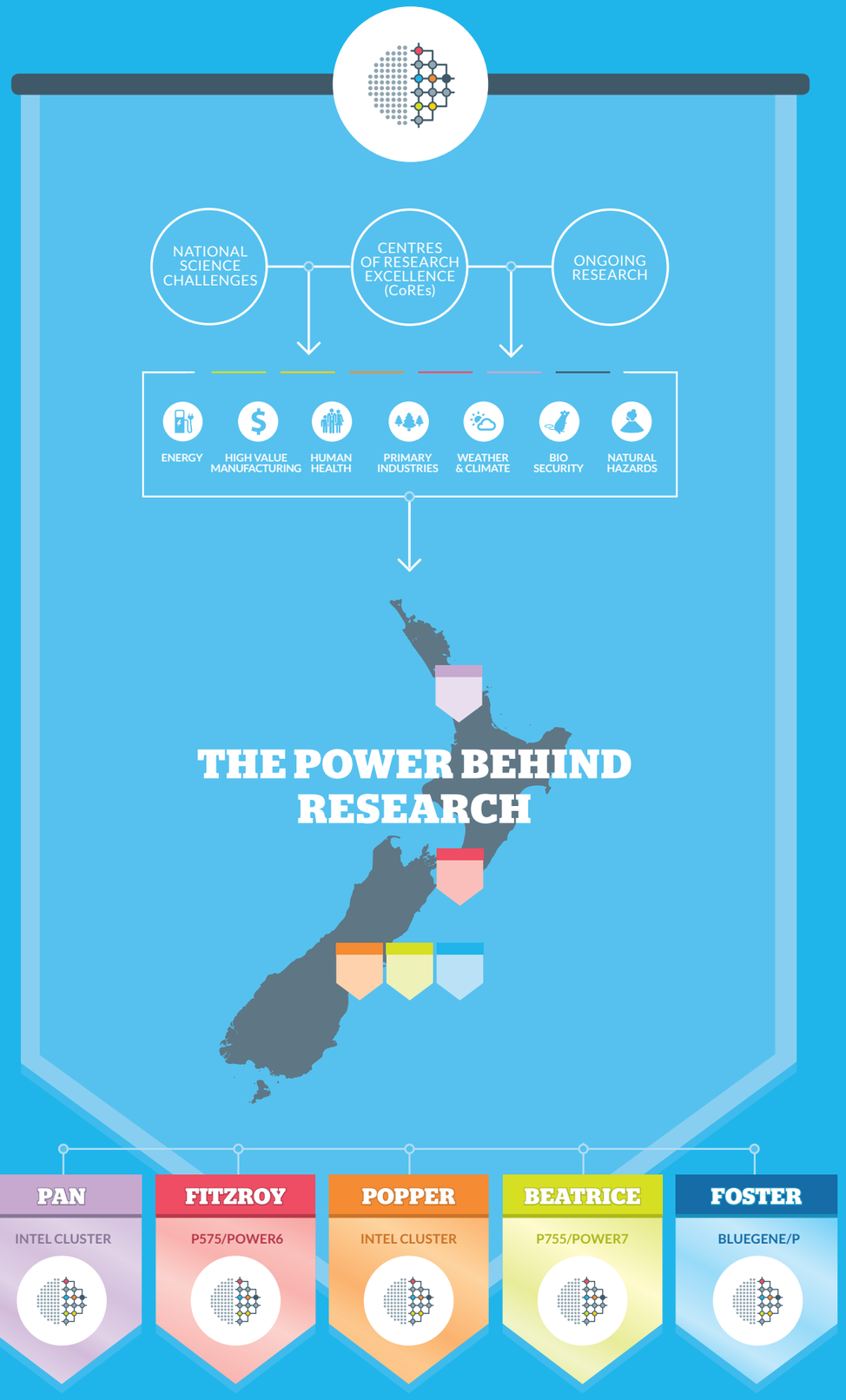
Andrew Farrell and Tim McNamara have now left the NeSI team. We wish them all the best in their future endeavours.

Computing capability for future prosperity

In October 2010, four collaborating universities and Crown Research Institutes submitted an investment case to the Minister of Research, Science and Technology.

The case for an eScience infrastructure would provide a virtual and distributed computational and data-intensive research platform for New Zealand's research communities. The proposal was successful and NeSI was established in July 2011. By coordinating investments across institutions and creating a connected infrastructure, NeSI makes available to public and private sector researchers significantly more HPC capability than would otherwise be the case.

