NeSI
New Zealand eScience Infrastructure

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Chair's report

2015 has been another intensive year at NeSI for both management and the Board, resulting in good progress across a range of activities, strategically and operationally. There have also been some significant changes in personnel, especially with management, in implementing changes in structure.

It is pleasing that we were able to conclude negotiations around major contracts with the Crown and NeSI's Collaborators. These contracts have now been executed and are being implemented.

The next steps for our National Platforms Framework are now underway. These include a revised capital investment plan based on a two-facility model. A pilot project to test cloud burst capacity is intended to provide additional flexibility and specifically to deal with peak usage.

Huge progress was made at an operational level to complete the successful transition from NeSI's original devolved structure to a unitary model, with the strengthening of the management team in key areas. All senior appointments have now been made and we are starting to see improvements in relationships with our research communities, which are now more complex with the impact of the National Science Challenges and the new CoREs. Considerable credit is due to Nick Jones and his team in achieving the transition, which had been the subject of a major planning exercise during 2014.

Our eResearch 2020 governance group, comprising Chairs and directors from NeSI, Research and Education Advanced Network New Zealand (REANNZ) and New Zealand Genomics Ltd (NZGL), consolidated further and is now leading strategy development around e-Infrastructure, although government policy settings and intentions are still unknown. My thanks are due to the work of John Raine who has now stepped down as Chair of REANNZ. REANNZ has an able replacement in Jim Donovan who has been on the governance group.

The National Research Data Programme has been soft-launched and NeSI has commenced capability work around research data support, focusing on digital skills and data analytics development at both researcher and institutional levels.

NeSI's partnership with NZGL has matured and strengthened and will assist their transition to a shared services model. Later in the year we welcomed Massey University as a subscriber and Rob Ballagh joined NeSI's Board to represent the University of Otago and Landcare Research.

To conclude, I would like to thank our Board and management who have worked together well on our new business model. Together with the eResearch 2020 governance group they are providing important leadership and support for the development of a robust national e-Infrastructure for New Zealand researchers and research institutions.

Rick Christie
Chair, Board of Directors

"Huge progress was made at an operational level to complete the successful transition from NeSI's original devolved structure to a unitary model, with the strengthening of the management team in key areas."

Director's report

During 2015 NeSI implemented a substantial reorganisation. A new business model was established and contracted with the Crown and Collaborators. This included a unitary organisation restructure and subsequent recruitment; implementation of new approaches to governance over future investments; shifting access and allocation from local to national; broadening NeSI's scope of services to address high-priority needs for skills training; and innovation within NeSI's infrastructure to incorporate 'Cloud' infrastructure.

For much of the year the team operated in a transitional state as new roles and routines were established, with intensive activity running from Q2 through the remainder of the year. 2015 has been a year of implementation, resulting in a more confident, focused, and flexible NeSI. I commend NeSI's transitional team, who have managed a successful shift from "local to national".

Building the new team has opened up opportunities for a lift in leadership, expertise and experience. We have recruited globally for all key roles, finding talented individuals both locally and offshore. The new team is near fully populated; you can feel the lift in energy and see the sharpening of our focus. We have augmented the team with decades of experience in international digital research infrastructure, computational science, multi-national professional services delivery, top-tier data analytics consultancy, and international leadership in digital skills development. We are now moving rapidly to embed our learnings from the past four years, while pushing ahead with ambitious plans.

Our teams are now operating along single functional reporting lines nationally; our people and platforms are allocated on the basis of best fit for purpose with national research needs; our future investments are driven by research priorities first, supported by our investing institutions.

The year also saw NeSI strengthen partnerships. The founding partnership between MBIE and the Collaborator investors was renewed, and remains fundamental to enabling NeSI's broader mission. Two additional partnerships were established, with Massey University becoming a subscriber to NeSI's services, and with NZ Genomics Ltd via a strategic alliance bringing together the power of both providers for researchers nationwide. The ongoing partnership with REANNZ and NZ Genomics within the eResearch 2020 initiative shifted focus to identify and map out sector-wide strategic opportunities for future infrastructure and skills, to address a critical gap in research data.

In 2016 the team are focusing on strategic research drivers and joint activities with National Science Challenges and Centres of Research Excellence. NeSI's Research Reference Group is now in place, providing expert advice on national and international research priorities and trends. Our renewed platforms investment plan moves to implementation – our platforms will be replaced by mid-2017 and at that point incorporate NZGL Genomics platforms, in time to herald a new era of converged data-intensive computational research in 2017, as Big Data and High Performance Computing converge.

Nick Jones

Nick Jones
Director

"Building the new team has opened up opportunities for a lift in leadership, expertise and experience. We have recruited globally for all key roles."

Board of Directors

The NeSI Board is responsible for strategy, policy, approving major initiatives and investments, as well as monitoring the NeSI risk register. Three of the collaborator institutions appoint a Director alongside an independent Chair and another independent member with expertise in the field representing the research sector at large. All Board members are focused on the interests of NeSI, being the effective delivery of national research infrastructure services.

Rick Christie
Chair, Independent Director

Prof. Andrew Rohl
Independent Director and
Professor of Computational Science
Curtin University

Dr Murray Poulter
Chief Scientist, Atmosphere,
Hazards and Energy
NIWA (Retired)

Prof. Rob Ballagh
Department of Physics
University of Otago

Stephen Whiteside
Chief Digital Officer
University of Auckland

Senior Management

NeSI has a Management team, led by a Director, who are responsible for executive management, planning and overseeing day-to-day operations. Activities are coordinated through nationally distributed functional teams across each of the investing institutions. NeSI also maintains Advisory Committees and Panels, including an independent Access Policy Advisory Committee to advise the Director on the ongoing development and periodic review of access policy.

Robin Bensley
Operations Manager

Nick Jones
Director

Brian Corrie
Solutions Manager

Georgina Rae
Engagement Manager

Michael Uddstrom
Platforms Manager

Our people

Operations

Robin Bensley
Operations Manager

Mike Ladd
Strategic Projects Manager

Kirsten Brown
Operations Coordinator

Laura Casimiro
Operations Administrator

Site Managers

Fabrice Cantos
Site Manager - NIWA

Nick Spencer
Site Manager - Landcare Research

Marcus Gustafsson
Site Manager - University of Auckland

David Maclaurin
Site Manager - University of Otago

Dan Sun
Site Manager - University of Canterbury

Engagement

Georgina Rae
Engagement Manager

Aleksandra Pawlik
Research Communities Manager

Platforms


Fabrice Cantos
Systems Engineer


Gene Soudlenkov
Systems Engineer


Michael Uddstrom
Platforms Manager


Aaron Hicks
Systems Engineer


Jose Higino
Systems Engineer


Greg Hall
Systems Engineer


Francois Bissey
Systems Engineer


Yuriy Halytskyy
Systems Engineer

The Computational Science team provides consultancy support to approved Projects. User training ranges from use of the HPC and data platforms to best practice software development methodologies.

Solutions


Alexander Pletzer
Scientific Programmer


Ruan Malan
Solutions Architect


Chris Scott
Scientific Programmer


Jordi Blasco
Systems Integrator


Brian Corrie
Solutions Manager


Ben Roberts
Application Support Specialist


Gene Soudlenkov
Application Support Specialist


Peter Maxwell
Application Support Specialist


Matt Healey
Application Support Specialist


Wolfgang Hayek
Scientific Programmer


Albert Savary
Application Support Specialist


Francois Bissey
Application Support Specialist

Progress towards our strategic goals

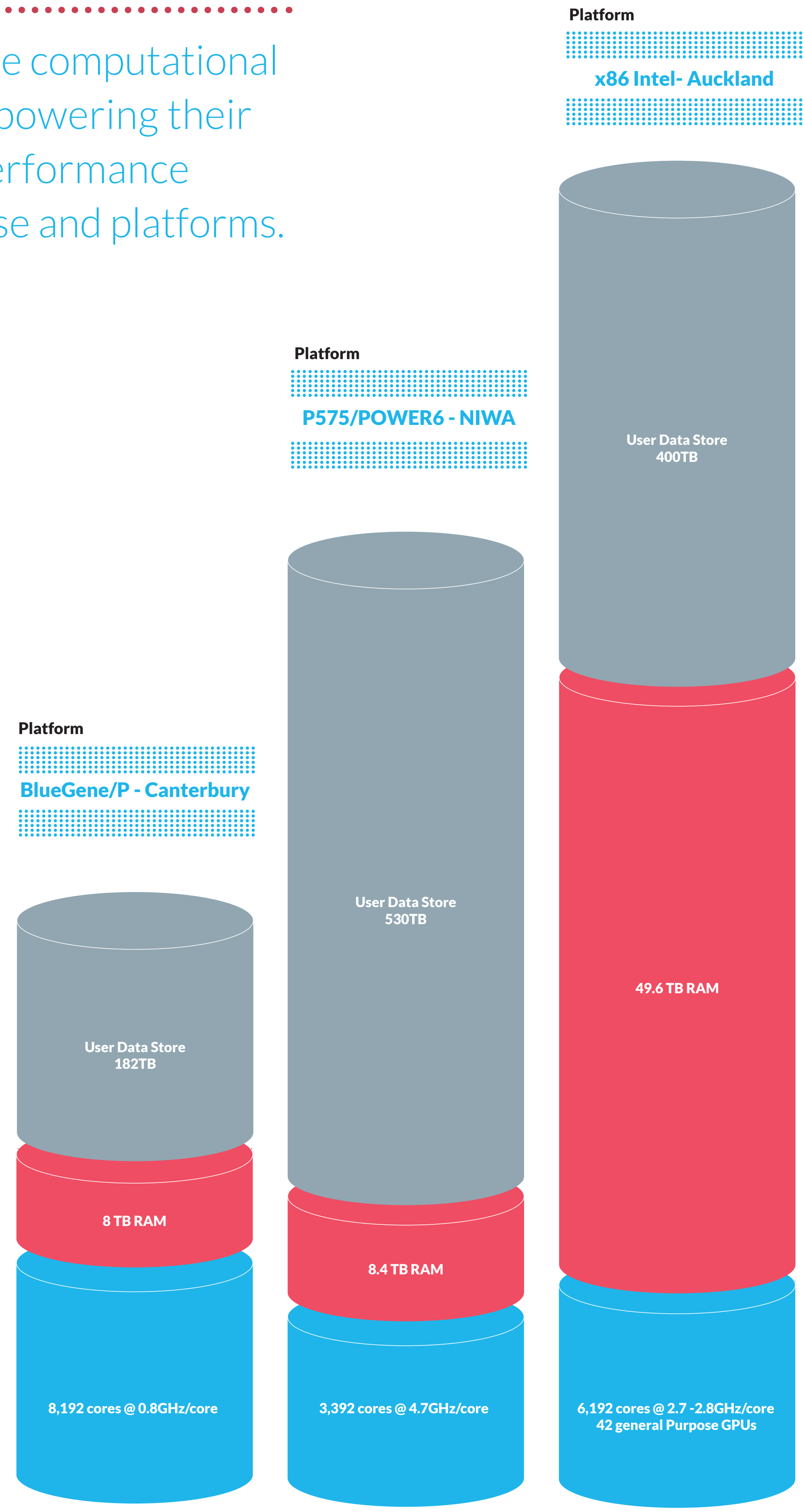
Throughout 2015 NeSI made the transition to one national team aligned by function (service line), and established an investment framework which prioritises a joint approach with research users and institutions. As a fundamental base to these shifts, NeSI developed a coordinated approach across all Collaborator institutions during 2015 to ensure efficient sharing of responsibilities, capabilities, knowledge, and work, gaining commitments to work together to continuously improve the implementation of NeSI as a national infrastructure.

This coordinated approach saw the following transition activities completed:

- NeSI Collaboration and Service Agreements were executed via a coordinated consultation process with all Collaborators, ensuring transparency and providing rich feedback mechanisms to ensure longer term buy-in to NeSI's organisational innovations.
- NeSI now operates as a national team, with team members delivering benefits to researchers across New Zealand independent of locations and affiliations.
- A new senior leadership team was recruited and will be in place as of March 2016, advancing NeSI's sector leadership and ability to influence as a voice for strategic change.
- National investment and procurement responsibilities now sit with the NeSI Board and management. With a focus on developing a national platform aligned to researcher needs, an annual investment Framework review was established, along with standards for investment cases and procurement processes.
- Common finance and reporting standards now underpin the collaboration across the five institutions and with government. All reporting and compliance obligations have been captured within an overall reporting framework to standardise the approach to financial and KPI data collection and reporting processes.

These fundamentals underpin much of the work the team now undertakes. The resulting simplified and consistent operating environment enables a greater focus on delivering value through services.

