NCI AUSTRALIA

ANNUAL REPORT

2016 2017

WORLD-CLASS HIGH-END COMPUTING SERVICES FOR AUSTRALIAN RESEARCH AND INNOVATION

The report is also accessible from the NCI website at www.nci.org.au

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Cover Image: *An overhead view of the Canberra city centre, visualised using a point cloud made with the Australian Capital Territory Government's publicly available LiDAR dataset. The high resolution LiDAR data allows viewers to distinguish individual trees and buildings, and enables uses from environmental management to urban planning. The point cloud was visualised by Dr Ajay Limaye from NCI's VizLab.*


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NATIONAL COMPUTATIONAL INFRASTRUCTURE

CONTENTS

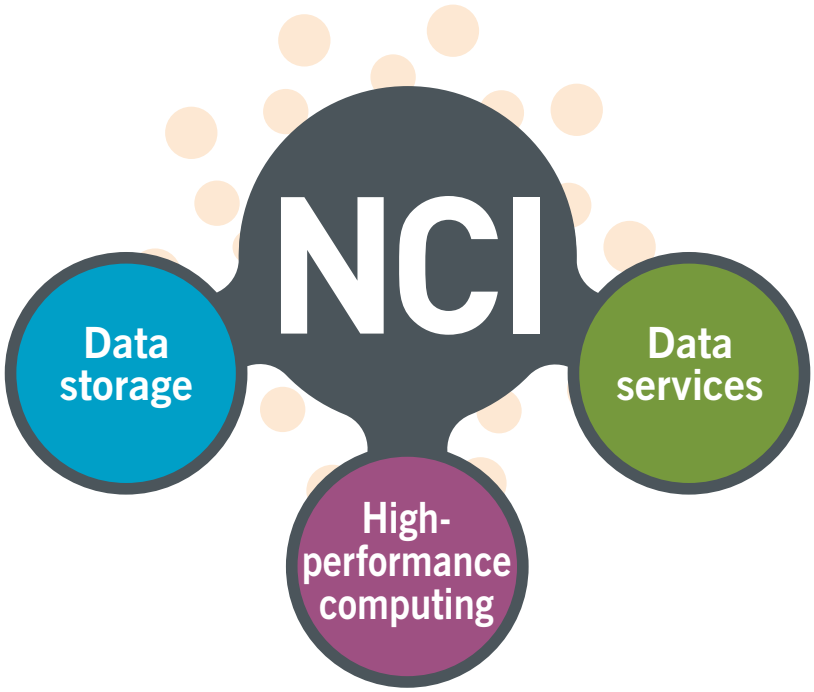
Our Mission

The National Computational Infrastructure (NCI) is a core part of Australia's advanced computing landscape. We are the leading organisation providing nationally integrated high-performance data, storage and computing services to Australian science, government and industry. Driven to raise the ambition, impact and outcomes of Australian research, NCI delivers on national priorities and research goals from across the scientific disciplines.

The National Science and Research Priorities developed by the Federal Government indicate the key areas for the nation to focus on in facing our biggest challenges. Through the National Collaborative Research Infrastructure Strategy (NCRIS), the Australian Government also provides world-class infrastructure to the research community. As an NCRIS facility, and through our focus on these priorities, NCI supports the most valuable research activities from across Australia.

NCI achieves its mission by bringing together the Australian Government and the Australian research sector through a broad collaboration involving the largest national science agencies, universities, industry and the Australian Research Council (ARC).

The wide variety of organisations that use our services speaks to NCI's national and strategic value. By combining the shared responsibilities of the Australian Government and the research sector in this highly integrated scientific computing facility, NCI provides world-class services to thousands of researchers every year. Our combination of infrastructure and expertise enables high-impact research and innovation that is otherwise impossible to undertake. It also delivers outcomes that inform and benefit public policy, and supports an internationally competitive research environment that attracts and retains leading researchers in Australia.



We are home to one of the nation's most powerful supercomputers, the nation's highest performance research cloud, some of its fastest filesystems and its largest research data repository. Our staff are renowned nationally and internationally for their expertise.

Since our early days as the Australian Partnership for Advanced Computing, established in 1999, NCI has been the leader in Australian high-performance computing. Today, our internationally recognised compute and data services continue to support Australian science from theoretical development through to commercialisation.

Our Objectives

Our objectives drive us to deliver transformational outcomes for Australian society, policy, industry and the environment.

- NCI is research- and outcomes-driven, innovating and evolving our service portfolio to deliver on researchers' requirements, institutional research needs, and national research priorities.
- NCI delivers a national benefit by enhancing the outcomes of individual research projects and longer run research programs undertaken by government, science agencies, universities and industry from across the country.
- NCI's research-driven agenda is underpinned by deep engagement with a broad range of research organisations, centres and communities across Australia and the world, which drives the relevance, agility and value of its services.
- NCI's infrastructure, expertise and experience deliver transformational outcomes that are on par with the world's best and, in some cases, are world-leading.

NCI is Australia's leading facility for scientific computing. By integrating all the elements required for compute- and data-intensive science within one organisation, we provide an unmatched service to the Australian research community. From highly compute-intensive research to the most interactive virtual data manipulations, NCI underpins many important Australian scientific research advancements. The services we offer are continually being improved, with world-leading innovations extending the possibilities for new kinds of research.

By providing high-performance computing, digital research environments and data services under one roof, NCI brings to the research community an all-in-one resource for Australian science. From the integration of the latest many-core and GPU accelerator technologies into our operational system, to the creation of leading data access platforms, NCI caters to all kinds of scientists and all kinds of research.

As Australian research becomes ever more reliant on computational methods, a reliable and innovative high-performance computing platform is required. That is why NCI is pushing the boundaries of what high-performance computing (HPC) and high-performance data (HPD) facilities can offer. The colocation of petabyte-scale data storage with a petaflop supercomputer is critical in making data science innovation possible for Australian research.

NCI is the backbone of many e-research tools: bridging the gap between data and compute, and opening up new opportunities for research engagement from broader sections of the scientific community. As a consequence, people working in industry, in small organisations, and in local councils can all make use of publicly available data resources for their own specific needs.

NCI is a highly integrated, advanced computing facility, dedicated to enabling research that benefits Australia and its national science priorities. By providing high-performance computing, data storage and data services under one roof, NCI brings an all-in-one resource for compute and data-intensive research to the Australian community.

Chair's Report

It is my pleasure to welcome you to NCI's 2016–17 Annual Report. This has been a significant year for NCI.

In May, we farewelled Professor Lindsay Botten, who retired after seven years as Director. During that time, NCI established itself as Australia's most integrated high-performance and data research service. Fittingly, the acquisition and deployment of a Lenovo cluster, funded by a $7 million grant from the NCRIS Agility Fund, saw NCI named again the fastest supercomputer in Australia, ranking 70th on the Top500 list released in June. Lindsay's legacy is not only significant for NCI but for Australian research that relies increasingly on high-performance computing and data services.

Lindsay will be succeeded by Professor Sean Smith, who will commence as Director in January 2018. Professor Smith, an internationally prominent computational chemist and nanomaterials scientist, is currently Founding Director of the Integrated Materials Design Centre at UNSW Sydney. Not only has he been a major user of NCI in his own right, but he will also bring to NCI his highly relevant international experience of the Oak Ridge National Laboratory user facilities.

Until Professor Smith takes up his appointment, the Board was extremely pleased that Dr Chris Pigram, the former CEO of Geoscience Australia and an NCI Board member, was willing to step in as Interim Director. Chris's detailed knowledge of the Government bureaucracy is proving particularly useful since the major issue facing NCI is the urgency around a replacement for the main compute facility, Raijin.

While the Australian Government's *2016 National Research Infrastructure Roadmap* explicitly recommended the urgent replacement of the ageing supercomputers at NCI and Pawsey, no action has yet been taken to implement this recommendation. Given the procurement of supercomputers can take at least a year, this hiatus is of increasing concern since Raijin will reach the end of its operational life at the end of 2018.