NeSI increasingly focuses on research underpinning New Zealand's social and economic wellbeing. NeSI provides thought leadership, identifying infrastructure and skill gaps that if addressed will significantly increase the sophistication and impact of e-infrastructure capabilities on research. NeSI delivers training workshops into research communities to lift skills across the sector, with a focus on applying high-tech capabilities into research. Similarly NeSI works with research institutions to identify bottlenecks in their institutional infrastucture that if addressed would improve the productivity and possibliities of research.



Our stable of supercomputers

PAN

INTEL CLUSTER

6000 CORES

RAM **2.7** GHz
CORES WITH 50 TB RAM

300 TB
USER DATA STORE

FITZROY

P575/POWER6

3392 CORES

RAM **4.7** GHz
CORES WITH 8.375 TB RAM

1600 TB
USER DATA STORE

POPPER

INTEL CLUSTER

40 CORES

RAM **3.03** GHz
CORES WITH 480 GB RAM 10 GPEs

BEATRICE

P755/POWER7

416 CORES

RAM **3.6** GHz
CORES WITH 1.625 TB RAM

182 TB
USER DATA STORE (BG/P &P&)

FOSTER

P755/POWER7

8192 CORES

RAM **0.8** GHz
CORES WITH 8 TB RAM

182 TB
USER DATA STORE (BG/P &P&)

NeSI has invested in eScience resources for providing HPC platforms, services for research data storage and transfer, and access identity federation. Allocations on HPC platforms are made to various national communities, with allocation classes including research, proposal development, postgraduate, institutional including by subscription and to collaborator investors – institutions that have coordinated their institutional investment into NeSI with agreement that in return they receive a proportional share of access to the HPC platforms at their sites. NeSI delivers the following eScience services in collaboration with infrastructure providers and institutions: data storage to researchers through the Data Fabric service; data transfer capabilities in collaboration with REANNZ so that researchers may transfer their data sets more quickly (this includes improvements to transfer end-points at NeSI sites and for end-points at other institutions); Tuakiri, which provides access federation to New Zealand researchers.

High Performance Computing

The HPC service supports researchers to run simulations and other compute-intensive tasks such as data mining. Visualisation capabilities are also an integral part of the service. The key benefit is that a user can scale out their work on machines that are orders of magnitude more powerful than their desktop or other local systems.

Data Services

NeSI offers a portfolio of services for research data storage, transfer and management for New Zealand researchers and research institutions. NeSI aims to make the management of data as simple as possible and the development of the NeSI Data Fabric tool enables researchers to upload, then collaborate and compute on project data. NeSI offers many ways to interact with this data and is engineering the system to operate at high levels of transfer performance across the country.

Education & Training

Providing training opens up avenues by which researchers can join the growing NeSI community of users, support knowledge transfer and enhance research capability in the sector. For example, researchers who acquire these skills can make better use of the massive scales of computing and sophisticated analytical software applications offered by today's advanced computing environments. Researchers are then able to achieve their goals faster, as well as apply advanced techniques and use the available technology with less assistance. NeSI has a leadership role in developing New Zealand's capabilities in scientific applications programming, alongside the advanced academic education programmes that provide conceptual grounding and applied skills to current students. NeSI facilitates the growth of essential skills and capabilities, focusing on enhancing New Zealand's computational readiness, including identifying essential future skills and capabilities to enhance research sector productivity.

The power of partnerships

NeSI is a leading example of a national collaboration across the research system. NeSI brings together high-tech skills and infrastructure from across its investors, connecting with a broader range of researchers around the country to enhance their research.

NeSI does this from within the sector as the specialist capabilities being harnessed aren't easy to build and sustain, and are strongly defined by the research they support. An unincorporated body, NeSI receives investment from New Zealand universities, Crown Research Institutes and the Crown. The investors are the University of Auckland, University of Canterbury, NIWA (National Institute of Water & Atmospheric Research Ltd), Landcare Research, the University of Otago and the Ministry of Business, Innovation and Employment. NeSI is constituted through a legal agreement between the five institutions, with the University of Auckland as the Host and legal contracting entity with the Crown.