NeSI's services address the computational needs of researchers, empowering their research through High Performance Computing (HPC) expertise and platforms.



High performance computing

Compute and analytics

NeSI's services address the computational needs of researchers, empowering their research through High Performance Computing (HPC) expertise and platforms. Our platforms underwent a modest increase in scale during 2015, with an upgrade of the x86 Intel platform aimed at supporting growth through to the planned platform replacement in mid-2017.

Building on an initial review to create a baseline in Quarter 1, in Quarters 3 and 4 NeSI implemented its first National Platforms Framework Review. This review included analysis of platform use over the last three years, stakeholder consultations, conducting a user needs survey, and an analysis of demand drivers and technology trends in HPC and data analytics.

The NeSI Board approved in principle a revised Framework, with stakeholder consultation and feedback meetings focused on addressing implementation risks continuing into early 2016 to inform final Board sign-off. The Framework review led to some excellent opportunities to engage with the research community and streamline the process for next year.

The revised Framework sees NeSI decommissioning the BlueGene/P platform by end of June 2016, and replacing both the POWER6 and x86 Intel platforms ready for production use by July 2017. To support future investment, a national approach to procurement was developed with consultation from Collaborators in the first half of the year. This will guide the major platform replacement project due to start in early 2016.

NeSI is enhancing HPC services, providing seamless access to Cloud compute services for high throughput, low data-demand research projects. In parallel to the National Platform Framework review, an RFP was initiated to support a Cloud Pilot project after consultation with partners REANNZ and NZ Genomics Ltd. Responses to the RFP were received and reviewed in October 2015, with an investment case approved by the Board during November. The Cloud Pilot project will be up and running in early 2016.

Early in 2015 a revised Access Policy was finalised and released, including replacement of cost recovery by a newly introduced subscription model for institutions. Replacement of cost recovery meant an increase in Merit projects in 2015, from 7 in 2014 to 20 in 2015, indicating NeSI is meeting its goal of making it easier for researchers to start projects with us. In 2016, full implementation of the revised Access Policy is a top priority, including the national approach to institutional allocations to allow increased mobility of research work across platforms, and improve overall fit-for-purpose use of NeSI infrastructure.

NeSI is enhancing HPC services, providing seamless access to Cloud compute services for high throughput, low data-demand research projects.

Consultancy and training

To fully exploit HPC requires significant expertise at the top end through the work of scientific programmers tuning and optimising research software codes. In general, the digital skills required to operate computing tools, applications and platforms are scarce, leading to an increasing need for basic to advanced skills training in digital research tools and methods. These skills are core to NeSI's purpose of growing the computing capability of New Zealand researchers.

In 2015 NeSI recruited a new team of scientific (HPC-focused) programmers to support research projects with Merit allocations. The team members' skills cover application porting, testing, application support, platform-specific optimisation (compute and input/output), custom HPC code design and development, data analytics and data visualisation. This team forms the basis for the further development of NeSI's consultancy service during 2016.

NeSI works with research communities in New Zealand to develop training and education programmes, and in a previous year carried out a gap analysis to identify key digital skills training needs. 2015 saw NeSI deliver the first phase of a sector-wide training strategy, leading the delivery of a series of national Software Carpentry events to uplift digital research skills sector-wide.

Software Carpentry is a highly successful international programme addressing gaps in essential digital research skills. Software Carpentry aims to make it easier for researchers to work digitally, and ultimately enhances the ability of researchers to answer computationally demanding research questions. NeSI has taken a lead over the last couple of years to bring this approach to New Zealand, and early in 2015 NeSI was part of a contingent to attend Software Carpentry Instructor training in Melbourne, producing New Zealand's first certified Software Carpentry instructors.

During the remainder of 2015 the team, in partnership with other institutions sector-wide, delivered seven Software Carpentry workshops, reaching more than 200 researchers and built partnerships which will see a significant increase in training events in 2016. This included workshops at the University of Canterbury, Auckland University of Technology, the University of Otago, Massey University (both Palmerston North and Albany campuses), Victoria University of Wellington, and Lincoln University. The team received enthusiastic feedback on these events and looks forward to continuing through 2016.

In addition NeSI delivered two specialised HPC courses and collaborated with NVIDIA, an industry leader in HPC accelerator technology, to deliver a workshop on General Purpose GPU-based scientific programming in Auckland in September.

A significant part of NeSI's training plan for 2016, finalised towards the end of 2015, involves scaling up New Zealand's ability to hold Software Carpentry workshops. Work was done in the latter part of 2015 on coordinating New Zealand's first Software Carpentry Instructor training, held late January 2016 in Auckland and certifying 20 new instructors. These instructors are each committed to supporting at least two workshops during 2016.

To support basic digital skills training such as Software Carpentry, NeSI provided sector leadership by supporting champions at the University of Otago and the University of Auckland to host their inaugural Research Bazaar (ResBaz) events in February of 2016. Pitching the concept, garnering support, sourcing funding and event organisation was all supported by NeSI and undertaken during 2015. Off the back of the success of the Dunedin and Auckland events, Victoria University Wellington is hosting a similar event in April 2016, also supported by NeSI.

NeSI works with research communities in New Zealand to develop training and education programmes, and in a previous year carried out a gap analysis to identify key digital skills training needs.

Partnerships

NeSI collaborates sector-wide to improve efficiency and effectiveness across the New Zealand research system. In 2015 NeSI signed on Massey University as its first subscriber, providing a strategic context for growing HPC support for researchers across Massey campuses.

The agreement provides Massey University with a fixed allocation of platform access. As a subscriber, Massey University is now included in the majority of engagement activities, consistent with the investing Collaborator organisations. Institutional reporting was prototyped based on the requirements of Massey University's subscription contract. NeSI then sought broader engagement with institutions to mature this reporting mechanism, to ensure the general solution meets the needs of Collaborators and Subscribers.

In March of 2015 NeSI hosted a successful eResearch NZ conference in Queenstown, with very high attendance. The new co-hosting arrangements with NZ Genomics Ltd (NZGL) and REANNZ delivered significant growth in all aspects of the programme, sponsorship, and participation. Handover to REANNZ as the 2016 lead host was completed immediately after the event.

The 2014 Annual Report and Review and the Plan for 2015 were submitted in the first quarter of 2015. The Annual Plan for 2016 was completed and submitted before the MBIE deadline of November 30 and reviewed in depth at NeSI's annual Team Retreat, in December.

The NeSI NZGL Alliance was launched in Quarter 3, based on shared directions established over the preceding 12 months. A briefing paper with findings and opportunities for an Alliance was presented to the respective Boards of NeSI and NZGL in July 2015. A media release was made in early September which clearly outlined the intention of both organisations to form an alliance. An implementation project was kicked off in October, with representatives from both NeSI and NZGL, and in early November 2015 the joint team held a two-day planning session to agree activities to implement the Alliance. During the remainder of 2015 the working party met regularly and good progress was made on joint training initiatives and business development.

Although the development of the Alliance is still just beginning there are already benefits from the closer relationship of the two organisations:

- Both organisations are exploring investing in complementary staff.
- A priority in 2016 is joint investment in platforms, with NZGL's needs incorporated during the 2015 National Platform Framework review.
- New prospects and customers are shared where relevant, with discussion focused on providing the best possible outcomes for researchers.
- Joint workforce development initiatives have already taken place, with more planned in 2016. Two NZ Genomics team members are now certified Software Carpentry instructors.

In order to make it easier to start working with NeSI, there is a need for increased services marketing. Due to limited capacity within NeSI this initiative was put on hold awaiting the recruitment of an Engagement Manager, a position which was filled in November 2015. This project is a priority in 2016.

The eResearch 2020 discussion document was completed and communicated to the sector early in 2015. In response to the document and after feedback from Minister Joyce, MBIE instigated a strategy development project – the eResearch Infrastructure Strategic Refresh. MBIE released the National Statement of Science Investment in 2015, which incorporates several themes common to the eResearch 2020 discussion document, such as a focus on research excellence, simplification of funding structures, and seeking stronger alignment between institutions and researchers.

As a result of MBIE's response to the eResearch 2020 work, eResearch 2020 has produced the National Research Data Programme, to be launched in March 2016. This proposes a programme of change across the New Zealand research sector aimed at transforming researcher's abilities to work with and create value from data.

Data sharing and transfer

Alongside computational work, researchers often need to share access to their data and transfer data to or from NeSI's HPC platforms and institutions. NeSI offers methods to access, share and transfer data, including via high-performance, secure, high-throughput data transfer services between HPC platforms and a user's institutional storage, via a localised Globus service.

This Data Transfer service was rolled out at all NeSI sites in 2015 and supports cross-site workflow for researchers, improving time-to-solution through the faster transfer of data. During this roll-out a reference architecture was developed and deployed, and will be refined during 2016 to include the Science DMZ concept with REANNZ. This will mean that the researchers can deploy their own data transfer nodes at their local institute, and participate in a national high performance data transfer network, thus making data transfer easier and more broadly available.

In 2015 NeSI conducted a review of its current data services to inform future directions, define a baseline for current services and prioritise future areas for development and investment. Recommendations included investment in dedicated staff to support data services, and incorporate covered data services in the planned platform procurement. These recommendations were augmented by another contained in the revised National Platforms Framework – prioritising the recruitment of a data analytics expert to lead NeSI's data-focused services evolution.

NeSI contributed to eResearch 2020s's development of the National Research Data Programme (see Partnerships), preparing for launch in March 2016.

Services innovation

NeSI innovated in the development and delivery of services by investing in organisational development and capability maturity, lifting NeSI's performance and effectiveness. With the significant increase in experience and expertise, NeSI's team are now positioned to provide improved services and stronger leadership across the research sector.

Quarter 1 of 2015 introduced significant improvements to strategic planning and execution, as NeSI's new strategy system became bedded down. An early indicator of this new approach was a more coherent, integrated Annual Plan for 2015, and greater clarity of focus and direction across the team. A key initiative within this plan saw NeSI transformed into a project-led organisation, implementing consistent project management practices to support operational delivery.

This paved the way for a focus during 2016 on further maximising benefits through building integrated high-level programme management practice.

The revised programmes will lift NeSI's performance as a service provider, focusing on end-to-end delivery of user services, and maturity of service delivery as a national infrastructure.

With these enhancements to NeSI's execution of strategy well underway, the team also invested in providing a more coherent service for NeSI users. A key opportunity is through developing an alliance with NZ Genomics Ltd. This alliance aims to reduce barriers to researchers whose needs are met by one or other of the alliance partners. In the latter part of 2015, the team set in place foundations for the delivery of joint services in 2016, with a shared project team established and shared plans agreed. Initial priorities for 2016 will be developing a joint platforms technology roadmap, aligned within NeSI's National Platforms Framework, and on joint training activities.

The goal is to establish clear areas for joint work, and build familiarity and understanding to enable both organisations to increase the service offered.

Performance in meeting our objectives

1. Support New Zealand's research priorities
2. Grow advanced skills that can apply high-tech capabilities to challenging research questions
3. Increase fit-for-purpose use of national research infrastructure
4. Make fit-for-purpose investments aligned with sector needs
5. Enhance national service delivery consistency and performance to position NeSI for growth
6. Realise financial contributions and revenue targets to enhance NeSI's sustainability

Support New Zealand's research priorities

1

New Zealand has identified a number of research priorities as outlined in the National Statement of Science Investment. These priorities can be broken down into Investigator-Led Science which includes the Centres of Research Excellence (CoREs), Mission-Led Science and Industry-Led Science.

With these national research priorities in mind, NeSI has provided research support to the following CoREs during 2015: The Bio-Protection Research Centre; Brain Research New Zealand; The Dodd-Walls Centre for Photonic and Quantum Technologies; MacDiarmid Institute for Advanced Materials and Nanotechnology; QuakeCoRE: Centre for Earthquake Resilience; Riddet Institute; the Allan Wilson Centre for Molecular Ecology and Evolution; and Gravida: National Research Centre for Growth and Development.

A specific example of how we are aligning ourselves with research priorities is our collaborative work with QuakeCoRE. We are working proactively with leaders within QuakeCoRE to develop an organisational-level relationship with the CoRE – working together to develop optimised, robust NeSI workflows which can be used across QuakeCoRE's projects and investigators. This will improve QuakeCoRE's time-to-solution and make it easier for their researchers to start working with NeSI.

NeSI refreshed its Access Policy early in 2015. One of the Allocation classes is Merit Projects, which allows researchers who have already received New Zealand-sourced grants to access NeSI platforms and consulting services, with the rationale that they have been identified as aligning with New Zealand research priorities by virtue of being awarded funding. In 2015, the Access Policy was updated, replacing the cost recovery aspect of the Merit Project Allocation class with a subscription-based revenue model for institutions. This change has resulted in a significant increase in the number of Merit projects from 7 in 2014 to 20 in 2015, showing NeSI has improved its alignment with New Zealand's clearly-defined research priorities.