The criticality of NCI to Australian research was further demonstrated this year by two new Flagship Scheme partners: the ARC Centres of Excellence in Future Low-Energy Electronics Technologies and in Exciton Science.

In December, NCI became the first Australian organisation to join the OpenPOWER Foundation, a global open technical community enabling collaborative development and industry growth. This is a testament to NCI's world-class standing.

Meanwhile, we have completed our major three-year collaborative project with Fujitsu to optimise ACCESS – the numerical weather and climate modelling suite used by researchers and government agencies across the country. The project outcomes have been impressive, including a 40% improvement in the overall performance of the current Australian Bureau of Meteorology forecast system, which delivers the nation's official climate and weather predictions. This outstanding result is indicative of the skill and expertise of NCI's staff.

I would also like to offer thanks to my fellow Board members for their dedicated service.

Emeritus Professor Michael Barber FAA FTSE, Chair, NCI Board

Director's Report

Since taking up the helm as NCI Director in May 2017 after the retirement of long-serving Director Professor Lindsay Botten, I have been impressed by the depth and breadth of the expertise and skills of NCI's staff. NCI is at the forefront, both nationally and internationally, of integrated supercomputing and data service environments – in large part a product of our dedicated and innovative technical and service teams.

The past 12 months have seen NCI's data services thriving (read more on page 36). The tireless work of our data services teams means the fruit of decades of publicly funded data gathering is now easily searchable online in one place.

NCI has made this data accessible to our users through a number of methods using NCI's National Environmental Research Data Interoperability Platform (read more on page 36), including direct access through NCI's supercomputer. These services are already in use supporting, for example, the Nectar Science Clouds and Virtual Laboratories programs, the Climate and Weather Science Lab, AuScope's Virtual Geophysics Laboratory,

HIGHLIGHTS OF OUR YEAR

Data Intensive Workshops, SC16 @ Salt Lake City

Announcement of $14 million Agility investment in NCI

2016 JULY AUGUST SEPTEMBER OCTOBER NOVEMBER DECEMBER

Intel Xeon Phi 'Knights Landing' CPUs installed

NCI joins OpenPower Foundation

and Digital Earth Australia (formerly known as the Australian Geoscience Data Cube).

Curating and making these petabyte-scale data collections available to Australian researchers was a key objective under the Australian Government's NCRIS RDSI/RDS project and is a tribute to the skills of NCI's committed staff.

Of course, our staff and users are supported by world-class infrastructure. This year our supercomputer received several hardware enhancements, including new Graphics Processing Units and an approximately 22,000 core Intel Broadwell Agility System. These changes represent a 40% capacity increase. NCI's global parallel filesystems were also upgraded this year to a combined total of 22 petabytes.

These augmentations to NCI's supercomputing and storage capabilities were made possible by a $7 million contribution from the Australian Government's NCRIS Agility Fund, matched dollar-for-dollar by the NCI Collaboration, a testament to NCI's role in the national R&D agenda and the value our partners place in world-class high-performance computing services.

I would like to take this opportunity to sincerely thank the NCI Board and my senior colleagues for their insightful guidance; the NCI staff for their dedication and work ethic; and of course all the people who use NCI's facilities and services and whose research goals shape and validate our existence.

Dr Chris Pigram
Interim Director, NCI

NCI adds ~22,000 core Intel Broadwell Agility System

/g/data1 updated with all new Fujitsu/ NetApp and HPE systems

Conclusion of NCI-Fujitsu ACCESS Code Optimisation project

Knights Landing Users Workshop from Intel

JANUARY

FEBRUARY

MARCH

APRIL

MAY

JUNE

2017

NVIDIA Pascal GPU nodes added

HPC Summer School

ISC17 @ Frankfurt

NCI named fastest supercomputer in Australia

Research Outcomes and Impact

1

National Benefits

NCI is a crucial component of the research process for thousands of Australian projects. Those projects span every scientific discipline, and go from pure research all the way through to direct industry applications. Our software and hardware infrastructure creates a place where the ambitious ideas of genomics, environmental science, chemistry and engineering can be investigated. The solutions we offer to researchers have a direct national benefit, helping advance the National Science Research Priorities through projects with highly impactful outcomes.

Addressing the National Priorities – Food, Soil and Water, Transport, Cybersecurity, Energy, Resources, Advanced Manufacturing, Environmental Change and Health – we support and enable projects that have an impact on people's everyday lives. NCI's work is in providing an integrated platform for thousands of researchers, and underpinning millions of dollars of investment in national research. NCI strives for a continual improvement of our national data access and analysis tools, making our huge data collections more useable and useful than ever before. These advancements go hand in hand with our high-performance computing systems, which continue to enable world-leading findings.

Research projects based at NCI touch on many of the Australian Government's major portfolios. Sitting within the Department of Industry, Innovation and Science, the nationally significant Australian Community Climate and Earth System Simulator (ACCESS) relies heavily on NCI systems and expertise for its extensive development. Similarly, the Copernicus Data Hub, managed by Geoscience Australia and hosted at NCI, provides the Australian

community with access to the latest satellite imagery from the European Commission.

Starting in 2016, with NCI as a national partner, the Australian Genomics Health Alliance (AGHA) aims to prepare Australia for the use of genomics in research and medicine. The AGHA's mission directly aligns with the Department of Health and the National Research Priorities, and its Data Federation and Analysis Program relies heavily on NCI. By taking advantage of the scalable computing and data infrastructure available, and by using secure data repositories in situ at NCI, the AGHA shows clearly how NCI can benefit Australian research. A list of the Government portfolios impacted by projects at NCI can be found in the Appendix, on page 90.

Applying HPC to Satellite Earth Observations

The Australian Geoscience Data Cube (AGDC) is a novel collaborative approach from Geoscience Australia, CSIRO and NCI for generating vast volumes of satellite earth observation and other geospatial datasets at the continental scale.

Soon to be replaced by the Australian Government-supported Digital Earth Australia program, the AGDC builds on 35 years of Landsat earth observation, and has evolved into a sophisticated system for managing and analysing varied earth observation datasets. This allows researchers to visually track changes in the Australian landscape – including bushfires, flood paths and land clearance – yielding valuable insights for agriculture, environment and resource management, and a variety of information products of value to industry.

The AGDC gives Australia a world-leading edge in the management of environmental data, and is the first time anywhere in the world that an entire continent's geographical and geoscientific attributes have been made available to researchers and policy makers– an achievement recognised by the AGDC winning the Content Platform of the Year at the 2016 Geospatial World Leadership Awards.