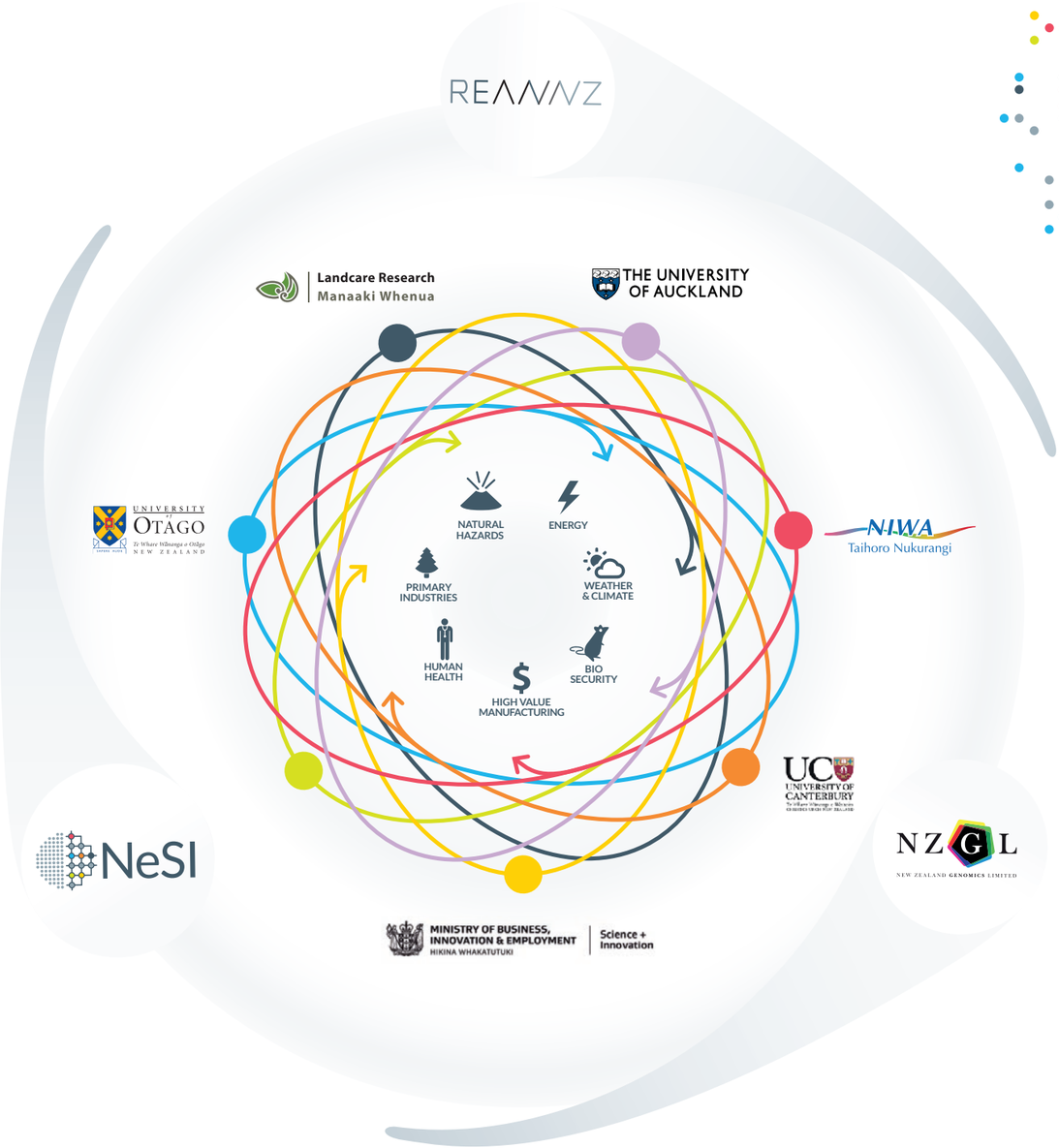
NeSI works alongside partners REANNZ and NZGL, building awareness of and confidence in applying eScience infrastructure and skills to research, and engaging with the research sector across research communities, institutions and government. This includes hosting training workshops, and collaborating on outreach events such as the annual eResearch NZ conference series.

NeSI strengthens international partnerships to translate needed skills and infrastructure capabilities into use in New Zealand. NeSI has supported the evolution of federated identity management capabilities in the sector, managing and delivering the Tuakiri services over the past two years in partnership with the University of Auckland. Similarly, NeSI is growing capacity in skills training for researchers, working alongside global leadership groups such as the Mozilla Science Lab within their Software Carpentry skills training for researchers programme.

New Zealand's path to prosperity, as a small nation, is paved with pragmatic and collaborative approaches to translating advanced practices and technologies into the research system – NeSI is a key enabler in making this happen.

eResearch Advisory Groups

In 2013 NeSI formalised a strategic joint working relationship with REANNZ and New Zealand Genomics Ltd, and also



acknowledges the valued input received from other key eResearch partners and advisors, in particular Prof. Mark Gahegan (Centre for eResearch, University of Auckland), Prof. Tim David (BlueFern, University of Canterbury)and Dr Michael Uddstrom (FitzRoy HPCF, NIWA).