NeSI's training events support New Zealand researchers to develop both their computing capability and supportive research communities. Training is discussed more comprehensively below.

Comprehensive implementation of an Engagement programme was not undertaken during 2015, largely due to a delay in the employment of Engagement team members. The Engagement Manager started in November 2015 and the Research Communities Manager starts in May 2016. The addition of these two new team members provides an opportunity for NeSI to further develop its alignment with research priorities.

In 2015, NeSI continued to be a part of the eResearch 2020 initiative. A position paper entitled 'National Research Data Programme' has been the focus for 2015. This programme identifies opportunities for action at a national level that will yield the greatest impact, and therefore benefit, for New Zealand researchers with regards to data.

Progress has also been made on the formation of an Alliance between NeSI and NZ Genomics Ltd. We anticipate the Alliance delivering streamlined services to Genomics researchers in New Zealand across all scales of need – making it easier for them to start working with NZGL and NeSI and improving researcher time-to-solution.

> We are working proactively with leaders within QuakeCoRE to develop an organisational level relationship with the CoRE.

Grow advanced skills that can apply high-tech capabilities to challenging research questions

2

The National Research Data Programme discussion paper put together by eResearch 2020 (a joint NeSI, NZGL, REANNZ initiative) has highlighted the need to grow data analytics skills of New Zealand researchers. Growing advanced skills in researchers was a priority for 2015 to enable researchers to answer more challenging research questions. To do this NeSI focused on making it easier to start working with NeSI through training, which addressed fundamental digital literacy skill gaps considered essential for computation research, such as the use of a command line and shell environment, collaboration on software code through version control tools, and scripting languages for programming and data analysis.

In 2015 NeSI implemented phase one of a new training strategy. Nine workshops and two specialised HPC courses were delivered by NeSI in partnership with institutions nationally and to various research communities across New Zealand.

NeSI also continued to raise researchers' awareness of the use of digital skills to accelerate their research through contributing to the eResearch NZ conference series. NeSI hosted the 2015 conference and supported REANNZ as a co-host of the 2016 conference. NeSI staff gave a range of well received presentations, some on our future plans and others in review of work done in 2015.

Increase fit-for-purpose use of national research infrastructure

3

NeSI manages two underpinning policies for improving the utilisation of NeSI Platforms through increasing fit-for-purpose allocations of researchers' applications to the NeSI HPC infrastructure:

1. Access Policy - The Access Policy provides the framework for NeSI to allocate researchers' computational projects to the most appropriate NeSI Platform. This allows NeSI to optimise the allocation of the capital equipment and expertise is managed for most efficient use.

2. Collaboration Agreement - The Collaboration agreement between the Host (University of Auckland) and the Collaborators (University of Auckland, University of Canterbury, University of Otago, National Institute of Water and Atmospheric Research, and Landcare Research) allows for the platforms owned by these Collaborator institutions and the people employed by the same to be pooled nationally and allocated to individual research projects by the team, based on fit-for-purpose criteria.

Both policies have yet to be fully implemented (that will occur in the 2016 calendar year). They do underpin the planning for new investments in platforms in the 2017 timeframe (*see Objective 4*).

Make fit-for-purpose investments aligned with sector needs

4

The NeSI Business Case establishes a new mechanism to make fit-for-purpose investments aligned with sector needs – the National Platforms Framework – a high level plan for nationally coordinated procurements.

This plan is reviewed annually, with the first review taking place in the fourth quarter of 2015. Investments have historically focused on HPC platforms, while opportunities in the Data Services area come into focus in 2016.

The 2015 review involved:

- Initial meetings with Collaborator and Subscriber key researchers to review their use of NeSI platforms over the period 2013 to 2015, solicit their current and future HPC requirements, and identify potential benchmark codes for use in future procurements.
- A review of Cloud computing opportunities (informed by a NeSI Cloud Pilot project) and HPC technology roadmaps, including assessment of potentially disruptive technologies that have come into view over the last year.
- Financial analysis of potential investment decisions on the Fund, being the virtual investment fund across Collaborators managed by NeSI.
- Revision of the National Platforms Framework informed by research directions and technology developments, detailing commissioning and decommissioning activities.
- Consultation with these stakeholders on the revisions, to ensure alignment and management of operational or implementation risks.

The NeSI Board approved the revisions to the Framework in principle, while Collaborators highlighted various operational and implementation risks. The consultation process on these risks is scheduled to be completed in the first quarter of 2016, for final NeSI Board approval in March 2016.

Enhance national service delivery consistency and performance to position NeSI for growth

5

NeSI's transition into a national organisation operating within functional teams created the opportunity for enhancing consistency and performance in 2015. Task assignment now occurs nationally, enabling better collaboration within teams and across institutions. Role clarity for team members has improved and role conflict decreased, increasing the efficiency of service delivery. NeSI's new organisational structure enables us to support researchers across sites as a seamless team. All of these enhancements were implemented starting in quarter two, taking effect as the new team was recruited and inducted into the new organisation structure and their new nationally aligned and consistent roles.

NeSI now has the foundations of a national data transfer network operating across all NeSI sites, enhancing service delivery consistency, improving time-to-solution and making it easier to support computational workflows across multiple NeSI platforms. These foundations will be built on in 2016, aimed at increased performance through partnerships with local ITS providers and REANNZ on Science DMZ and last mile connectivity to research data stores and lab instruments and equipment.

NeSI's project management capability has matured over 2015, giving us a consistent approach to the way we run projects to deliver benefits.

Realise financial contributions and revenue targets to enhance NeSI's sustainability

6

Our Collaborators' financial commitment, as a ratio of Crown contributions, is a financial indicator of the health of the NeSI partnership. The contract requirement is total Collaborator contributions and Collaborator commitments to reinvestment amount to at least 95% of the total Crown Contributions by the contract end. As at December 2015 the ratio of Collaborator Commitments to Crown Contributions is 79.0%, life-to-date, which is lower than budget-to-date (85.6%) and contract end target (95.6%).

The majority of the under performance of the ratio due to unspent Crown funds alongside deferred reinvestment in platforms, now timed for mid-2017. Sector revenue is $76.0k, $19.7k lower than life-to-date budget of $95.7k.

NeSI - a national organisation

NeSI is a collaboration of five institutions coordinating investments in partnership with the Crown. This collaboration is constituted through a legal agreement between the University of Auckland, the University of Canterbury, the National Institute of Water and Atmospheric Research (NIWA), the University of Otago and Landcare Research, with the University of Auckland as the legal contracting entity with the Crown, commonly referred to as the Host. A set of operating principles defined in the Collaboration and Services Agreements forms the basis for governance, management and operations.

Governance

NeSI's Board is responsible for strategy development, policy, approving major initiatives and investments, as well as monitoring the NeSI risk register. Five of the Collaborator institutions appoint four Directors, alongside an independent Chair and another independent member with expertise in the field representing the research sector at large. All Board members are focused on the interests of NeSI, being the effective delivery of national research infrastructure services.

In 2015 the NeSI Board was comprised of the following members:

- Rick Christie, Independent Chair
- Prof. Andrew Rohl, Independent, Professor of Computational Science, Curtin University
- Dr Murray Poulter, Retired Chief Scientist, NIWA
- Prof. Steve Weaver, Deputy Vice-Chancellor (Research), University of Canterbury
- Stephen Whiteside, Director Organisational Performance & CIO, The University of Auckland
- Prof. Rob Ballagh, Department of Physics, University of Otago