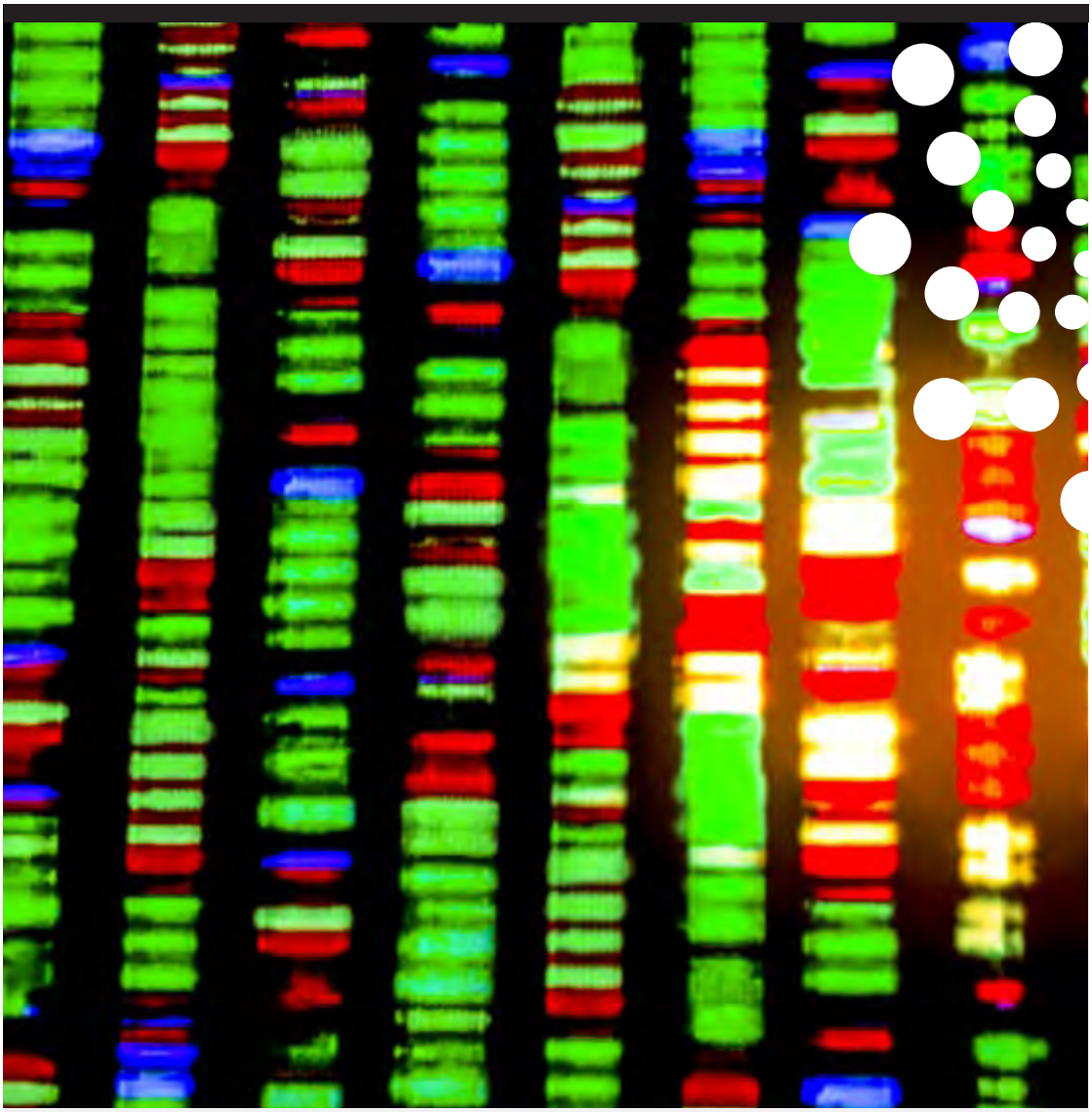
NCI's integrated high-performance computing and storage platform, along with its expert data services team, provides the high-performance infrastructure and the capability needed to process and analyse petabyte-scale datasets.

Before the creation of the AGDC, satellite imagery and other geospatial datasets were downloaded, analysed and provided to users on a custom basis–a lengthy, high-cost approach that could only be used for a single purpose each time. Rapidly processing large data sources into usable products, such as bringing analysis time from months down to hours for the award-winning Water Observations from Space project, makes the

previously impossible task of continental scale analysis now achievable.

Through its access point via NCI's NERDIP platform (see page 36), this data is widely available to the research community, allowing investigators to gain new insights into the Australian landscape as it changes over time. The new datasets support modern techniques for advanced analysis and use in agriculture, environment and natural resource management.

This Australian technology has opened up international partnerships, with development now taking place on the world stage. The underpinning satellite data is prepared by the same open source Open Data Cube technology that the AGDC is based on, and this has now been adapted for use in countries such as Cameroon, Columbia and Kenya. This extends its reach well beyond its original Australian application by local agencies, such as the Murray-Darling Basin Authority.



Thousands of genomes prepared for clinical use

In late 2016, biologists from the Garvan Institute of Medical Research and The Australian National University's John Curtin School of Medical Research took 1,206 human genomes and, in one night of computation at NCI, realigned them to the human reference genome and identified the genetic variations they contained. Genome alignment is a technique for stitching together the many snippets of the genomic sequence that are produced by sequencers in the lab. There are millions of such snippets in any sequenced genome, and altogether they make up a file around 50 gigabytes in size.

The alignment process involves many steps and requires the computer processors involved to be constantly reading and writing new data from the genomic dataset into hard drives. As such, the entire process is constrained by the speed of those hard drives and the filesystem that manages the storage. Typical computational setups might manage to do around 30 alignments at a time, so the fact that 1,206 could be done at once at NCI was truly groundbreaking.

NCI's high-performance filesystems, which include the two fastest in the Southern Hemisphere, are used to store all kinds of data, from Earth observations through to astronomical modelling. In the case of human genomics, the filesystems make it possible for genome alignments to be done as fast as possible. Genomics is one of the computational tasks that is the most reliant on rapid communication between the filesystem and the processors.

Dr Dan Andrews, Program Manager at the NHMRC-funded Australian Genomics Health Alliance (AGHA), says "The combination of vast computing capacity coupled with the finely tuned fast storage that NCI provides helped us scale up the software to work with more than 1,200 genomes at once. Aligning that many genomes in one night is a clear demonstration of the NCI computational capacity - that couldn't have been done elsewhere in Australia."

The genomes came from Garvan's Medical Genome Reference Bank (MGRB), supported by the AGHA. The MGRB is a groundbreaking database of human genetic information that will comprise more than 4,000 complete human genomes from disease-free seniors when complete.

Once the genomes are all assembled in the database, researchers and clinicians can query the fully anonymised information. To get to that stage, though, the genome sequences need to be aligned in a supercomputer. Working with this many genomes makes it impossible for an individual laboratory to deal with the data on its own. Instead, NCI provides the high-performance data and compute infrastructure that makes it possible.

As the field of computational biology develops, the improved software and knowledge gained through research such as this will allow hospitals and clinics to incorporate genomics into their daily operations. The use of genomics in medicine brings a huge potential for faster diagnosis and treatment of rare diseases. NCI is proud to be a part of the crucial early developments that will make this possible.

Impactful Science

Researchers turn to NCI to advance their projects because the varied computing and data innovations we provide are not found anywhere else in the country. This makes NCI the home of some of the most impactful science in Australia, and a key factor in hundreds of important scientific developments each year.

The science that comes out of NCI is due in part to the large number of national agencies, universities, medical research institutes and industry groups that form the NCI Collaboration. Together these organisations provide more than 6,000 researchers every year with compute resources, and many thousands more with access to data collections and the tools to analyse them.

We are helping to develop the capability of the university sector, home to much of Australia's research activity, in efficient use of high-performance computing resources. Many scientists can benefit from using such a facility, and dedicated workshops and training sessions run throughout the year are designed to teach both basic and advanced uses of the NCI facility.

The NCI Collaboration opens high-performance computing up to more Australian researchers, but for those who are not part of a participating institution, we also provide access to resources through the National Computational Merit Allocation Scheme. This annual, open access scheme lets researchers from any publicly funded research organisation apply for computational resources on the country's high-performance computing platforms, including NCI, the Pawsey Supercomputing Centre, MASSIVE and Flashlite. For 2017, NCI provided more than half of the total resource allocation, totalling more than 110 million hours of computation spread across 157 projects.

NCI continues to develop partnerships across the scientific research space (see Growth in the NCI Partnership on page 21), with the aim of reaching even more users and facilitating their interactions with the data collections and computing systems in new ways. As data science becomes more prevalent across all domains, new researchers stand to benefit from having access to well-managed and highly curated data collections. At the same time, they have a growing need for the specialised computational resources to analyse it all.

By providing all these capabilities integrated within one facility, NCI is enabling research in new ways, developing researcher skills, contributing to our international competitiveness and bringing about impactful science outcomes. The case studies throughout this report highlight significant new findings with clear future benefits for Australian industry and society.