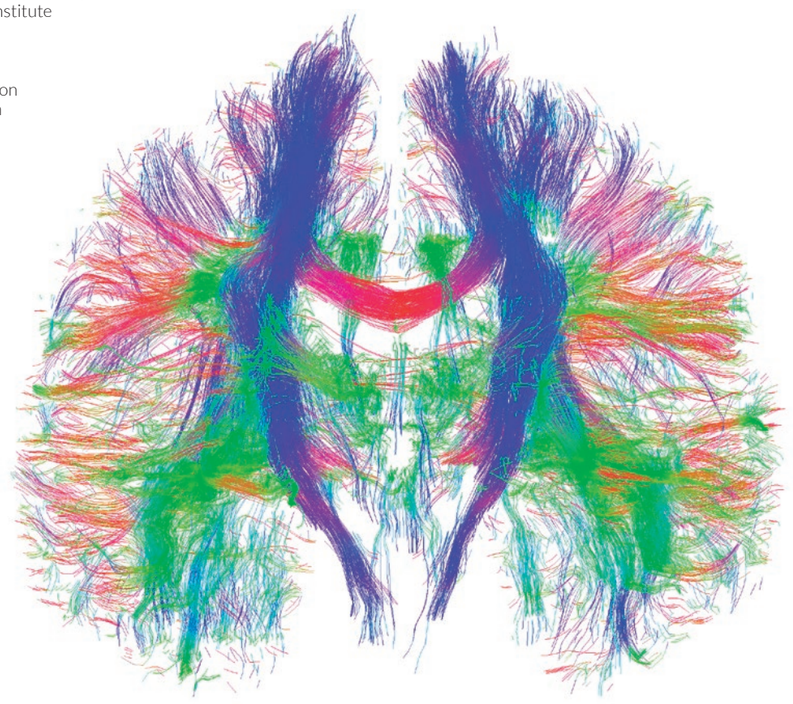
NeSI also regularly benefits from the advice of its Access Policy Advisory Committee members – Prof. Shaun Hendy of the University of Auckland, Dr Vernon Choy from the Health Research Council of NZ, Dean Peterson formerly of the Royal Society of NZ, and Craig Holmes of MBIE – who provide feedback on access and allocation mechanisms to aid NeSI in achieving its goals.

Outreach & Partnerships

NeSI is a trusted partner, building awareness of and confidence in applying eScience infrastructure and skills to research through engaging with the research sector across research communities, institutions and government. NeSI strengthens international partnerships to translate needed skills wand infrastructure capabilities into use in New Zealand, including by subscription and by collaborator investors.

Case study 1.

Dr Daniel Myall, Computational Neuroscientist, NZ Brain Research Institute

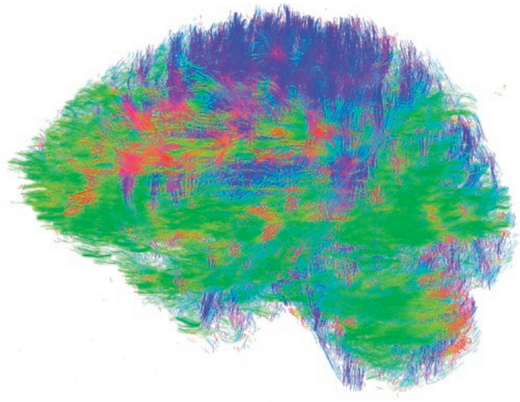


A map of axon pathways in the brain

Helping refine Parkinson's disease analysis

A science researcher developing predictive models for pre-clinical detection of cognitive decline in Parkinson's disease says NeSI is enabling him to conduct his research more effectively.

"A probabilistic analysis of the major axonal pathways in the brain takes around 18 hours on a single core ... On a 32-core node it runs in 35 minutes."



Around 10,000 New Zealanders suffer from Parkinson's disease. This degenerative disorder of the central nervous system does not only limit a patient's movement, says Dr Daniel Myall, a computational neuroscientist at the New Zealand Brain Research Institute in Christchurch. "Many, though not all, Parkinson's patients eventually also develop cognitive decline, which then becomes the most burdensome aspect of this progressive condition."

There is currently no treatment for cognitive decline in Parkinson's disease, so there's a need to detect those who are at high risk of cognitive decline so they can be targeted in forthcoming therapeutic trials.

Myall is part of a team that has a database of brain scans and longitudinal cognitive measures of people with Parkinson's disease at its disposal, but analysing this data in order to extract useful measures of brain structure and function – and then combining these into a model of the probabilistic risk of cognitive decline – is computationally demanding.