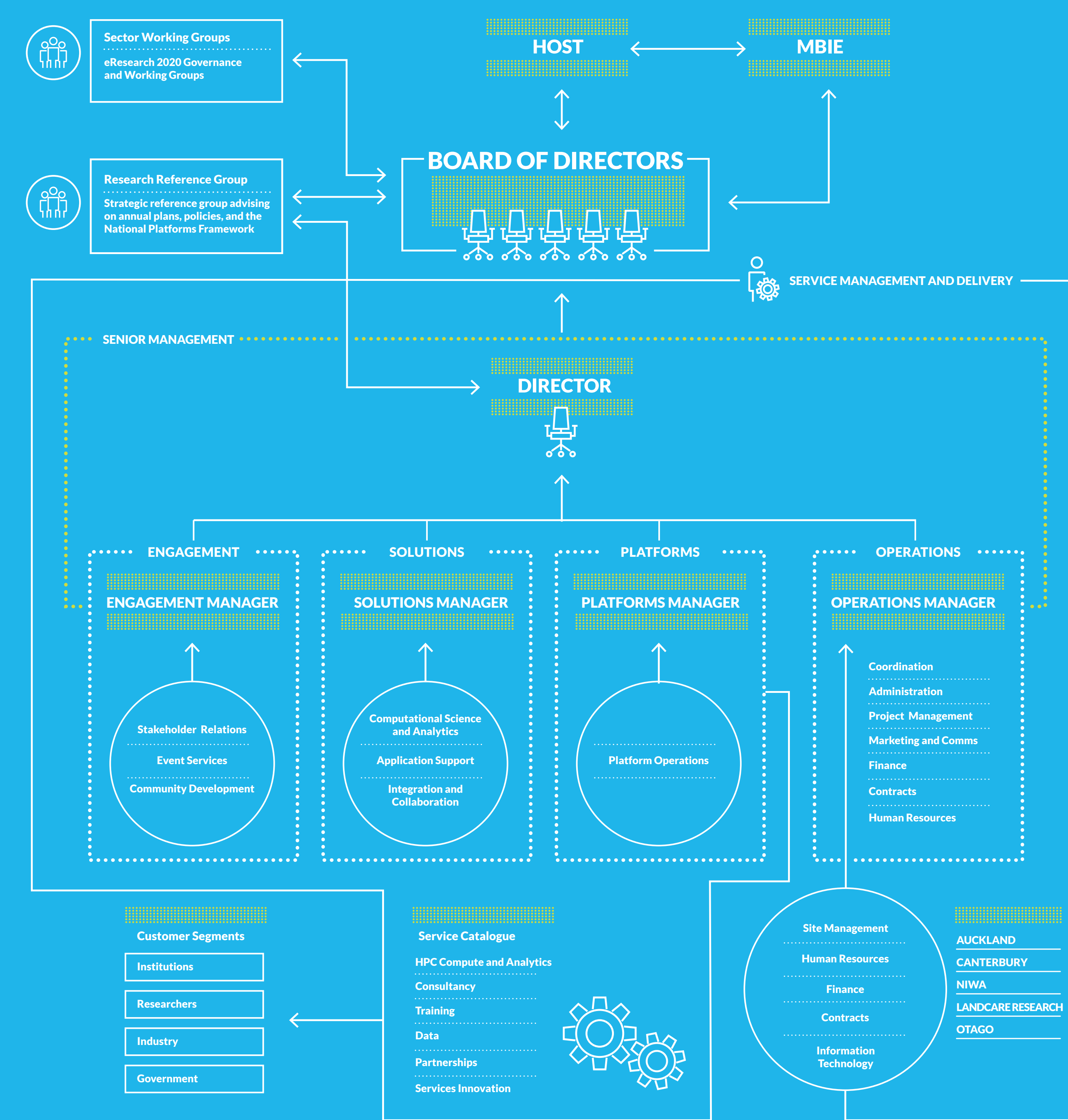
Advisory

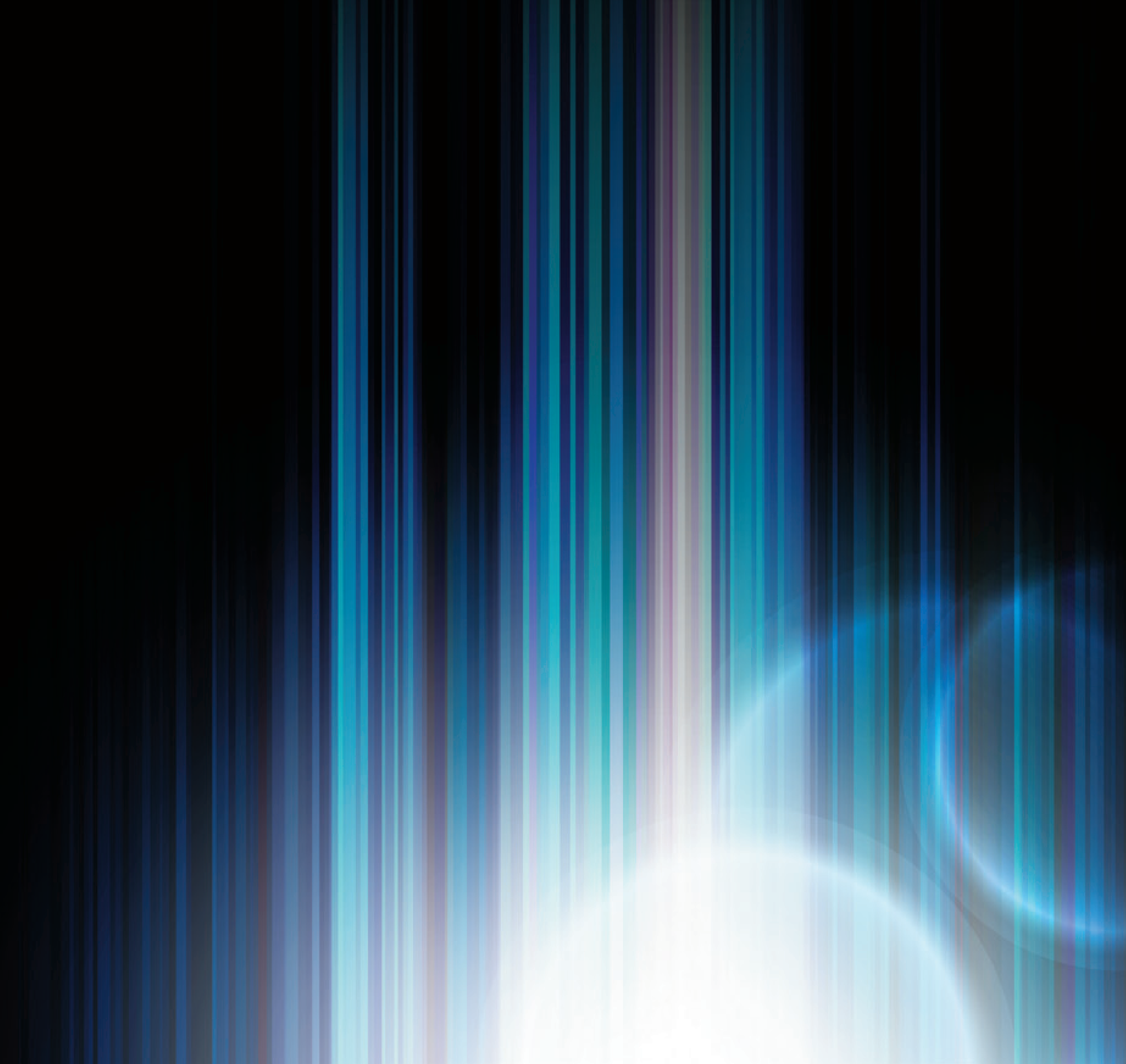
Towards the end of 2015 NeSI established the NeSI Research Reference Group, an advisory group made up of eight research community leaders with strong technical knowledge on the impact of eScience as an enabler to research. The Group has a key role in providing timely advice and input on strategic and policy matters of interest to NeSI, especially those most relevant to researchers.

- Dr Joseph Lane, Chair, Senior Lecturer (Physical and Theoretical Chemistry), University of Waikato
- Dr Nauman Maqbool, Group Leader Knowledge & Analytics, AgResearch
- Prof. Cristin Print, Molecular Medicine & Pathology, The University of Auckland
- Prof. Ian Foster, Department of Computer Science, University of Chicago
- Dr Susan Wells, Associate Professor, Epidemiology and Biostatistics, The University of Auckland
- Dr Sam Dean, Chief Scientist - Climate, Atmosphere and Hazards, NIWA
- Prof. Blair Blakie, Department of Physics, University of Otago
- Prof. Barbara Chapman, Department of Computer Science, University of Houston and Professor, Institute for Computational Science, Stony Brook University.

Organisation Design

NeSI is a virtual organisation embedded within research institutions across New Zealand. We value our role alongside researchers, on the front line of research. Operating within sector institutions creates spaces for collegial relations and trust, underpinning our ability to influence and inform. Our contributions increase the productivity of research, requiring working knowledge of the means by which research is performed. NeSI's organisational design is focused on retaining this position within the sector, while ensuring strong alignment and efficient delivery against our strategic goals and more immediate plans.





NeSI 2015 case studies

The theory of ultra-cold atomic gases

Searching for earth-mass planets around Alpha Centauri

Decoding the bovine genome

Investigating the reliability of bloodstain pattern analysis

Software Carpentry in NZ: the seed has been planted

Quantum trajectories: a story of qubits and photons

Scouring continuous seismic data for low-frequency earthquakes

Multi-scale modelling of saliva secretion

The theory of ultra-cold atomic gases

Gases have recently been cooled to a billionth of a degree above absolute zero, at which point everyday thermal noise is almost totally absent and the quantum mechanical behaviour of the particles is revealed.

Researchers at the Dodd-Walls Centre for Photonic and Quantum Technologies, including Dr Danny Baillie of the Department of Physics, University of Otago, have used NeSI's resources to help analyse the use of ultra-cold atomic gases.

Gases have recently been cooled to a billionth of a degree above absolute zero, at which point everyday thermal noise is almost totally absent and the quantum mechanical behaviour of the particles is revealed. Magnetic fields and lasers are used to confine and manipulate the gas, and even control how the atoms or molecules interact with each other. The properties of the gas can be measured in real time, typically with optical imaging, which can be used to measure the gas density on micrometre length scales. These systems are of interest in physics for fundamental studies of quantum physics and for applications into next-generation atomic clocks and quantum computers.

A feature of these ultra-cold gases is that the interactions between the particles are extremely well characterised, offering the opportunity for first-principles calculations to compare with experiment.

A recent development in the field has been the production of cold samples of dipolar particles, in which the interactions between the particles is like that between two bar magnets: both long-ranged and dependent on the orientation of the particles. This interaction leads to new physical phenomena that can be explored in these systems, however the partially attractive character of the interaction (e.g. two bar magnets placed head to tail attract each other) also means the gas can be unstable and collapse, meaning the gas is lost to the experiment. When a collapse occurs it involves a complex interplay of the geometry of the confined gas, the temperature of the system, and the precise properties of the interactions.

"By using NeSI's resources we were able to simultaneously use almost a thousand cores, which enabled us to complete the work in a fraction of the time it would've taken using only local resources."

This work establishes a comprehensive theory for the conditions where the gas is stable, which is vital to providing a map for experimentalists for how to prepare and manipulate these systems.

According to quantum mechanics, particles of the same species are fundamentally indistinguishable: if two of them were exchanged it would be impossible to tell. Particles come in two flavours depending on the number of constituent electrons, protons and neutrons: an odd number and they are fermions; an even number and they are bosons. For fermions, the effect of exchange gives rise to the Pauli exclusion principle: two of them cannot occupy the same quantum state. The coldest bosons occupy the lowest energy state, a Bose Einstein Condensate. The exchange effect means that cold fermions are significantly more stable than bosons. Fully allowing for the exchange effect is computationally difficult: it is necessary to model both the density of the particles and their relative position. Even exploiting the cylindrical symmetry of the problem, the system has four effective dimensions and interaction effects need to be solved self-consistently.

Due to this difficulty, the researchers' earlier work[1] was not able to fully allow for the exchange effect, but this was rectified by using their newly developed algorithm[2] with the computational power provided by NeSI's Pan Cluster.

Dr Baillie says, "By using NeSI's resources we were also able to evaluate the stability at our full range of temperatures in parallel, simultaneously using almost a thousand cores, which enabled us to complete the work in a fraction of the time it would've taken using only local resources."

Fig.1 shows that the exchange effect is significant.

FIGURE. 1

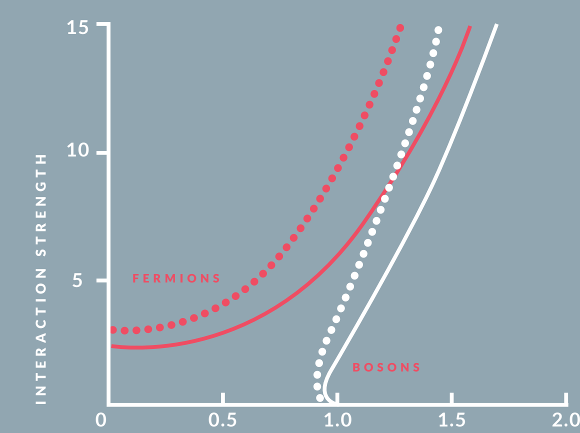


Fig.1 Relationship between interaction strength and temperature at the instability point for a pancake geometry: fully allowing for exchange (solid) makes the gas less stable than earlier work (dashed). Note that fermions (red) are more stable than bosons (white).

Searching for earth-mass planets around Alpha Centauri

Researchers at the University of Canterbury have been conducting an intensive observational campaign with the aim of detecting Earth-mass planets in our closest neighbouring star system – the binary stars of Alpha Centauri – including those which may lie within the respective habitable zones around either star.

Several methods can be employed to detect extrasolar planets (planets around stars other than the Sun). PhD candidate Christoph Bergmann and his supervisor, Professor John Hearnshaw, used the so-called radial velocity method (or Doppler method), whereby the tiny reflex motion induced on the star by the gravitational pull of an orbiting planet is detected. The underlying physical principle is the well-known Doppler effect.

Starlight collected with a telescope is fed into a spectrograph, which disperses the light into its different wavelengths (or colours). By precisely measuring the position of the spectral lines, the star's radial velocity, which is the line-of-sight component of its velocity through space, can be determined. If there is a periodic variation in a star's radial velocity, the presence of an orbiting companion can be deduced. This can either be another star or a planet. In the latter case however, the signal is several orders of magnitudes smaller because planets are considerably less massive than stars.

Over the course of about six years at Mt John University Observatory by Lake Tekapo, Bergmann and Professor Hearnshaw collected tens of thousands of spectroscopic observations of both components of the Alpha Centauri binary system, as well as several hundred observations of four other binary stars . All observations were taken with the 1-m McLellan telescope at Mt John University Observatory by Lake Tekapo, in conjunction with the HERCULES Spectrograph. Both the telescope and the spectrograph were designed and built by the Department of Physics and Astronomy at the University of Canterbury.

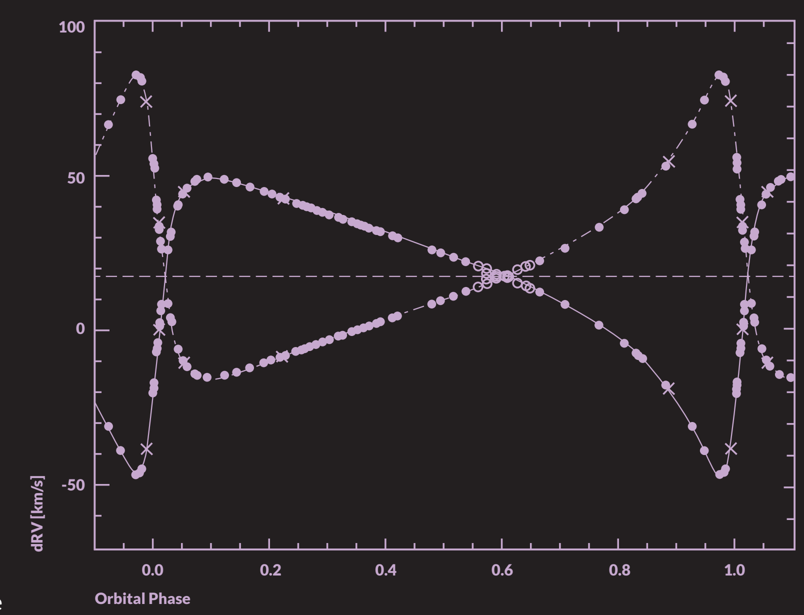
Because the angular separation between the two components of the Alpha Centauri system is very small, some light from the other star would be included in the observed spectrum most of the time. This spectral cross-contamination resulted in a spurious shift of the measured radial velocity relative to an uncontaminated observation. To make things worse, the amount of contamination was different for every spectrum observed. The standard modelling technique therefore had to be extended to include both stars at a variable light ratio in the modelling process. All other unresolved binary stars present a similar, yet slightly simpler case, as the light contribution from the two stars does not change.

> "We were able to calculate radial velocities for all our 50,000 observations within about a week – a task that would have otherwise taken several months of computational time."