Awards

NCI user Professor Carola Vinuesa has been named as part of the team that secured the NHMRC's top Project Grant application for 2017. Her research is internationally recognised, pioneering the use of personalised medicine to tailor treatments based on the genetic sequences of patients.

NCI user Professor Michelle Coote has been awarded a 2017 ARC Laureate Fellowship to develop new classes of chemical catalyst for assembling complex molecules and materials. The aim is for the catalysts to provide significant practical benefits to industry.

Building a new global tsunami model

Every few years, tragedies on coastlines around the world remind us of the risk that we face from tsunamis. The 2011 Tōhoku earthquake and tsunami demonstrated just how vulnerable we are, and that research is required to better understand the risks we face.

With help from NCI, Geoscience Australia (GA) has recently developed a Global Probabilistic Tsunami Hazard Assessment (PTHA) in collaboration with an international team of tsunami hazard scientists. This is a computer model that simulates thousands of different earthquake-generated tsunami scenarios around the world. It covers most of the world's coastline, giving vital information about which countries and regions are at risk from tsunamis.

The PTHA model considers thousands of different earthquake-generated tsunami scenarios and their probabilities of occurring. Statistical analysis of the suite of scenarios allows estimation of the likelihood of a tsunami of a particular height hitting the coast anywhere in the world. With this kind of information, tsunami hazard scientists can look further into the high-risk areas and do more detailed modelling to support national and local scale risk reduction measures. The work is also useful to global institutions such as the United Nations Office for Disaster Risk Reduction, which needs consistent global analyses to help understand the global-scale

exposure of nations to natural hazards and prioritise risk reduction efforts.

Dr Gareth Davies, a hydrodynamic modeller from GA involved in producing the PTHA, says, "This model gives us a global picture of tsunami hazard, something that we have never had before. With a better understanding of the global distribution of tsunami hazards, we can prioritise regions for further high-resolution studies, and ultimately, contribute to tsunami risk reduction measures which reduce the impacts of tsunamis on society."

Because the model needs to be run thousands of times to make the statistics robust enough, each time with slightly different parameters, the computing power required is beyond a small-scale computational system. Instead, to simulate the approximately 20,000 scenarios that make up the PTHA, GA uses NCI to do the equivalent of 2,500 days of computing, all over the span of a few days. By using many processors simultaneously on NCI's systems, GA can produce all the data they need to put together their rigorous hazard assessment.

Davies says, "This global PTHA could not be run without access to NCI's infrastructure. The high-performance computing systems make it possible for us to run complex algorithms at a global scale. The data we've produced here is already being used to help guide our future tsunami work."

The data output from the PTHA is a combination of tsunami wave run-up height and earthquake frequency estimates, which together give an estimate of the likelihood and potential impact of a tsunami hitting the coast at any one time. That picture of tsunami hazard produced by the PTHA helps identify where higher resolution localised studies would be most helpful. These can then help governments and planning authorities with important decisions about how best to develop or secure coastal areas.

The partnership between GA and NCI is what enables innovative and impactful research outcomes. By connecting researchers with the advanced computing infrastructure that they need, we make possible previously unattainable findings.

Growth in the NCI Partnership

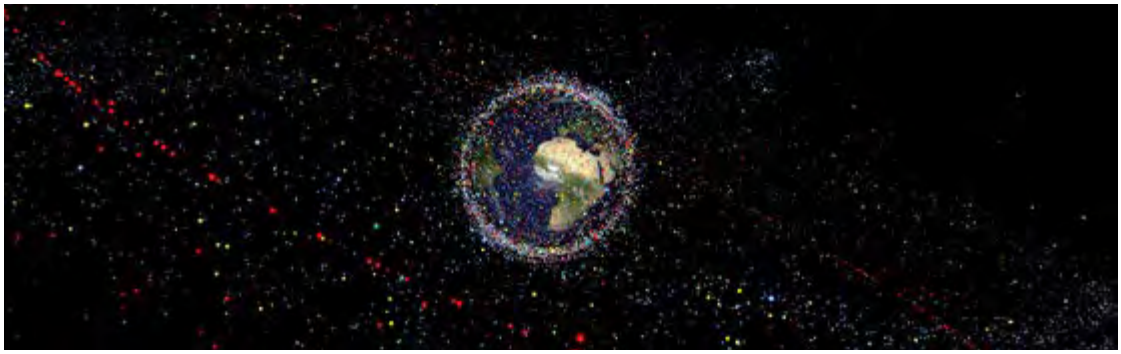
Since the launch of the Raijin supercomputer in 2012, a key part of NCI's operational model has been the NCI Collaboration. Starting with a membership of three – the ANU, the Bureau of Meteorology and CSIRO – the Collaboration has since grown to include more than 20 partners, including universities, national science agencies, research institutes and Collaborative Research Centres. The Collaboration provides the majority of the funding required for the day-to-day operation of NCI's high-performance computing and data activities.

The Collaboration is crucial in providing ongoing cutting-edge computational platforms to scientists all over the country, and the continuing growth in the number of partners demonstrates the increasing demand for NCI services throughout the scientific research sector. This is a testament to the high quality and reliability of the NCI systems, and the breadth and depth of the expertise of its staff. It also highlights the need for such computing resources to be increasingly available to Australian researchers over the coming years.

The 2016 update to Raijin was funded by the Australian Government's NCRIS Agility Fund and a dollar-for-dollar matching contribution from the NCI Collaboration. This investment, and the Collaboration's commitment to supporting the growth of HPC for their researchers, highlights the importance of having a network of similarly focused institutions working cooperatively on advanced data and computing systems.

NCI also provides support to nine Australian Research Council Centres of Excellence through our Flagship Scheme. This gives nationally recognised research groups with a commitment to high-impact science in Australia access to supercomputing resources at a fraction of the cost of alternative commercial arrangements. This year, the new Centres of Excellence in Future Low-Energy Electronics Technologies (FLEET) and in Exciton Science join the six continuing Flagship Centres – the Centres of Excellence for All-Sky Astrophysics, Climate System Science, Electromaterials Science, Particle Physics at the Terascale, Nanoscale BioPhotonics and Ultrahigh Bandwidth Devices for Optical Systems – to share in 25 million compute hours on NCI's HPC systems. The new partners have a clear future-focus, looking at nanoscale electronics and at the various ways they might be used in the future to improve our computing and communication systems.

We have also continued to expand our support for the growing field of human genomics. Through our support of the NHMRC-funded Australian Genomics Health Alliance (AGHA), a growing dataset of genomic information is now becoming available to researchers across the country. NCI plays a key role in the AGHA's data management and analysis research program, helping to develop new ways of securely storing and providing access to sensitive datasets.



An image of the human-made space junk around the Earth, from the European Space Agency.