Access to NeSI presents Myall and his team with an opportunity to conduct its research faster. "NeSI provides resources with enough processing power and memory to enable pre-processing and model formation to be performed in a reasonable time – days as opposed to months," says Dr Myall.

Myall's model of cognitive decline is trained on data from 170 individuals with multiple measurements over time. Those predictions will then be validated. "Over the next two years many of these individuals will be followed up. Success is determined by how accurate the predictions are compared to the actual change in cognition."

The study should provide a clear indication of the ability to predict cognitive change based upon modern brain imaging techniques, says Myall. "The primary methodology is to use existing magnetic resonance imaging (MRI) analysis packages to extract measures of brain structure and function and then use Bayesian techniques to optimally learn from this what measures are most useful for predicting future cognition."

Myall trained in mathematics before he moved into medicine, and he also has extensive experience in computing and programming. For his PhD Myall developed a virtual environment platform and used it to examine motor adaptation in Parkinson's disease. Myall says his main computational challenges now relate to adapting the MRI analysis software to work well on NeSI, and implementing the Bayesian learning algorithms to work efficiently in a high performance computing environment.

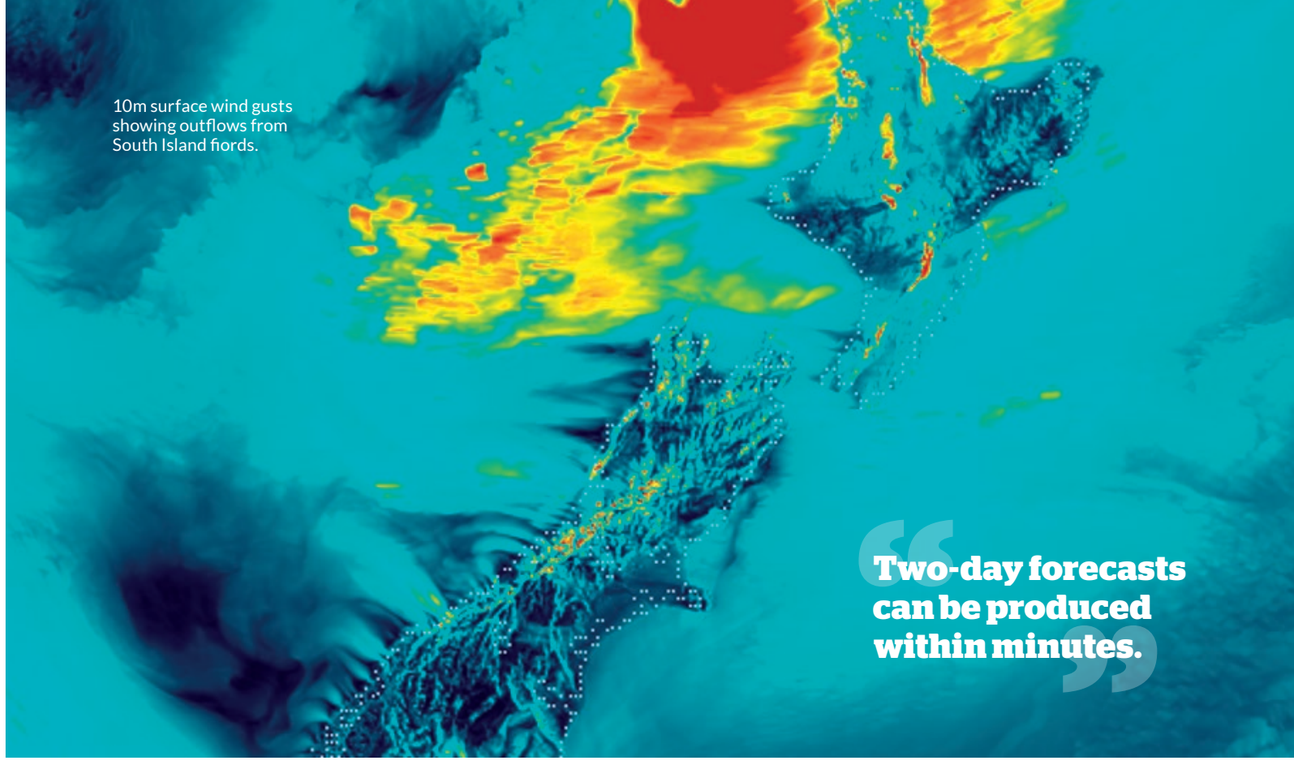
Members of NeSI's computational science team have provided Myall with technical assistance. This has included integrating his software with a parallel job-scheduling system that allows users to run more jobs in less time by matching the processing needs and priority of each with available computational resources to maximise resource use.