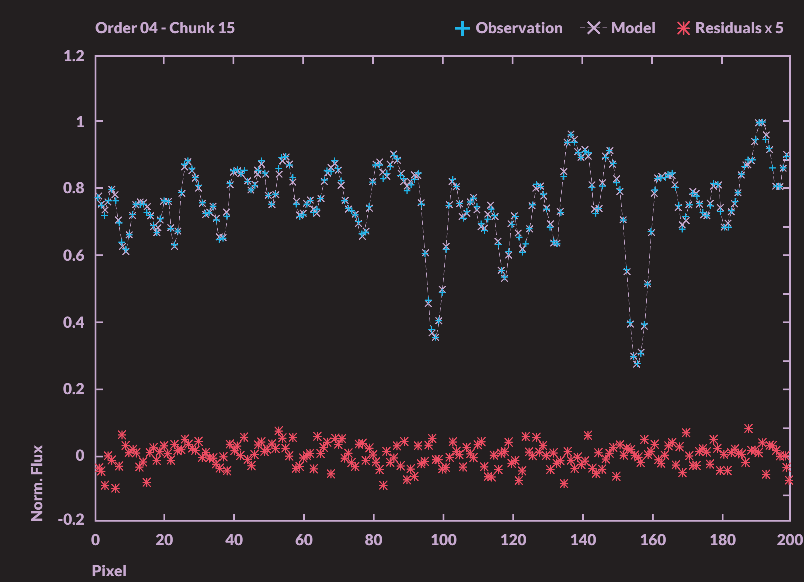
For the purposes of wavelength calibration, an iodine gas cell was placed in the light path. As the starlight passes through the iodine cell, a dense forest of absorption lines is superimposed onto the stellar spectrum. To determine a star's radial velocity, the observed spectrum is modelled by combining template spectra for the star as well as for the iodine. Bergmann further extended the reduction code used in this research so that a second stellar template was included in the modelling of the observations, providing a newly developed model which included up to 19 free parameters, making the modelling procedure computationally expensive.

The pipeline is written in FORTRAN77 and typically the radial velocity extraction from an observed spectrum takes of the order of 5-10 minutes on a standard PC. In total there were almost 50,000 observations that had to be processed with this pipeline. Furthermore, as the code was still being developed and refined, the researchers went through several rounds of reducing the entire data set. Bergmann says "This would not have been possible without the use of NeSI's supercomputing resources. Dr François Bissey assisted us in setting this pipeline up and a method was devised to break down the computational task into several jobs that could be run simultaneously. That way we were able to calculate radial velocities for all our 50,000 observations within about a week – a task that would have otherwise taken several months of computational time."

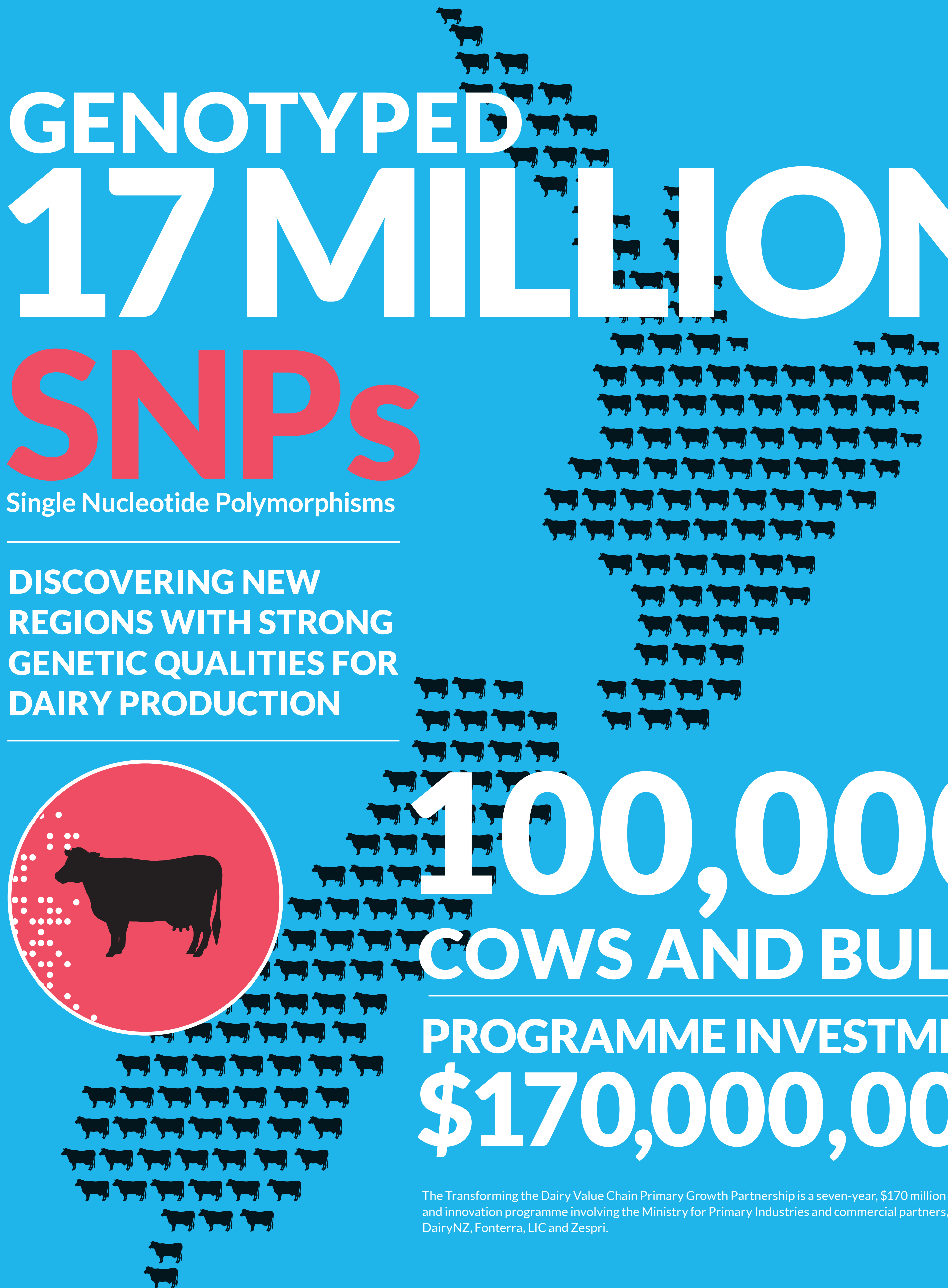
With the full set of radial velocities of Alpha Centauri at hand, the researchers were able to analyse the data and look for signals caused by potential planets. While no planets were found around either of the two components, upper mass limits could be derived and hence the presence of planets more massive than about 14 Earth-masses in orbits with periods of less than 30 days could be excluded around both stars. For alpha Centauri B (the less massive component), the existence of planets with more than 3 and 4.5 Earth-masses could also be ruled out in orbits of less than three and five days, respectively. Furthermore, Bergmann and Professor Hearnshaw were able to compute orbital solutions for binary systems with unprecedented precision.



Example of a radial velocity curve of a binary system observed for this work together with the best-fit orbital solution.



Example of a small chunk of the observed spectrum together with the best-fit model. The residuals have been multiplied with a factor of 5.



GENOTYPED 17 MILLION SNPs

Single Nucleotide Polymorphisms

DISCOVERING NEW REGIONS WITH STRONG GENETIC QUALITIES FOR DAIRY PRODUCTION

100,000 COWS AND BULLS

PROGRAMME INVESTMENT $170,000,000

The Transforming the Dairy Value Chain Primary Growth Partnership is a seven-year, $170 million research and innovation programme involving the Ministry for Primary Industries and commercial partners, including DairyNZ, Fonterra, LIC and Zespri.

Decoding the bovine genome

Maksim Struchalin and fellow researchers at LIC, Livestock Improvement Corporation, have been conducting a world-leading PGP-funded study on sequencing the genome of dairy cattle which will be of enormous benefit to the dairy industry, the national economy and will also help researchers better understand human genetic disorders.

The main aim of the project is to discover new regions in the bovine genome that are responsible for important dairy traits such as milk volume, protein and fat concentration in milk, amongst others. Knowledge of such genomic regions will allow for more accurate selection of bulls with desirable genes, which can then be passed on to their female offspring. The cows with those genes are more likely to produce milk of higher quality and/or greater quantity, thus increasing the potential of generating income for the dairy industry and boosting the New Zealand economy.

> "The NeSI cluster allowed us to run analyses in one week which otherwise would have taken maybe 100 years of computational time."

The bovine genome consists of three billion elementary building blocks called nucleotides and about one percent of them vary amongst the population. Those varying nucleotides are called Single Nucleotide Polymorphisms (SNPs). SNPs are known to bear partial responsibility for phenotypic differences between individual animals – what makes animals different from each other. The researchers aimed to find the SNPs that are responsible for bovine performance. LIC researchers genotyped (measured) approximately 17 million SNPs in more than 100,000 cows and bulls. Thus, the data set is represented by a matrix of about 100,000 rows and 17,000,000 columns. Because many of the animals are closely related, there is nonzero covariance between rows (individuals) of this matrix – this reflects the fact that relatives share some portion of genetic material. Likewise, there is nonzero covariance between columns (SNPs), reflecting the presence of so called linkage disequilibrium between SNPs and the presence of genetic strata in the sample, i.e. clusters of genetically similar animals.

Such complex data demands special care. A few truly associated SNPs might result in millions of observable correlations between SNPs and a trait of interest. The vast majority of correlations would therefore be false positive associations reflecting how these animals were sampled rather than an underlying, biologically relevant genetic model. The main difficulty therefore lies in selecting the small number of true positive associations from amongst millions of false positive ones.

"The NeSI cluster provided priceless resources that allowed us to work with such complex data," explained Dr Struchalin. "In our analysis, we had to transpose, inverse and multiply large matrices which requires us to use nodes with lots of RAM. Using a large number of computational cores allowed us to run analyses in one week which otherwise would have taken maybe 100 years of computational time. Moreover, NeSI provided us with enough disk space to store countless terabytes of our data and generated outputs."

"The technical and consulting support provided by NeSI staff was extremely important and, in some cases, crucial for our project. We received a lot of valuable advice on how to accelerate and optimise our computations. Prompt responses from the NeSI team to our requests helped us solve our problems in a few minutes, which in turn allowed us to focus on scientific research rather than on dealing with technical issues.

Undoubtedly, the amount of data and the complexity of analysis will continue to grow in the future. This makes it very important to have such computational resources as NeSI."

"Without an organisation like NeSI, and the services that they provide, it is unlikely that we would have been able to advance the research methodology to a bayesian framework."

Dr Niki Osborne in the Bloodstain Pattern Analysis lab at the Institute of Environmental Science and Research.

Investigating the reliability of bloodstain pattern analysis

Psychological scientist Dr Niki Osborne, from both the Department of Psychology at the University of Otago and the Institute of Environmental Science and Research Ltd (ESR), spends her days looking at blood spatter.

Her recent research project on the topic of bloodstain pattern analysis (BPA) is helping to progress a research programme critical to New Zealand's criminal justice system. In utilising NeSI's facilities, Niki was able to take her research to the next level by grounding it in a computationally complex Bayesian framework.

"Without an organisation like NeSI, and the services that they provide, it is unlikely that we would have been able to advance the research methodology to a Bayesian framework. Doing so gave us not only the required computational power to run large effective-n Bayesian tests, but also the methodological freedom to plan subsequent scaled-up Bayesian tests in an iterative research paradigm. It's only a matter of time now before more psychological/health/social scientists cotton on to this massive opportunity for research advancement that NeSI provides. We're just glad to be at the forefront of it. Cheers NeSI."

The impetus behind Niki's current work is the 2009 National Research Council report into the state of forensic science, which made specific reference to vulnerabilities to cognitive bias in forensic science, and called for research to understand and address these, including BPA.

BPA is a pattern recognition task in which interpretation of the size, shape, and distribution of bloodstains can provide valuable information in a crime scene investigation. This analysis can help to piece together the events of the crime and in some cases might help to distinguish between, for example, homicide and suicide, or self-defence and murder.

In the course of a bloodstain pattern analysis, analysts can be exposed to a plethora of information, such as police investigators' theories, witness statements, type of injuries sustained by the victim, or the type of weapon used. All of this information may – consciously or subconsciously – influence how analysts interpret the bloodstain patterns. Given that a large degree of contextual information in BPA is unavoidable, research to investigate how contextual information might influence BPA decisions is paramount.

Niki's team with the help of NeSI, found that the provision of contextual information can influence the interpretation of bloodstain pattern evidence. This finding highlights the need for context-management procedures in BPA.

Software Carpentry in NZ: the seed has been planted

“It was overwhelming to witness all 40 seats fully booked within six hours. We noted a strong demand from the humanities and social sciences.”

Since 2014, after having identified a skills gap within the research community, NeSI has run a series of workshops to upskill researchers in digital research tools and methods becoming an official affiliate of the Software Carpentry Foundation.