Solutions for cryptography in the quantum age

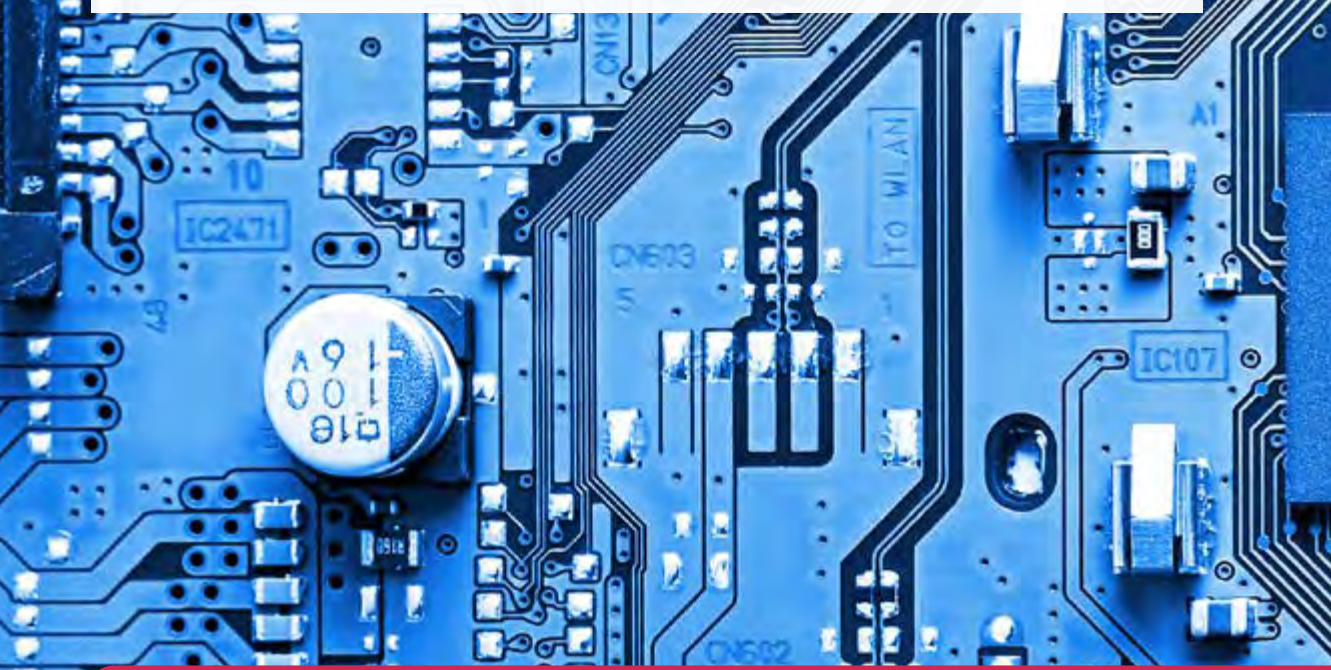
The future of computing is quantum computers, a new kind of machine that will be able to do calculations in completely different ways from the computers we are used to. This will open up new doors for research, technological development and deep learning, but will also mean a shift in the way computers communicate securely between themselves.

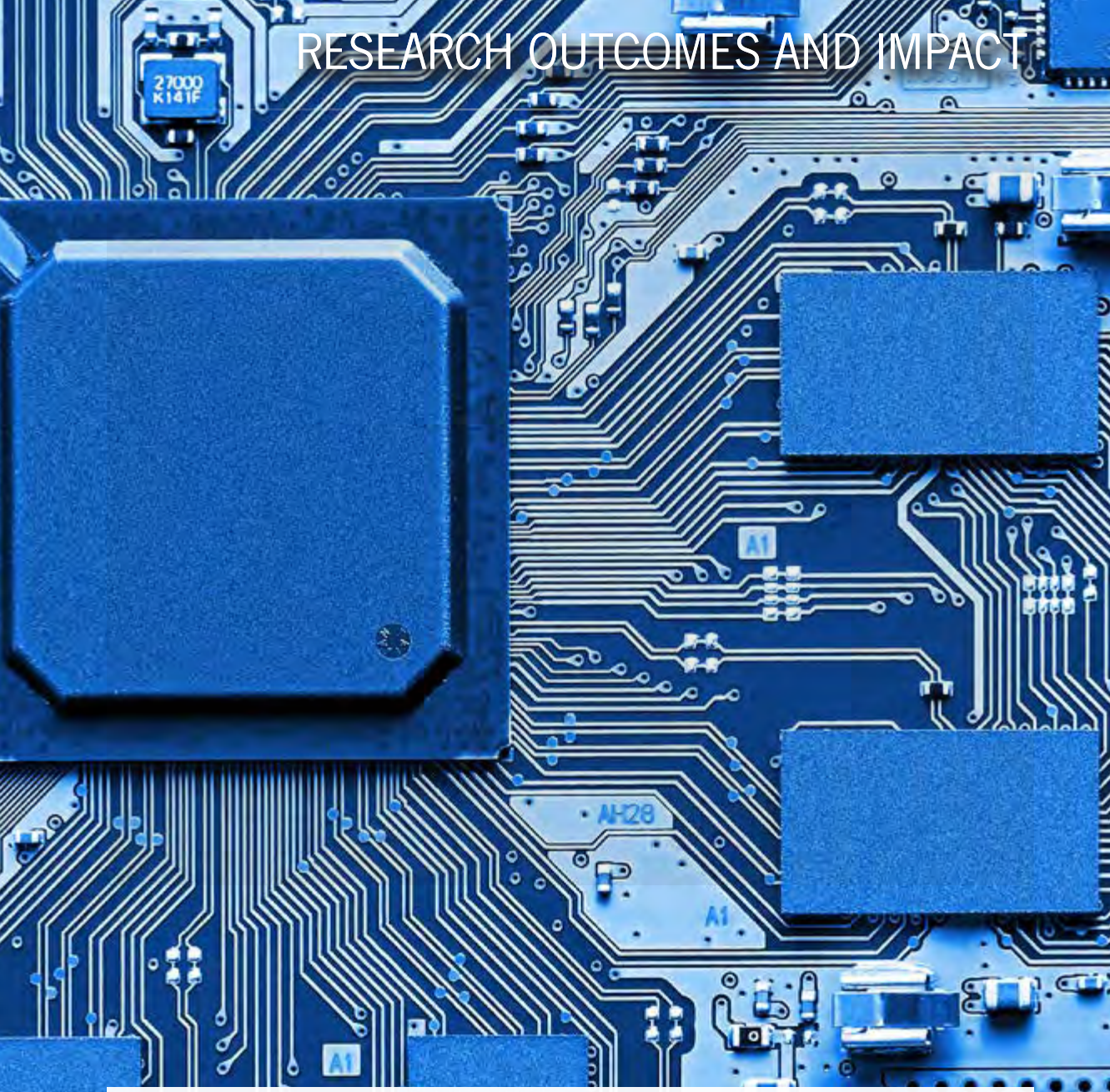
Specifically, quantum computers will be able to break through the encryption systems we currently use to communicate securely over the internet. This means that bank transactions, data transfers and private communications could all become easily accessible to someone with a quantum computer.

The challenge for researchers in the field of cryptography is to find new ways of encrypting internet communications, ways that are resistant to quantum computers. Dr Thomas Plantard from the University of Wollongong is working to understand a new kind of cryptography we might use for this, based on large lattices. Lattices are large grids of numbers, and will be a key part of future encryption processes.

Dr Plantard uses NCI's supercomputer to test the various ways that lattice problems can be solved by quantum computers, alongside standard computers. By tweaking the variables and optimising his codes, he can find a lattice size that will be suitably resistant to quantum computer solving.

A bigger lattice is better, but if it is too big then the encryption and decryption process becomes too hard for the devices on either end of the communication to handle.





That is where high-performance computing can help his research: it gives him practical results that can help him understand the theory underlying his codes. He says, "The next few years will be crucial for the development of these quantum-resistant systems. We have to do the work now so that we can implement these solutions before quantum computers become more common."

While still in early development, quantum computers will have a big impact on certain sectors of the research-computing world. Getting ahead of them in designing security systems is critical in maintaining the secure communications we are used to today.