"A probabilistic analysis of the major axonal pathways in the brain takes around 18 hours on a single cpu core," says Myall. "This can be efficiently parallelised, and on a 32-core node runs in 35 minutes. This makes it much easier to iteratively refine and improve the analysis, as we don't have to wait days for a single analysis or months to analyse the entire collection of data."

Once Myall's software is fully integrated with the scheduler Myall hopes to be able to determine changes in the pathways of over 300 brains in various states of cognitive impairment.

For Myall and his research peers, access to NeSI's HPC network means they don't have to buy and maintain their own workstations and it allows large computational tasks to be completed quickly when required.

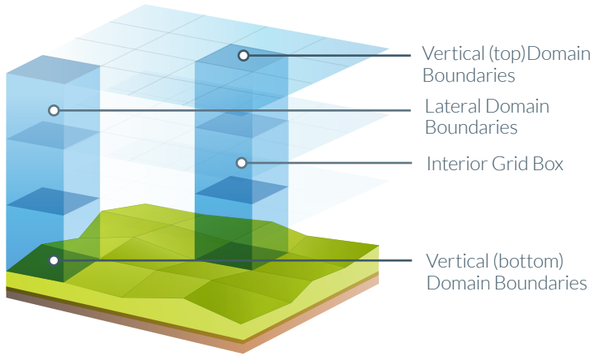
Improving New Zealand's weather fore-casting ability



10m surface wind gusts showing outflows from South Island fiords.

"Two-day forecasts can be produced within minutes."

A typical two-day forecast takes approximately 11 minutes to complete, using 256 processors across 8 nodes.



Limited Area Model — NWP Limited Area Model domain showing how it is discretised into a horizontal (x, y) grid, vertical layers (z) - which near the surface are terrain following, but become smoother with height. (Courtesy of the UCAR COMET programme.)

A team of meteorologists at NIWA, led by principal scientist Dr Michael Uddstrom, has been looking into how to improve weather forecasts for New Zealand. The team has been developing a new numerical weather prediction model for the country that will be much more capable of representing the unique features of our environment, such as the geography of the Southern Alps.

Numerical Weather Prediction (NWP) is a term used to describe the use of computer modelling to predict the weather. More formally, the intention of NWP is to predict the future state of the atmosphere using data gathered from observations of its current state and the application of a set of numerical approximations to the equations of fluid dynamics and physical processes. Those processes include convection, boundary layer turbulence, radiation, cloud physics, microphysics and orographic drag.

For the last few years, NIWA has operated the New Zealand Limited Area Model, or NZLAM. In this model, New Zealand and its surrounding seas are divided onto a 324x324 horizontal grid, while the atmosphere is split into 70 vertical levels, from the surface to approximately 80km above sea level. Each horizontal grid square is about 12km (0.11 degrees) in length.

Observational data for New Zealand's atmosphere is typically provided via satellite, in particular from instruments on board NOAA-14 and NOAA-15. Additional data is provided from ship, airplane readings and weather stations from around the country. These data are then inserted into the model using a process called data assimilation, where the model state from a previous forecast is altered to include the new observations and becomes the initial state for the next forecast.

During the course of this assimilation process, a number of processing, data cleansing and bias correction steps are carried out to ensure no erroneous data is included that could lead to problems running the model.

NeSI's computing platforms, in particular the synergy of many processors, large amounts of memory and extremely fast interconnects, enable a two-day forecast to be produced within minutes. On FitzRoy, a typical two-day NZLAM forecast takes approximately 11 minutes to complete, using 256 processors across 8 nodes.

There is a difficult trade-off in NWP between accuracy and speed. A more accurate model is much more computationally intensive. With access to HPC facilities through NeSI, NIWA is able to increase the accuracy of the modelling while retaining the speed necessary for effective planning.

A finer grid enables the model to more accurately represent the topography of the region of interest and the surface processes occurring at the smaller spatial scales. Unfortunately, as the number of grid points increases, so does the number of calculations and the communication overhead that is imposed between each region to progress to the next step in the simulation.

In parallel to NZLAM, NIWA has recently begun running a 1.5km resolution NWP model called the New Zealand Convective Scale Model (NZCSM). This model uses initial conditions interpolated from NZLAM onto a 1.5km grid. This first guess is then adapted to match up-to-date observation data. The domain is divided into a horizontal grid of 1200x1350 1.5x1.5km squares and has 70 vertical levels that cover the lowest 40km of the atmosphere.