Software Carpentry is an international research computing skills training initiative. The foundation has gained tremendous experience in providing researchers with high-quality training since 1998 worldwide. Software Carpentry training is typically given as a two-day ‘boot camp’ and covers essential digital skills and tools such as basic task automation using unix shell, programming concepts (Python or R), version control and collaboration using GIT and data management with SQL. It promotes an active, ‘hands-on’ approach to learning, in which a team of certified instructors is supported by a number of helpers.

NeSI’s Computational Science team members John Rugis and Sung Bae became certified Software Carpentry instructors in February 2015 and began a nationwide series of workshops in collaboration with six universities at seven campuses, holding training events at the University of Canterbury, Auckland University of Technology, the University of Otago, Massey University at Palmerston North, Victoria University of Wellington, Massey University at Albany and Lincoln University between February and November 2015.

Each training event had 30~40 participants from various research fields, the majority from science and engineering, and a significant number from a broader range of disciplines. NeSI’s training programme manager, Sung Bae, notes “It was overwhelming to witness all 40 seats fully booked within six hours. We noted a strong demand from the humanities and social sciences.”

Feedback responses following the training workshops were very positive. NeSI adopted an industry-standard approach to evaluate the quality of training offerings, and Software Carpentry events scored an overall rating of 4.34 out of 5.00. One of the most received requests was a call for Software Carpentry or similar training on a regular basis.

To accommodate this growing need from the New Zealand research community, NeSI hosted New Zealand’s first Software Carpentry Instructor Training from January 28 to 29 2016. Aleksandra Pawlik from the Software Sustainability Institute UK, a certified Software Carpentry instructor trainer, teamed up with NeSI’s John Rugis to train candidates from various research institutions and universities. There are now 20 new certified instructors in New Zealand, and a commitment from each new instructor to run two workshops during 2016.

NeSI plans to work together with the new instructors and host more Software Carpentry events at their local institutions on a regular basis. “The seed has been planted and watered. In 2016, we will make it grow together with the community,” says Bae. “If we keep the momentum and excitement from the research sector going, we will see a growing number of community-driven training activities in New Zealand.”

Photo credit: Sung Bae

Quantum trajectories: a story of qubits and photons

For many, the theoretical physics question Canela is pursuing is a challenging concept, however the applications or perhaps implications of the research are something with potentially wide-ranging effects.

Victor Canela arrived on New Zealand's shores three years ago. His sole reason for coming to New Zealand – being able to work on one of physics' biggest questions – how do we get from A to B, when we don't even know where B is?

Victor says, "During my undergraduate degree, I learned about quantum mechanics and the strangeness of the microscopic universe and became very interested in quantum optics: the study of the interaction between light and matter in the tiniest of scales – photons and atoms. Coming to New Zealand to work with Prof. Carmichael at the University of Auckland has been a great experience as he has done fundamental work on the field."

Quantum optics - an interesting field

"The system we study is called a one-atom maser, similar in operation to a laser, with microwaves instead of light. We simulate a stream of two-level atoms (nicknamed quantum bits or qubits in analogy with the classical computer bits) interacting with photons in a box. We are interested in controlling the properties of the photons by modifying properties of the stream of qubits."

It is not surprising that a young researcher would choose this field. In 2012, Serge Haroche and David Wineland were recipients of the Nobel Prize for Physics for experiments that realised the delicate interaction of matter and light.

Canela himself is very good at explaining the fundamentals of his research: "The difficulty in studying and simulating these systems is that none of them are closed; they have losses and in general have a complex interaction with the outside world. Computationally speaking, the simulations are too complex to handle. A way around this is to introduce random fluctuations to our system and thus mimic the effect the outside environment would have. These are the so-called quantum trajectories."

"Individual quantum trajectories are created with random processes, so we don't know in advance where they will go. What we do know is that their ensemble average gives us information of properties of the system that we are interested in, such as how many photons are inside the box."

The power of HPC

When run in serial, one trajectory after another, it would take about 1200 core-hours to obtain useful data (nearly two months on your standard desktop computer). Canela was already aware of NeSI's Pan cluster and had optimised his code for running in an HPC system. Upon attending a Hacky Hour hosted by team members of the University of Auckland's Centre of eResearch and NeSI, Canela met NeSI's Jordi Blasco. It was during one of these Hacky Hours that Blasco and Canela were able to optimise Canela's code, speeding up the processing time by a factor of 150.

Blasco explains, "We realised that the problem could easily transform into a highly decoupled problem with parameter switching workflow. In less than one hour working with the Fortran code, the application was able to run several independent trajectories at once."

Thanks to the Intel VTune Amplifier reports, they were able to identify the major bottlenecks in the code. After a few meetings optimising parts of the code, Canela and Blasco finally achieved an overall improvement in speed of up to 600 times faster. What's next for Canela?

"We have been successful in simulating the interaction between qubits and photons and have devised ways to control the photon number. Such quantum control is of big interest to the community as it provides tools for the development of a quantum computer."

What's next for Canela

Findings such as those above are only the beginning for Canela's thesis:

"The control mechanisms we have developed have allowed us to simulate the creation of states with particular photon statistics and we have been able to explore different parameters regimes, thanks to the NeSI Pan Cluster. We aim to expand our simulations and include more sources of noise such as one would have in an experiment."

Victor Canela is using NeSI to help answer the question: how do we get from A to B, when we don't even know where B is?

Scouring continuous seismic data for low-frequency earthquakes

"As a PhD student close to completion, the speed-up afforded by the NeSI infrastructure and the ease of migration came at a crucial time. Everything was straightforward and well-documented, and the expertise of the technical team was invaluable."

Researcher Calum Chamberlain servicing the Solution Ranges seismic site above the Landsborough Valley. **Photo credit:** Adrian Benson.

PhD Candidate Calum Chamberlain, at Victoria University of Wellington's School of Geography, Environment and Earth Sciences, has used NeSI's Pan cluster in an attempt to further our ability to understand the properties of earthquakes and faults, which is often limited by what earthquakes can be detected.

Large earthquakes, while easy to detect, occur infrequently, whereas small earthquakes occur frequently, but are hard to detect due to low signal amplitudes. The detection and analysis of small earthquakes is particularly important when considering faults that are likely to generate large earthquakes, but have not generated such an earthquake within recorded history.

New Zealand's Alpine Fault is thought to be capable of generating large (magnitude 7-8) earthquakes around every 330 years, with the last large earthquake thought to have occurred in 1717 AD. In this context, understanding how small earthquakes are distributed along the fault in both space and time may help us to understand how the next Alpine Fault earthquake will behave.

To enable the detection of small earthquakes associated with the Alpine Fault, Chamberlain and his colleagues recorded background seismic waves for the last 61/2 years on a network of highly sensitive seismometers deployed in the high Southern Alps in shallow boreholes and on the surface. To take advantage of this large dataset (~1.5 TB), they adapted a cross-correlation detection method in which previously detected earthquakes were used as templates to scan through the data and find similar events (video).

This method has specific benefits for earthquakes that repeat, which, as Chamberlain explains, "is interpreted to mean that slip (the relative displacement of two formerly adjacent points on the opposite sides of a fault) is recurring on the same patch of a fault multiple times." In particular, it is better at detecting the seismic signatures of recently recognised "slow slip" earthquakes (commonly known as "silent earthquakes") than standard detection methods. Slow-slip events have been documented on many major faults throughout the world using observations of continuous global positioning system (GPS) networks and are thought to transfer stress from the deep extent of these faults to the shallow earthquake-generating areas in the cooler, more brittle crust.

Due to the Alpine Fault's geometry and sparse network coverage, GPS cannot currently be used to detect slow-slip events. However, these slow-slip events often generate low-frequency seismic energy composed of lots of small low-frequency earthquakes (LFEs). Therefore, these LFEs can be used as proxies indicative of slow slip.

The research team had previously generated a preliminary catalogue of LFEs beneath the Southern Alps, and showed that they occurred near the inferred deep extent of the Alpine Fault. By looking at changes in LFE detection rate with time, they found that the deep extent of the Alpine Fault is sensitive to stresses caused by large regional earthquakes.

"Our previous study was limited by our ability to generate templates to use in the cross-correlation method," says Chamberlain, "so to improve on this preliminary catalogue we had to include more LFE sources as templates to target. To allow the use of much greater numbers of LFE templates, we developed a multi-parallel workflow in Python. Applying this workflow to many thousands of LFE templates, however, required more computational power than we originally had access to."

However, for the second study, NeSI provided the researchers with access to the Pan cluster HPC platform which allowed them to take advantage of the multi-parallel workflow. "This resulted in greatly reduced computational times — from several months on a standard four-core machine to less than ten hours on Pan for the full 61/2 year-long dataset", Chamberlain explains. "Setting up our codes to run was straightforward and data transfer using Globus was quick thanks to the assistance and expertise of the NeSI team. We were able to transfer our 1.5 Tb dataset to Pan in less than 24 hours, allowing us to quickly migrate to the cluster."

"The speed-up provided by Pan has allowed us to experiment with new objective methods of constructing templates and detecting small earthquakes in the continuous data. This speed-up also enabled us to undertake much more experimentation, allowing us to test and develop our methods dramatically faster than we would otherwise have been able to. As a PhD student close to completion, the speed-up afforded by the NeSI infrastructure and the ease of migration came at a crucial time. Everything from the original application procedure to complex job management was straightforward and well-documented, and the expertise of the technical team was invaluable."

This research was funded by the Marsden Fund of the Royal Society of New Zealand, the Earthquake Commission, and Victoria University of Wellington

Multi-scale modelling of saliva secretion

"Thanks to NeSI, we were able to render higher quality images and run many more simulation variants than would have been possible on a desktop computer."

Prof. James Sneyd

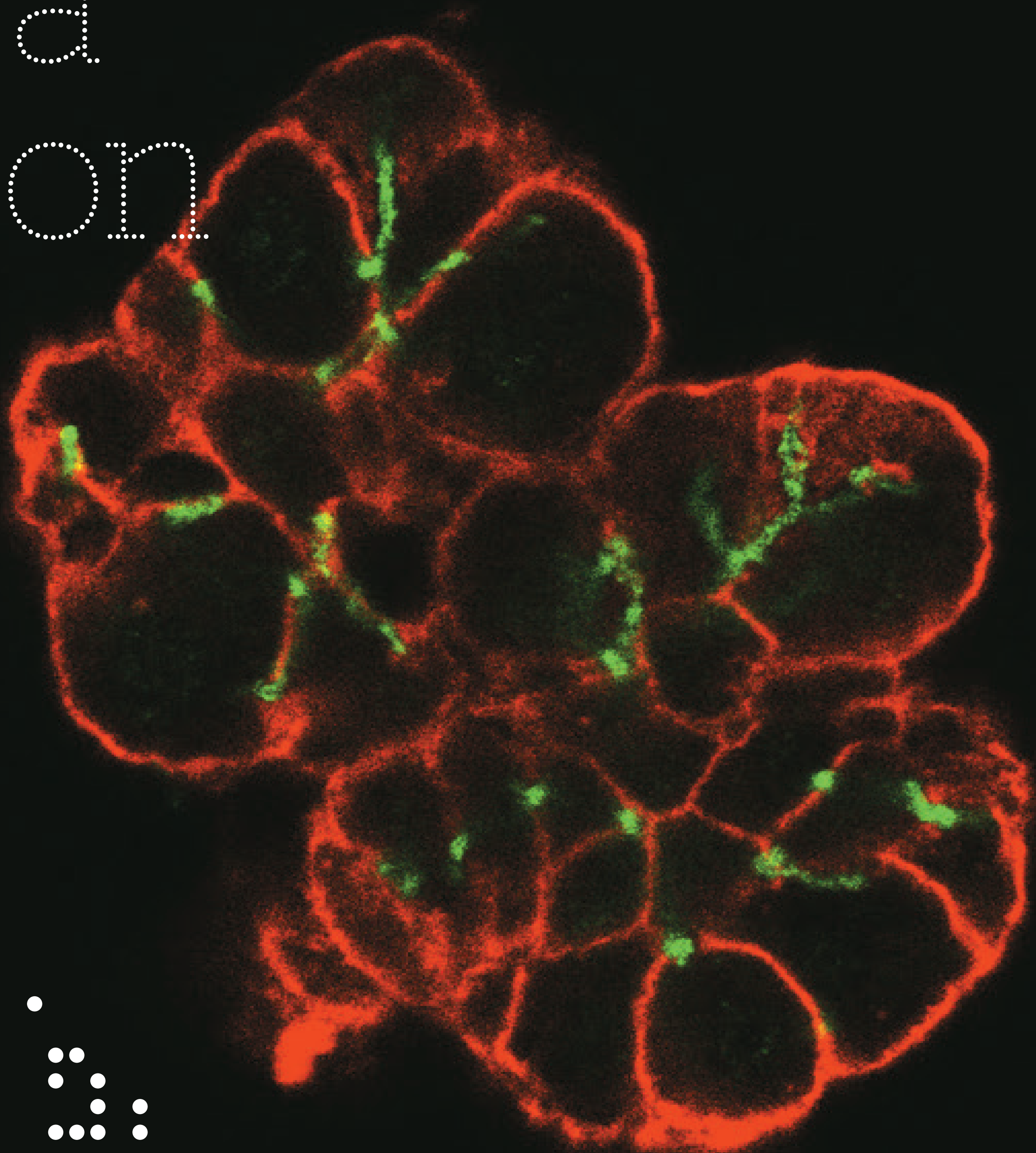


Figure 1: Colour coded digitised image slice (from Prof. David Yule's laboratory at the University of Rochester)

Biological samples of salivary cell clusters were digitised and the image slices used as the basis for a full 3D graphics model reconstruction of one cluster of cells. The 3D model was then used as a basis for simulations and visualisations.