Innovations Enabling New Science

2

Sediment-filled floodwaters near the Junee State Forest 120 kilometres northwest of Rockhampton during the 2017 Queensland floods. Processed by the European Space Agency using modified Copernicus Sentinel data - CC BY-SA IGO 3.0

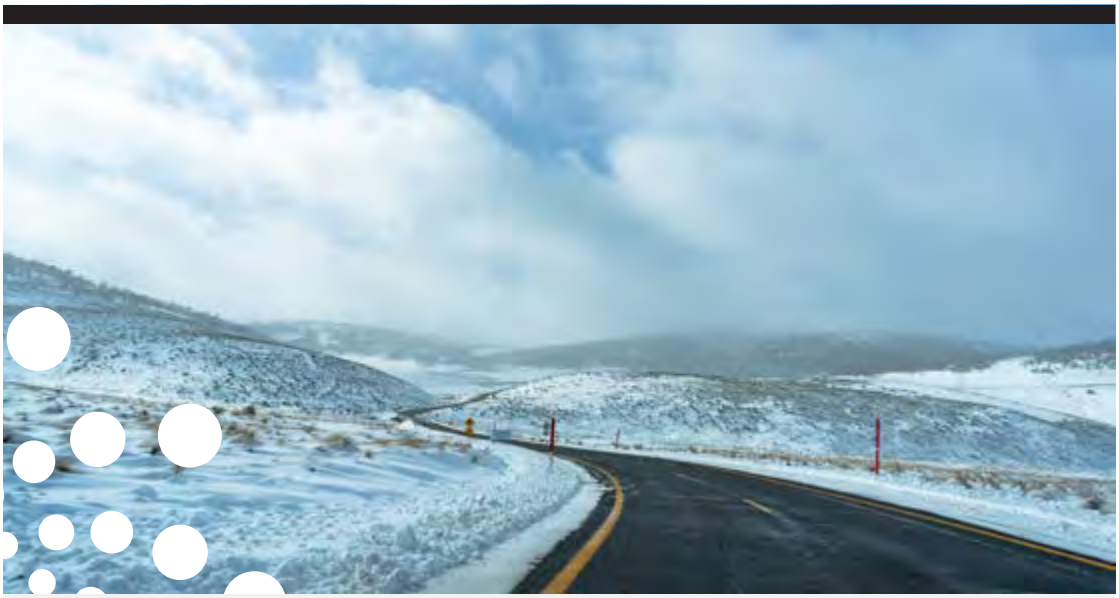
Computational Science

NCI is well placed to address nationally significant grand-scale computational challenges that require the full capability of the biggest HPC environments. Targeting both simulation/modelling-intensive and data-intensive applications, this work aims to transform leading scientific applications to take better advantage of HPC resources. The work has focused on community-identified cases with requirements to improve performance, all while increasing modelling resolution or large-scale data communication for processing, assimilation or analysis.

Improvements in application performance come not only from investing in the latest technology, but also come increasingly through optimising and modernising the software code. The scale and complexity of the needed transformation means that ongoing dedicated investments in software, algorithms and overall improved numerical methods are now essential for making progress to meet current and future requirements. The modified software is then fed back to the relevant modelling community, who can take advantage of the improvements and apply them to their growing list of use-cases and products.

NCI's work has focused on the priority science areas for our partners, and particularly those which contribute to important societal outcomes. These include:

- Climate modelling and Numerical Weather Prediction, including in support of ACCESS, the Australian Community Climate and Earth System Simulator, (see case study below) and the development of the Bureau of Meteorology's advanced Storm Surge Forecasting System (see case study on page 29)
- Geoscience modelling and simulation, and the analysis of significant datasets of natural resources in the Australian region
- Earth observation data analytics for a range of applications, including many for government-related policy-directed outcomes
- Bio-informatics pipelines that leverage the significant investment in genomics research and instruments and their increasing need for computational and data analysis.



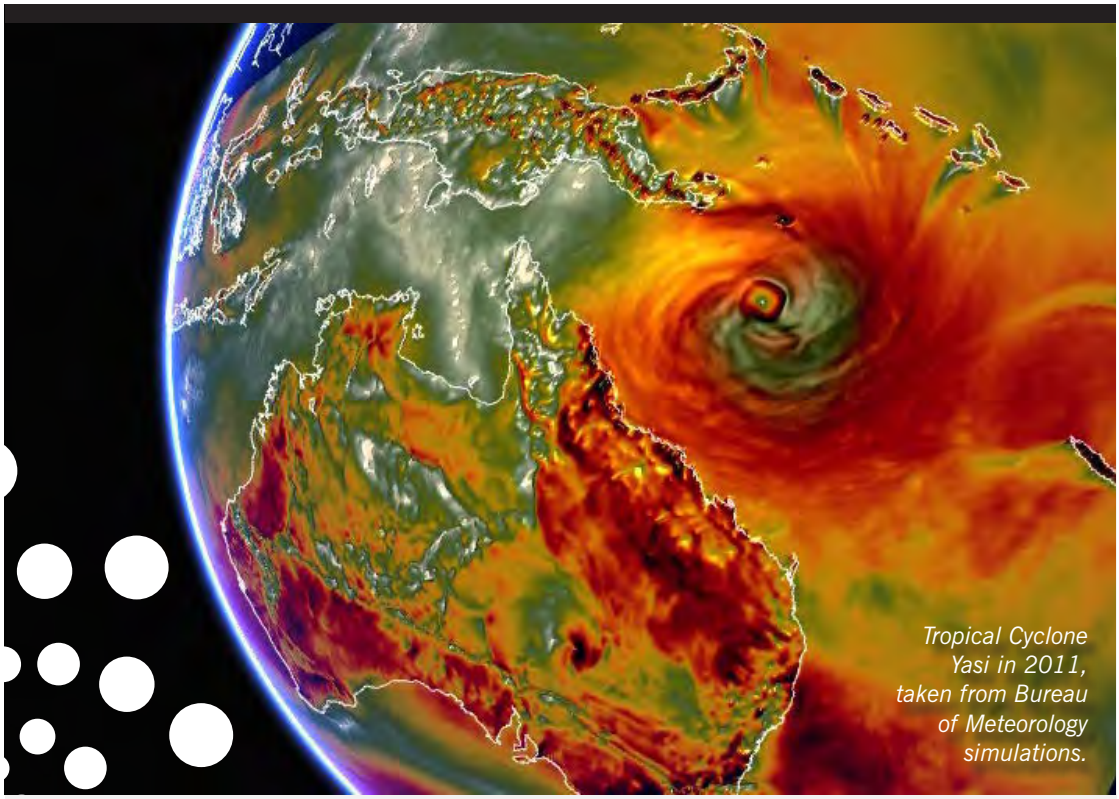
Improving Australia's weather predictions

The Australian Community Climate and Earth System Simulator (ACCESS) is Australia's national weather forecasting and climate prediction system, providing world-class modelling infrastructure to the Bureau of Meteorology, CSIRO, the ARC Centre of Excellence for Climate System Science and other university researchers around the country, as well as global collaborators.

The role of NCI, as highlighted in the *2016 National Research Infrastructure Roadmap,* is as a piece of critical infrastructure for delivering Australia's weather and climate prediction system to the whole research community, including innovative research addressing how the mean state and climate extremes affect us. The outcomes of improvements to ACCESS directly enhance the work of other sectors such as business, industry, government and environmental management.

ACCESS is a complex coupled-system model that comprises atmosphere, ocean, sea-ice, land and other components derived from the best models of the UK, USA, France and Australia to provide our national weather and climate prediction capability. The model's complexity and design enables it to be used over a range of time scales: from hours for extreme weather events (storms and bushfires), through to days for general weather prediction, months and years for seasonal prediction, and centuries for long-term climate change modelling. The outcomes for Australia are wide-ranging and underpin services that provide multi-billion dollar benefits for agriculture and industry. These include improved weather prediction and more accurate seasonal prediction, improved risk management and public safety during extreme weather events, and the provision of essential tools and information systems for long-term policy and decision-making.

ACCESS is developed through a collaboration of the Bureau of Meteorology, CSIRO, the academic community through the ARC Centre of Excellence in Climate System Science and NCI. NCI's role is essential, not only as the collaborative, integrated development platform but also through its unique expertise in optimising the performance of key model components. Performance improvements of 30–40% and much higher code scalability (up to 20-fold improvements, with some codes now exploiting up to 20,000 cores) enable greater operational efficiency and productivity for the Bureau and the broader research community. This leads to a faster time to results, more accurate simulations that enable new scientific outcomes and insight, and heightened prediction capability. These contributions are fed back into international systems through the UK Met Office and the National Oceanic and Atmospheric Administration in the USA, and are essential in such a world-class collaboration.