This resolution produces a model 15 times larger than NZLAM computationally, but still only covers a much smaller geographic area. It also requires a lot more computational power to produce a forecast in a timely manner. Currently, a 36 hour forecast by NZCSM takes 130 minutes to complete using 810 processors spread across 13 nodes of FitzRoy. The resolution difference between those two models means that while they will both be able to predict which cities will be affected by storms, NZCSM should be able to predict which suburbs will be heaviest hit.

In its current form, NZLAM is unable to adequately resolve important features of New Zealand's unique landscape, such as the Southern Alps. More accurately representing the geography, soil conditions and other physical processes that affect the weather will all combine to improve the accuracy of NWP in New Zealand.

As well as providing improved accuracy generally, finer resolutions also enable far better modelling of severe weather events.

Case Study 3.

Professor Emily Parker
University of Canterbury

Understanding biomolecular enzymes to develop new therapies

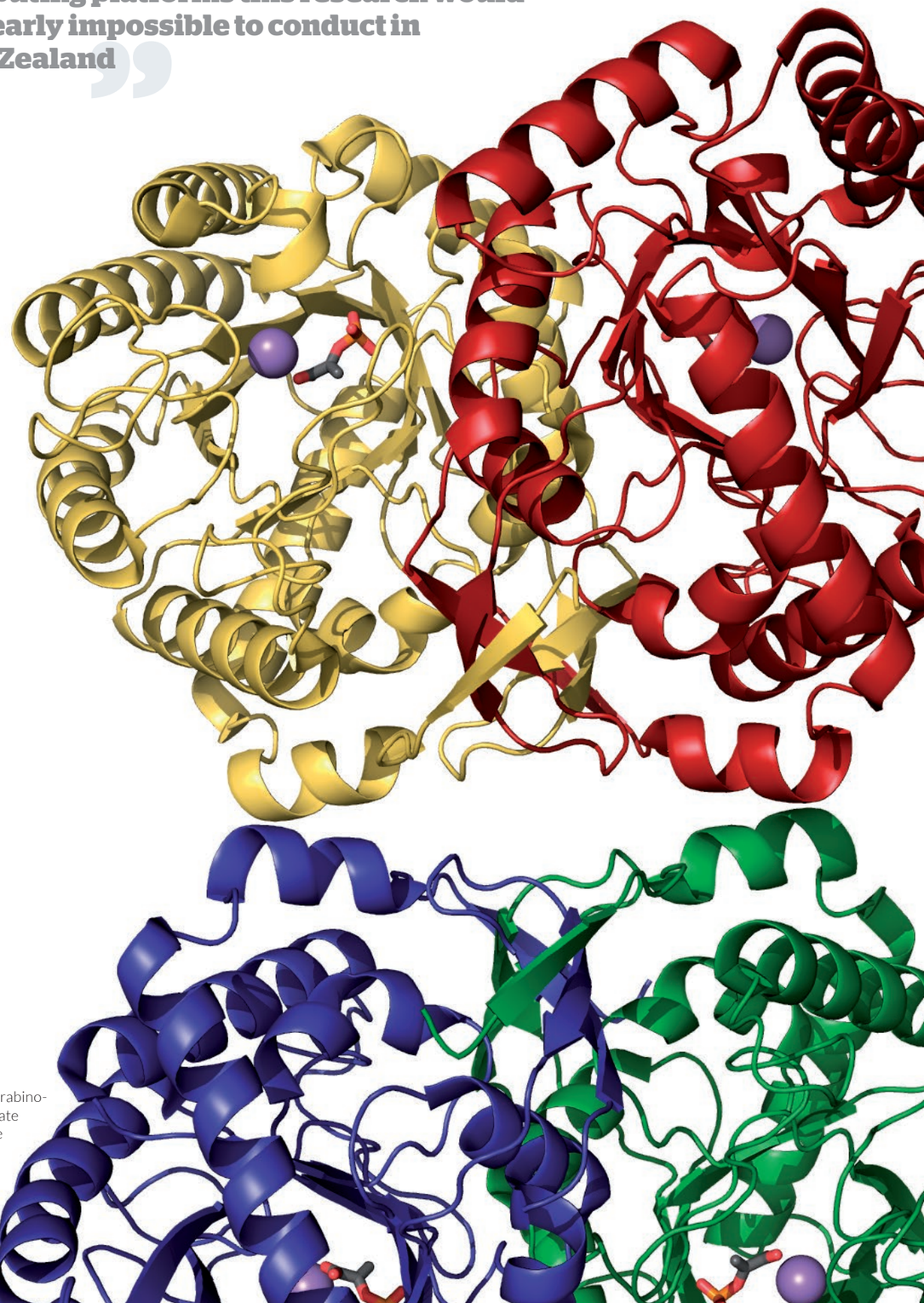
With support from the Marsden Fund and NeSI, a University of Canterbury group has been able to carry out research that may lead to novel antibacterial and antifungal agents.