Background

The current study examines the structure and function of cells in the salivary gland at the microscopic level. Recent advances in microscopy techniques have enabled us to acquire the data necessary for 3D reconstruction of cell structure. We have crossed the threshold into the world of physically accurate cell level modelling, simulation and visualisation.

This work was conducted by Prof. James Sneyd and Dr Shawn Means from the Department of Mathematics at the University of Auckland, in collaboration with Prof. David Yule from the School of Medicine and Dentistry at the University of Rochester. James Sneyd is a Professor of Applied Mathematics whose specialist research area is mathematical biology and physiology – i.e. studying how body parts work. Support from NeSI for this project was led by Dr John Rugis whose expertise in computer modelling and graphics complemented the HPC compute resources that NeSI also provided.

This interdisciplinary project encompasses a range of activities targeting anatomical data-based structural modelling of individual salivary cell clusters, solution of cellular calcium dynamics function in full 3D simulations, interactive visualisation of resultant calcium waves and validation of results by comparison to experimental data. The model will be used to test duct cell function and for the testing of pathological conditions. The overall project is funded by the National Institutes of Health, USA (Sneyd, Yule).

Current activity and results

Real biological samples were digitised using fluorescent markers and confocal microscopy. A sample image slice in which individual cell outlines can be seen is shown in Figure 1. The cell membranes are colour coded red and the interconnecting lumen is colour coded green. Note that the saliva secreted from the cells is transported through the assumed tube-like lumen structure.

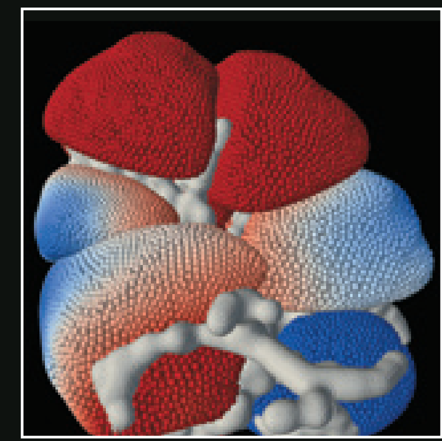


Figure 2: Full 3D mesh model of a cluster of cells.

The full collection of 32 images was used as the basis for a full 3D graphics model reconstruction of one cluster of cells as shown in *Figure 2*. The tube-like structure of the lumen can now be clearly seen. This anatomically correct model was used in turn as the basis for the creation of a 3D tetrahedral mesh suitable for finite element simulations.

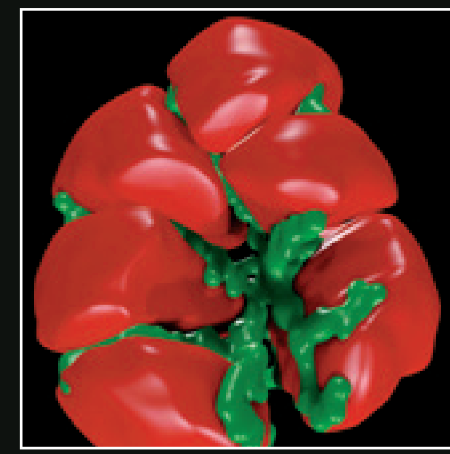


Figure 3: Simulation output snapshot.

The same underlying 3D graphics mesh was used in the animated visualisation of the calcium concentration simulation time series results. One time series frame is shown in *Figure 3*.

The NeSI Pan cluster at the University of Auckland was used for both graphics model rendering and running the finite element simulations.

"The Pan cluster is an ideal platform for the application in that it will also enable us to scale up the model to include many more cells." Dr John Rugis

What's next

As expected, simulation results for each of the cells differ somewhat. Further work will include a detailed analysis of how cell geometry affects the generation and propagation of calcium waves within each cell. We also plan to construct a larger model based on new digitisations using refined microscopy techniques.

Ground-motion simulations of earthquakes in the North Island of New Zealand

Seismologist Yoshi Kaneko of GNS Science has used an advanced 3D wave propagation code on NeSI's Power 6 supercomputer to simulate complex seismic wave propagation generated by earthquakes in the North Island of New Zealand.

With help from Dr Francois Bissey of NeSI's Computational Science team, Yoshi and his research colleagues simulate seismic waves from well-studied, local earthquakes to understand the influence of large-scale geological features on the resulting surface ground motions. The team constructed a computational mesh that includes surface topography, bathymetry and the latest 3D geological/seismological model of the North Island and the northern South Island. Without NeSI's supercomputer, they cannot run the software with a sufficient resolution.

"Without NeSI's supercomputer, we cannot run our simulations with a sufficient resolution."

In addition, the researchers have been developing a set of potential rupture scenarios for great earthquakes in the lower North Island. Since the Hikurangi subduction is potentially the largest contributor to seismic hazard in the lower North Island including the Wellington region, understanding physical factors controlling the levels of ground motions from destructive subduction earthquakes is critical for seismic hazard assessments.

A showcase of global research data initiatives

The recent 6th Plenary of the Research Data Alliance (RDA) brought together 603 experts in research data to coordinate and share their work. With a membership from 103 countries of 3200 individual experts and 39 institutional members working within 63 Interest and Working Groups, RDA has grown quickly within three years to become the most coherent organisation supporting the evolution of common research data capabilities internationally.

RDA, as a member-driven organisation, attracts experts from within research disciplines and across enabling functions. In producing recommendations on best practice on a specific topic, Working Groups within RDA expose the latest international thinking in any area, and as such are a rich source of relevant information.

Several sessions brought together thought and practice from national data services and infrastructures, of particular relevance to the formative National Research Data Programme in New Zealand.

Some of the key deliverables discussed, and in some cases released, at RDA Plenary 6 included recommendations on connecting datasets on the basis of co-authorship or joint funding, biosharing registries, repository audit and certification, practical policies, data publishing models and services, metadata standards directories and catalogues, and wheat data interoperability.

If the New Zealand research sector is to take advantage of the many opportunities on offer, we will need to grow our engagement with RDA's communities. If you are currently involved in research data projects or activities, please take a few minutes to look around the RDA communities and reach out to those involved, they are always keen to hear from new colleagues.

Quasi-2d Gallium Nanomaterials

Through an extensive series of computational simulations and analysis on NeSI's Pan and Foster systems, Dr Krista G. Steenbergen and Dr Nicola Gaston have recently unlocked the secret to greater- than-bulk melting of gallium nanoclusters.

Alongside silicon, gallium plays a major role in our modern technological world as a semiconductor component. It is a unique metal with many interesting properties, including how it melts.

Normal metals, such as alumunium or silver, melt at very high temperatures (650–950^0 C). A chunk of gallium metal, however, will melt in the human hand, needing less than body heat (37^0 C) to liquefy. At the nanoscale the intrigue continues: compared to larger chunks, smaller bits of matter typically melt at lower temperatures owing to a greater percentage of surface area which is more susceptible to temperature. However, a minuscule amount of gallium remains solid at more than 250^0 C. The origin of this strange "greater-than-bulk" melting phenomenon has long remained a mystery, making it difficult to technologically exploit.

Dr Krista G. Steenbergen (Massey University, Albany) and Dr Nicola Gaston (Victoria University of Wellington) have recently unlocked the secret to greater- than-bulk melting of gallium nanoclusters. Through an extensive series of computational simulations and analysis on NeSI's Pan and Foster systems, they discovered a counterintuitive quasi-two-dimensional (quasi-2D) liquid structure in nanoscale gallium. At the nanoscale, typical liquids adopt a spherical geometry as this geometry minimises the surface area. In gallium however, liquid nanoclusters prefer a flattened-elongated, quasi-2D structure that actually maximises the surface area.

On a practical level, the stability of the gallium surface structure has already found application in the growth of gallium nitride (GaN) films - where the stable gallium surface bilayer controls the kinetics of the film growth and results in improved morphology. GaN is a powerful semiconductor material used for high-performance transistors and integrated circuits. At a fundamental level, these findings solve a ten year-old mystery, and reveal the importance of both shape and dimensionality in the melting of nanoscale systems.

Fast cosmology with machine learning

Estimating the parameters of theoretical models using experimental data can be computationally intensive. Dr Grigor Aslanyan and his colleagues from the Physics department at the University of Auckland have developed a machine-learning algorithm that can greatly reduce the computational power required.

"What distinguishes our algorithm from previously developed similar tools is its ability to estimate and control the error it makes."

The machine learning algorithm uses the results of likelihood calculation to train itself, and after some training period is able to accurately approximate the likelihood function very rapidly for certain points in the parameter space, instead of doing the slow likelihood calculation.

Dr Grigor Aslanyan and his colleagues tested their algorithm on the standard cosmological model – more commonly known as the Big Bang theory.

The standard cosmological model is described by six parameters, which include the amount of dark matter and dark energy in the Universe as well as its expansion rate. Using the CMB radiation data, a likelihood function is constructed, which can tell which values of these parameters are more likely. "By probing many different values, we are able to determine the values of the parameters and their uncertainties from the data."

"The use of the NeSI computational resources was crucial for completing this project", explains Dr Aslanyan. "Since the main aim of our algorithm is to reduce the computational time of computationally very intensive problems, we would not be able to do any runs on a desktop. The cosmological example that we worked on typically requires a few days on about 50 CPU cores. We had to do many runs for many examples to be able to configure the details of our algorithm. Moreover, our algorithm is designed to take advantage of parallelism. Running the algorithm on many parallel nodes would have been impossible without the NeSI cluster."

"Our algorithm is designed to take advantage of parallelism. Running the algorithm on many parallel nodes would have been impossible without the NeSI cluster."

The evolution of single and binary stars

The evolution of a single star like our Sun is relatively well understood. While the very first computations of a star's evolution would take weeks to complete, today on NeSI's Pan cluster, a highly detailed model can define a star's entire evolution in about five minutes.

However only a quarter of stars are thought to be born as single stars, while half have a companion star and are in a binary system. The remaining quarter are in higher order multiples. The evolution of a binary star is different as the stars can get in each other's way and exchange mass and angular momentum, dramatically altering their evolutionary outcome.

"Today on NeSI's Pan cluster, a highly detailed model can define a star's entire evolution in about five minutes."

The Binary Population and Spectral Synthesis (BPASS) team, led by the University of Auckland's Dr JJ Eldridge and the University of Warwick's Dr Elizabeth Stanway, have been using NeSI's Pan cluster to model the evolution of stars, including that of seldom studied binary stars.

Until now the evolution of binary stellar systems has only been studied by a few groups, as this issue vastly increases the initial parameter space for the evolution of a star. This is due to the need to vary the initial masses of two stars and also the initial separation, as stars in tighter orbits are more likely to interact earlier in their lives than a wider binary. So, rather than requiring a few hundred models, something approaching a few hundreds of thousands of models are necessary. This would take approximately a year on a single desktop computer, but with NeSI's platforms it might take only a week to run the models, even after having to rerun different models because of any numerical problems.

Using NeSI's Pan cluster, the BPASS group have been able to create a detailed set of stellar models that include binary interactions. While the first version of the BPASS included only 15,000 stellar models, use of the cluster enabled the researchers to increase the resolution of their initial parameter grid by a factor of ten to nearly 200,000 models. This in turn increases the accuracy of the predicted stellar populations, which are now state of the art and have been made freely available on the web for astrophysicists to use.

Predicting druglikeness in new compounds

Scientists in New Zealand and overseas are always on the hunt for new drugs, both naturally-occurring and synthetic, to treat illnesses and chronic conditions. In recent decades, as computers have become more powerful and more readily available, scientists have been relying more on computational methods such as computer-aided drug design to identify drug candidates. These techniques are quick and relatively inexpensive per compound, so when it comes time to synthesise drug candidates we can focus our efforts and resources on those compounds most likely to be viable.