Tropical Cyclone Yasi in 2011, taken from Bureau of Meteorology simulations.

Preparing for the Bureau of Meteorology's new Storm Surge System

Tropical cyclones are usually associated with destructive winds and heavy rain but they can also cause widespread damage and loss of life due to the forcing of water onshore as they cross the coast, known as a 'storm surge'.

Predicting the increase in sea level above the normal tidal range is a critical part of the Bureau of Meteorology's warning services. For example, during Tropical Cyclone Debbie in March 2017, the combination of high winds, tides and intense low pressure caused the water level on the coast to rise by over two metres above normal in some places. Warnings from the Bureau assisted emergency managers in deciding to advise coastal communities in North Queensland to evacuate well ahead of the storm onset, thereby avoiding being caught in a life-threatening event.

The Bureau of Meteorology has been significantly upgrading its modelling systems to improve the accuracy and timing of their storm surge forecasts. The accuracy of the new system comes from running a high-resolution dynamical storm surge model for the actual forecast track, as opposed to previous techniques that used parameterised pre-computed scenarios using straight line tracks. By running the model many times to allow for the range of possible alternate tracks, an understanding of the uncertainty of the predicted storm surge can be

obtained. The more forecast runs the system has to work with, the better the uncertainty in the forecast can be represented.

For the region of coastline that a cyclone will pass over, the height at which the sea level will peak is the most critical piece of information. Due to large tidal ranges experienced over much of Australia, the timing of the surge is also very important. While the storm surge model takes into account many complex details about the atmosphere, wind speed, tides, cyclone movement, intensity and symmetry, the final product can be as simple as a single data point showing this peak sea height.

Computational Scientist from the Bureau of Meteorology Dr Justin Freeman says, "Managing a large number of simulations as fast as possible introduces some new challenges – especially as this is needed to help with timely emergency response."

As part of the development of the new system, the HPC Scaling and Optimisation team from NCI analysed the model and made improvements to ensure optimal use of the modern HPC infrastructure. As a result, the Bureau can now produce one 3-day forecast run in under 6 minutes.

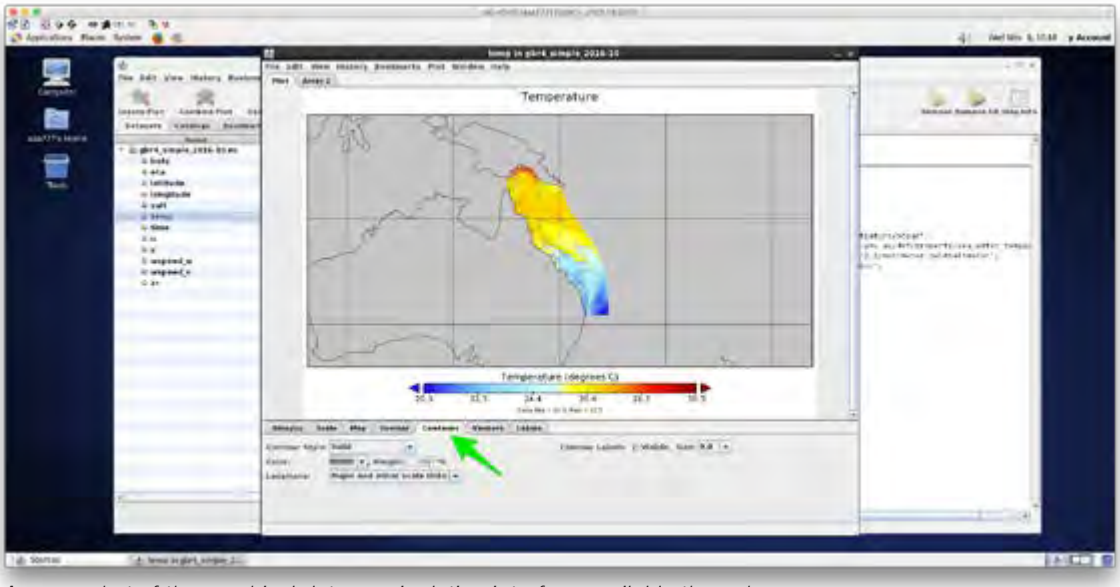
Dr Freeman and his team have been testing the model improvements using historical storm data and comparing the model's results with the location and sea height from the real observations. This testing has included the most recent Tropical Cyclone Debbie scenario to ensure that the most up-to-date information is considered. As a result of this work, the Bureau is preparing to introduce the new storm surge model for the coming 2017–18 cyclone season.

Data Science

Data science at NCI is about extracting information from data. The last ten years have seen an acceleration in the range of data science techniques being used by the research community. This has required both an improvement in the quality and organisation of the data, as well as the development of a range of digital environments that make it easier for researchers to analyse the data via software and analytics tools. These environments include anything from simple community data portals through to more advanced analysis platforms and virtual laboratories.

NCI supports data science through collaboration with community-specific virtual laboratories like the Climate and Weather Science Laboratory (CWSLab), Australian Geoscience Data Cube (AGDC), and the Virtual Geophysics Laboratory (VGL), as well as through provision of a wide range of tools and resources via the Virtual Desktop Infrastructure (VDI). These platforms open up high-performance data analysis to a wide range of researchers by providing a graphical interface and logical structure, through which datasets are accessed.

NCI's VDI (see Case Study on page 34) is an easy-to-use graphical interface that makes it possible for researchers to securely access and analyse data using its vast catalogue of scientific software. This saves time and data replication costs, as well as providing access to



A screenshot of the graphical data manipulation interface available through NCI's Virtual Desktop Infrastructure.

a high-performance computational and data infrastructure. NCI has a particular focus on making very large reference datasets suitable for the increasing need for programmatic access to data.

Programmatic access means that the data supports a diversity of digital environments and enables the application of new techniques. This approach has enabled new methods for extracting information using data science techniques – from Python analysis notebooks through to deep learning and machine learning. As the data is transformed for programmatic access, we have worked with individual research communities to upgrade their software and provide training on how to take advantage of the new capabilities.

NCI's effort to provide easier access to research-ready data (such as the Copernicus Regional Data Hub, see Case Study on page 38) is already enabling new approaches to scientific problems and will continue to lead the way in innovative data-intensive research.

NCI's VizLab also assists researchers with visualisations of scientific datasets and their findings (see case study on page 32). These visualisations use NCI's integrated HPC–data environment and expertise, and provide striking and detailed scientific visualisations for researchers to use to explain their findings. The process of visualising involves a collaborative team approach – harnessing the expertise across scientific and technical approaches. Using visualisation techniques provides a new way of analysing datasets or model outputs, which in turn leads to additional understanding and may potentially spark new scientific insight.

New ways of interacting with environmental data

Monitoring a forest plantation used to present a significant challenge, requiring spending hundreds of hours measuring tree heights and locations out in the field. Now, the development of new methods of near surface remote sensing is making it easier than ever to measure and map forests in three dimensions on a regular basis, but at the same time is producing more data than can be easily dealt with.

Recently, researchers have been facing an exponential growth of this problem as more and more drones and automatic monitoring stations become cheap and easy tools for research, producing large quantities of data that, while amazing in their novelty and complexity, still have very few tools available for viewing and interacting with them intuitively.

NCI's VizLab and Dr Tim Brown from The Australian National University's Research School of Biology are producing new software that will allow easy visualisation of these types of environmental data, especially in the form of point clouds. Point clouds are a type of three-dimensional model of the environment produced from drones flights and laser scans. They can be used to map the size, location, colour and other important characteristics of objects in the environment at high resolution. This data, gathered over an entire forest, can provide a clear image of what each individual tree looks like, how it grows over time and where it is placed in relation to the others.