Professor Emily Parker from the University of Canterbury is leading a research programme into molecular understanding of the process behind allosteric regulation. The aim of this work is to investigate the possibility of developing therapies that would interfere with a metabolic pathway that affects bacteria, but not humans.

Allosteric regulation is ubiquitous and crucial to metabolic control. By temporarily altering the catalytic efficiency of individual enzymes, allosteric activators and inhibitors can have profound effects on diverse cellular processes. A particular focus of the studies is the enzyme at the start of the "Shikimate pathway". This important metabolic pathway is used by bacteria and many other organisms to synthesise a range of essential amino acids. The clinical significance of this pathway is that it is not used by animals.

The computational resources for modelling these molecules and their reactions over the timescales required to shed new light on the phenomenon are immense. Without access to NeSI's high performance computing platforms this research would be nearly impossible to conduct in New Zealand.

"Without access to NeSI's high performance computing platforms this research would be nearly impossible to conduct in New Zealand"



3-deoxy-D arabino-heptuloxsonate 7- phosphate synthase (DAH7PS)

Case study 4.

Single sign-on helps education sector access services

Tuakiri
NEW ZEALAND ACCESS FEDERATION

“ You need local, on-the-ground expertise to draw on. Once Tuakiri came along and became its own national service, things very quickly started to work. ”

eTV, the Education Television and Video Communications Trust, uses the Tuakiri Federation Service to help it deliver video and other content more efficiently to New Zealand education providers. eTV selects programmes and posts them on its website where they're available to eTV members for viewing, downloading and embedding. Fast and reliable broadband are obviously prerequisites for eTV to operate these services effectively.

Tuakiri, New Zealand Access Federation Inc., is a single sign-on access federation service delivering access federation to web application services through its central federation registry. This means it allows authentication and user attributes to cross organisational boundaries, simplifies user access and promotes better security of access. The advantage of Tuakiri's service capabilities to eTV's members is that it allows staff and students role-based access to their organisation.

Case study 5.

Asking for help leads to a 1300x speedup

“[This] enabled us to complete the entire computation within 24 hours.”

Processing times for a geographer were able to be dramatically reduced after a request for help went to NeSI's computational science team. As a result, for the Australian subset of the data, processing time was reduced from 6.5 hours to 17 seconds.

This 1376-fold speed increase was due to algorithmic changes suggested by NeSI's Dr Sung Bae. The researcher's custom Python code was found to be using an inefficient search algorithm running largely in serial. Sung was able to improve both the search algorithm as well as the parallelism of the software. Those improvements compounded to produce the impressive result.

Our strategic direction

New Zealand aims to be in the first world of developed economies and societies in terms of the quality of our research and the impact of research on our society and economy. The expectation is that this will be achieved through cross-institutional initiatives supported by organisations such as NeSI.

Our major initiatives for the future are:

- eResearch 2020 - a strategic forum coordinated by NeSI, NZGL and REANNZ, focusing on future eResearch capability and skills needs across the New Zealand research system and providing integrity to NeSI's planning for the future. There are immediate activities that researchers need/want NeSI to help with. Examples include helping align organisations on standards, policies, tools, and strategies, and supporting the development of data infrastructure and related capabilities. Institutions are indicating that they no longer wish to operate in isolation.

- Taking a New Zealand-wide focus to annual planning of the acquisition and/or utilisation of NeSI's infrastructure, rather than exploiting individually purchased equipment for national use. This opens up options such as the adoption of cloud services or making use of international facilities.

- Revising arrangements for access to improve non-NeSI Investor uptake. This will include introduction of a subscription model to allow more institutions to invest in NeSI, and to broaden NeSI's income base.

Aiming to enhance researcher capability, NeSI will:

- Focus more of our investment on supporting research, including investing more in skills training and capability development.

- Aim to increase researcher literacy in computational and data intensive methods and tools, enabling our researchers to better realise the potential of computation and analytics to enhance research outputs.

This sets the tone for 2014, where NeSI will consolidate around the core investments already made, focus on enabling an increasingly broad and rich scope of research activity, and work alongside infrastructure partners REANNZ and NZGL, and other institutions and communities, to ensure the research system is supported by well-integrated high performance infrastructure.

NeSI anticipates a demanding year ahead supporting growth and development of the research sector, towards increasingly collaborative approaches that enable the sector to sustainably address national needs. NeSI's team looks forward to working closely with individual researchers on their research projects, and alongside research communities to contribute to economic, social and environmental prosperity across New Zealand.

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