Besides the drug candidate's effectiveness in treating the target disease, we test for "ADME-Tox", which stands for Absorption, Distribution, Metabolism, Excretion and Toxicity. Even if a compound is shown to be extremely potent and effective in treating the disease, an unfavourable ADME-Tox profile means it is not a viable drug candidate. Perhaps the drug will just get flushed out of the body without being absorbed into the blood stream, or maybe it is absorbed too well and builds up in the body, or has unacceptably bad side effects.

When investigating a compound's ADME-Tox profile, one of its key physical properties is the compound's pKa, which is a measure of acidity. The lower a substance's pKa, the greater that substance's acidity (though a substance with a high pKa isn't necessarily a strong base, just a very weak acid). Strongly acidic compounds tend to be highly water soluble but unable to pass easily through membranes such as the intestine. They also pose toxicity problems. On the other hand, very weak acids are often highly insoluble in water and so will have difficulty being absorbed into the body, transported to the correct places, or excreted once their work is done. The goal, therefore, is to identify those compounds that fit the desired pKa range for any given application.

While a compound's pKa can be easily measured, this requires a physical sample which is often not available in the case of drug candidates that are being virtually screened. We are instead looking for a way to predict pKa values using computed data. One of the most significant components of a compound's pKa is its proton affinity, which is the energy needed to remove the most weakly attached hydrogen atom from a single molecule of the compound.

Computation of a proton affinity requires quantum-mechanical approaches, demanding much greater computational resources as the size and complexity of the chemical system increases. Once we started running our calculations on the NeSI clusters insteak of on desktops, we were able to greatly increase our throughput of new molecules as we could calculate the proton affinities of several molecules per day – a roughly 20-fold increase in research productivity.

Computational multiscale modelling of failure in flax fibre composites

Natural fibre composites (NFCs) using flax and hemp have seen increased adoption by European automobile manufacturers due to benefits such as reductions in weight, cost, and CO2, less reliance on foreign oil sources, and recyclability. However, low confidence in current failure estimation methods means that designs are not as efficient as they could be.

Structural application of NFCs requires more accurate failure prediction than what is currently available, and such predictions can be achieved through computational multiscale modelling.

Shyam Panamoottil, a PhD candidate supervised by Dr. Raj Das and Associate Professor Krishnan Jayaraman at the Department of Mechanical Engineering, University of Auckland created on a computational multiscale model to provide a means for more accurate failure prediction.

With the assistance of Gene Soudlenkov from NeSI's Computational Science team, the solutions for all the numerical models were performed using the Abaqus finite element software, combined with user-defined Fortran subroutines. Using NeSI facilities was essential for the two-scale coupling, since calls to the mesomodel from the Fortran code associated with the macromodel could not be performed from a local computer. Additionally, several iterations of numerical solutions to determine RVE sizes, and for mesh convergence were required.

"Access to the NeSI x86 Pan cluster meant that several of these jobs could be run simultaneously, with more resources available per job, significantly reducing the overall time required to obtain results by several months," says Shyam. "To date, 8417 core hours have been used, of which about 750 hours have been parallel jobs using 4 cores. Preliminary findings using low time step resolution show reasonably good agreement with the experiment data."

> "My two-scale simulations could not have been performed without the use of NeSI's HPC clusters."

Visualisation of Canterbury earthquake simulations

In September 2010 and February 2011, two major earthquakes caused widespread damage in Canterbury by ground shaking and liquefaction. 185 people lost their lives and the recovery cost is estimated to be as high as NZ$40billion.

Associate Professor Brendon Bradley of the University of Canterbury, in collaboration with Rob Graves from the US Geological Survey, has used parallelised software designed for 3D seismic wave propagation simulations on NeSI's BlueGene/P supercomputer to develop a sophisticated earthquake model which he then used to simulate all the events in the Canterbury earthquake sequence. This software uses fourth order spatial and second order temporal differences to solve the elastodynamic wave equation, and simulates wave propagations through the earth's crust resulting from earthquakes.

To aid understanding of output from the earthquake simulation, Dr Sung Bae from NeSI developed a visualisation workflow that converts the raw ground motion data obtained from the simulation to VTK (Visualization Toolkit) format, and visualises the ground motion on Canterbury's 3D landscape map.

This visualisation workflow has been successfully applied to the 2010 Boxing Day aftershock simulation. The simulated result of this event contained ground motion data of 67,200 points measured every 0.1 seconds (a total of 27 million measurements). Bae then produced a 40-second long video with NeSI's Visualisation Cluster.

Bradley's team has recently completed the simulation of Alpine Fault scenario using 8192 cores of BlueGene/P and the visualisation workflow is expected to lead to a better understanding of future major seismic events.

Understanding mechanical signalling in the microcirculation

A layer of proteins lining our blood vessels called the Endothelial Glycocalyx Layer (EGL) protects the vessel walls from potentially harmful levels of fluid shear stress. However, the EGL must also allow the vessel walls to receive mechanical information about the flow of blood in the vessel in order to trigger biochemical events.

A current hypothesis is that much of the mechanical load is carried through the solid portion of the EGL, rather than through its hydrating fluid. However, the fragile nature of the EGL has made this theory difficult to conclusively prove this idea in experiments.

> "Our computational challenges were significant and required the high performance computing facilities available through NeSI."

PhD students Pavel Sumets and Tet Chuan Lee investigated this idea, under the supervision of Dr Richard Clarke, Dr John Cater and Dr David Long at the Department of Engineering Science, University of Auckland. Since modelling the microstructure of the EGL in all its complexity is computationally infeasible, they adopted a volume-averaged macroscopic level description, using Biphasic Mixture Theory. In an attempt to represent physiological reality as closely as possible, the geometry that they have used in the simulation was informed by actual biological data obtained from colleagues Dr Jennifer Bodkin and Prof. Sussan Nourshargh at the Centre for Microvascular Research, William Harvey Research Institute, Barts and The London Medical School, Queen Mary University of London.

Dr Richard Clarke says, "The computational challenges were significant, and required the high performance computing facilities available through NeSI. For simulations using an idealised two-dimensional geometry, construction of the computational system was distributed across 96 cores, each requiring 1.5Gb of memory, with a total solve time of 600 CPU hours for each of the 10 physiological scenarios considered. For the three-dimensional simulations using the biologically informed geometries, each simulation required up to 30,000 CPU hours at the highest resolution."

This computational study will now be extended to incorporate some of the non-homogeneities associated with the EGL's geometry, as well as electromechanical effects. There is some debate around the extent to which these effects are important in allowing the EGL to recover its shape after being crushed by passing blood cells, as compared with elastic restoring effects. It is hoped that future computational studies will be able to help shed some light on this issue.

Manipulating the photon number: simulating a controlled interaction of light and matter

Victor Canela is doctoral candidate in physics at the University of Auckland studying a quantum optics system called a micromaser, or one-atom maser. Together with his supervisor, Prof. Howard Carmichael, they simulate a microwave cavity through which atoms transit and interact with the electromagnetic field inside.

Their current project focuses on the number of photons in the cavity, and how this evolves with changes to the atomic flux. In particular, the researchers wanted to produce sub-Poissonian fields with large photon numbers or states of the field with both high and a definite number of photons.

Numerically, the problem is no more complicated than solving a set of linear ordinary differential equations (ODEs) and in order to achieve the steady state solution a big number of time-steps in the order of 1010 must be completed to obtain sufficient averages of photon numbers.

> "Jordi Blasco and the NeSI Computational Science team enabled us to achieve over 600 times improvement in the speed of the simulation workflow."

The simulation ran successfully in the NeSI Pan cluster but reliability and speed was an issue. Jordi Blasco, a member of the NeSI Computational Science team, recommended that the compilers be switched from GCC to the Intel compilers and add guided auto-vectorisation flags. Without touching the code, the simulation then ran close to three times as fast.

Jordi also proposed transforming the problem into a highly decoupled problem with parameter switching workflow so as to run several independent trajectories at once. Rather than take around two or three weeks of serial CPU time, more than 100 trajectories could be run, finally providing a major impact in the wall-time by decreasing the whole simulation runtime by 100 times.

Continued close work with Jordi means the overall improvement in speed in the simulation workflow is now over 600 times, enabling researchers to probe regions of higher atomic fluxes and develop various mechanisms of active control to manipulate the photon number and produce sub-Poissonian states of the electromagnetic field with more than 50 photons.

With the optimised code, the researchers can now also include more sources of noise in the system such as spontaneous emission of the atom or a variable coupling between the atom and field, making the simulation more robust.

A new spatial model for estimating New Zealand soil carbon

Dr Stephen McNeill, Dr Allan Hewitt (Landcare Research), and Dr Andrew Manderson (AgResearch) lead a project that sought to build a model that estimates the total carbon content in the soil for every location over the landscape, as well as the uncertainty in the estimates.

Carbon content is a major factor in the overall health of soil and we know that humans strongly influence the amount of carbon in the soil through losses induced, for example, by tillage and erosion, and gains sustained by re-vegetation and changes in land-use practise.

The researchers used a method from data mining ("boosting") to find out the best set of map layers to predict soil carbon. Boosting is a method that can readily accept a large number of potential predictors of soil carbon, testing each predictor and their interaction in a systematic manner. This boosting method can be quite slow and provides a model that is difficult to interpret. So the result from data mining was used as a starting point for a conventional statistical model-building exercise, but it was a crucial step that drastically reduced the time taken to develop the final model for soil carbon.

A critical step in the research was the development of a model for the uncertainty of the soil carbon estimates, which is the range of soil carbon values within which one might find the "true" value of soil carbon, given some set of climate, terrain, and other landscape conditions. Model uncertainty is essential if the uncertainty or confidence estimates are needed in downstream agricultural and climate change models that rely on these soil carbon estimates. This model is currently being used in a collaborative project with the University of Sydney to develop fine-spatial-scale models of soil carbon; this work is funded under the Global Research Alliance (GRA).

One key diagnostic step in the generation of the soil carbon stock model was to confirm the distribution of the model coefficients. This can be done is to use a bootstrap analysis. Using this approach on a modern Windows machine this job was estimated to take about 21 days of computing time, which was not considered practical. Using the NeSI high performance computing platform 'Pan' at the University of Auckland, we were able to substantially reduce this time by implementing the bootstrap analysis in parallel. We used R with the snow package to allocate the various bootstrap iterations to R tasks, assembling the data in the calling task on return. Using this approach, the job was carried out over less than a day of computing time, and the subsequent analysis of the results confirmed the appropriateness of the soil carbon model developed.

> "Using NeSI resources we substantially reduced the compute time of our data analysis from 21 days to less than one day."

Improving the treatment of heart disease

One in four people will die from a blockage in one of the coronary arteries, preventing supply of blood and oxygen to the heart. A common treatment for narrowed arteries is 'Percutaneous Coronary Intervention' or PCI, where a stent is inserted into the narrowed blood vessel and expanded to hold it open. The expansion of the stent compresses the abnormal build-up of atheroma narrowing the artery. This is a highly effective and relatively low risk treatment, unfortunately, stents fail in 25% of patients, when the previous narrowing reoccurs within the stent.

Stents change blood flow, which in turn alters the growth of tissue, and thereby affects treatment outcome. Currently, there are more than 250 different stent designs available, each of which has a different effect on the 3D pattern of blood flow. The stent design is therefore critically important in determining treatment success or failure.

> "Improving stent design by measuring the impact on blood flow may significantly reduce stent failures and ultimately save lives."

Clinical trials with groups of patients have been unable to define the stent design features which determine success or failure due to the complexity of the problem.

Susann Beier, a PhD candidate in Faculty of Medical and Health Sciences at the University of Auckland conducted on the link between stent design features, the changes they cause in blood flow (haemodynamics), and the impact on patient outcome.

Computational Fluid Dynamic (CFD) modelling was used to quantify the haemodynamics for various stent designs. This allowed the calculation of blood velocity, the stress the blood flow induces on the vessel wall, and to detect regions of rapid changes by simulating the vessel shape, circulation and blood rheology. Two commonly used stent designs were modelled to determine their respective strengths and weaknesses.

Each simulation contained approximately 20 million elements, and used multi-threading over six cores with 40CPU with 20GB memory each, and took around 48 hours to solve. This task would have not been possible without the use of NeSI's Pan cluster, as the memory requirements would have exceeded local desktop capabilities well before a possibly month long solution was obtained.

Due to having access to the Pan platform we are now extending our research to more complex vessel geometries such as vessel branching. Having gained a greater understanding of the features that are critical to idealised stent design, the next milestone is to model a stented coronary artery from an actual patient. This is a highly complex undertaking but the knowledge that can be gained will have an important impact in the treatment of patients with heart disease.

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