Point clouds of an area can be gathered from airplanes, drones or from the ground;

A point cloud of one of the forests within the National Arboretum in Canberra, based on data from Dr Tim Brown's research.

the challenge is bringing all those separate datasets into one single viewer. NCI is building the software and data management systems that will allow multiple point cloud sources to be viewed simultaneously, in virtual reality. This requires accurate GPS data to accompany each dataset, and access to storage and cloud services which provide the computational power needed to integrate all the data together.

Dr Brown's team, along with the ACT Government and CSIRO, has spent the last few years gathering point cloud data in the ACT. Dr Brown's dataset focuses on a forest in the National Arboretum, and when paired with the others, forms a detailed map of the changes in the forest over the last few years.

Critically, once you have multiple point clouds taken of your area of interest over a period of time, you can create a time-lapse component to the visualisation and see the trees grow and the landscapes change. The new tool allows data such as tree height, growth rate or even tree genetic variation to be mapped onto each tree. Dr Brown says, "More and more researchers would like 3D models of their plants, but there aren't any tools designed for interacting with a time-lapse stack of point clouds and their associated data. The ability to continuously measure the world in very high resolution has the potential to revolutionise scientific research.

"With tools such as those we are creating, in a few years, a researcher could call up a hologram of their forest on their desk and tap a tree to show the data associated with it. They could rearrange the forest by height or growth rate or genetic markers. They could discuss an analysis with a colleague on the other side of the world while simultaneously viewing the same 3D model in real-time."

Virtual Desktop accelerates epigenome alignment

When genes and proteins inside a cell are damaged, it can result in diseases such as cancers, diabetes and obesity. Understanding exactly how this damage affects DNA is key to understanding and developing early and effective treatments, and raises the chances of a treatment succeeding.

Epigenetics is the study of how gene expression is regulated inside cells, as it provides extra information above the DNA sequence code. With the advance of Next Generation Sequencing (NGS, a massive parallel sequencing technology), epigenetic DNA modifications can be profiled on a genome-wide scale. NGS produces large datasets of short DNA sequences that need to be mapped to the genome before use. It is essential that researchers use high-performance computing systems for this mapping, called genome alignment, so that they can gain the biological insights from within the epigenetic sequence datasets. The sequence datasets require computational pre-processing for quality control before the data can be analysed with confidence.

Dr Phuc Loi Luu, a senior bioinformatician from the Epigenetics Research Laboratory of Professor Susan Clark at the Garvan Institute of Medical Research, performs the pre-processing and alignment of whole genome bisulphite sequences (WGBS) to study DNA patterns specific to cancer. The computational alignment workflow includes a 64-step process and takes 3 to 4 weeks to run on the in-house cluster.

Recently, by using NCI's Virtual Desktop Infrastructure (VDI) to submit jobs to Raijin, Dr Luu built a pipeline to connect all the steps and run as a single process in a secure and easy-to-use environment.

Dr Luu has optimised his new pipeline for the VDI and obtained a significant reduction in run time from three weeks to four days, rapidly speeding up the workflow and making it more efficient and cost-effective.

"The DNA sequencing machines are now much faster than they used to be, but until this point, the way of working with large data in the WGBS alignment step has not been keeping pace. With the move to NCI, in a single secure environment, we don't have those problems any more.

"Now, right after the sequencing is performed, I can give biologically meaningful data to wet-lab biologists in 4 days instead of 3 weeks of processing time. The speed of processing allows for immediate insights into the data to accelerate the research and design of the next experiments," Dr Luu said.

The reduction in time spent calculating is not the only benefit that Dr Luu sees from the VDI.

"The easy-to-understand desktop interface of the VDI makes it much simpler for biologists with no programming knowledge to work on the analyses. The convenience of being able to log in from anywhere and monitor progress is a significant improvement," he said.

Dr Luu first learnt about the VDI at the HPC Summer School that NCI organised for users in February 2017. Since then he has made use of the high-performance computing, data storage, data tools and computational expertise available at NCI.

Data Services

NCI's data services are built to provide new and useful ways to access and use data. As an international leader in the fusion of high-performance computing and data science, NCI has championed a transdisciplinary approach to data access, which is creating exciting opportunities for research across multiple domains. This is particularly so in the Earth system sciences, which require analysis at ever higher resolutions and across multiple scales and domains.

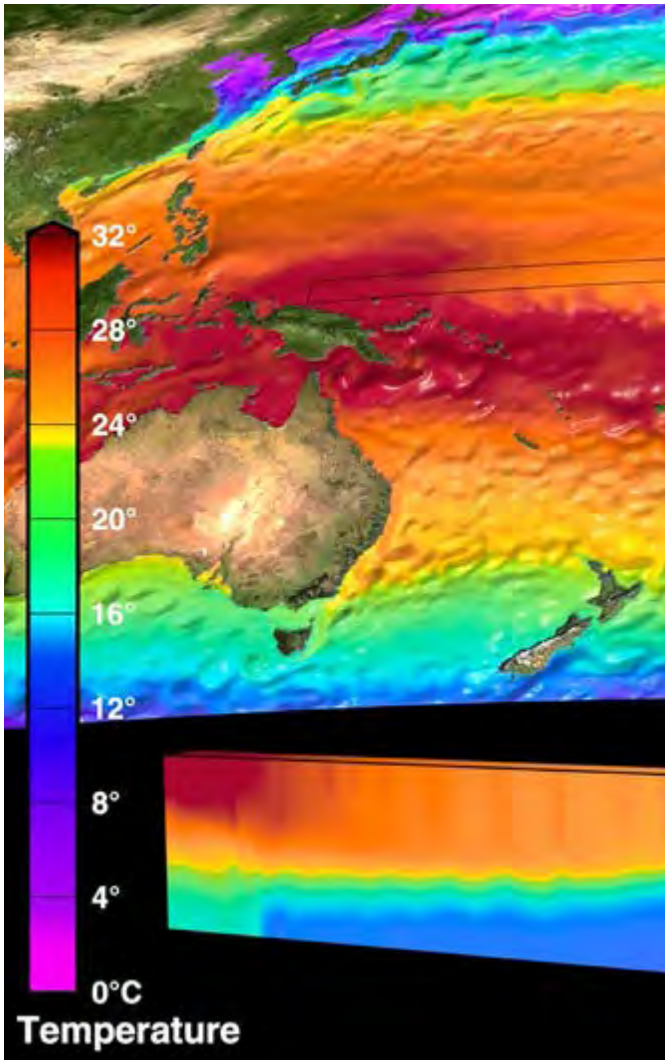
NCI aims to provide a trustworthy high-performance data platform that enables researchers to use data in a high-end computational and data-intensive environment. The aim is for the data to be suitable for use by a range of communities while solving discipline-specific needs. This includes enabling the integration of both small and large scale information.

The new National Environmental Research Data Interoperability Platform (NERDIP) developed at NCI has been designed to meet a broad range of these use cases and harnesses the large corpus of data that has been assembled at NCI. The platform uses modern data standards to ensure that the range of data provided is a vast improvement for research within a single domain. Previously, no single science domain had been able to access all the data made available to it.

NERDIP also enables interoperability across the different science domains – whereby any improvements to the repository are made accessible to the widest scientific community possible. By adopting the guiding principles for Findable, Accessible, Interoperable and Reusable (FAIR) data publishing (see text box on opposite page), NCI is also increasing the value of the datasets by extending their potential use in new and innovative ways.

Over the last year, we have made considerable advances in scalable server-side computing by using NCI's co-located computational power and data. The NCI-developed GSKY service (see case study on page 40) provides a new approach to online analysis and visualisation of environmental data. GSKY (pronounced ji-skee) provides an ability for users to interact with datasets and the information they contain using standard community protocols.

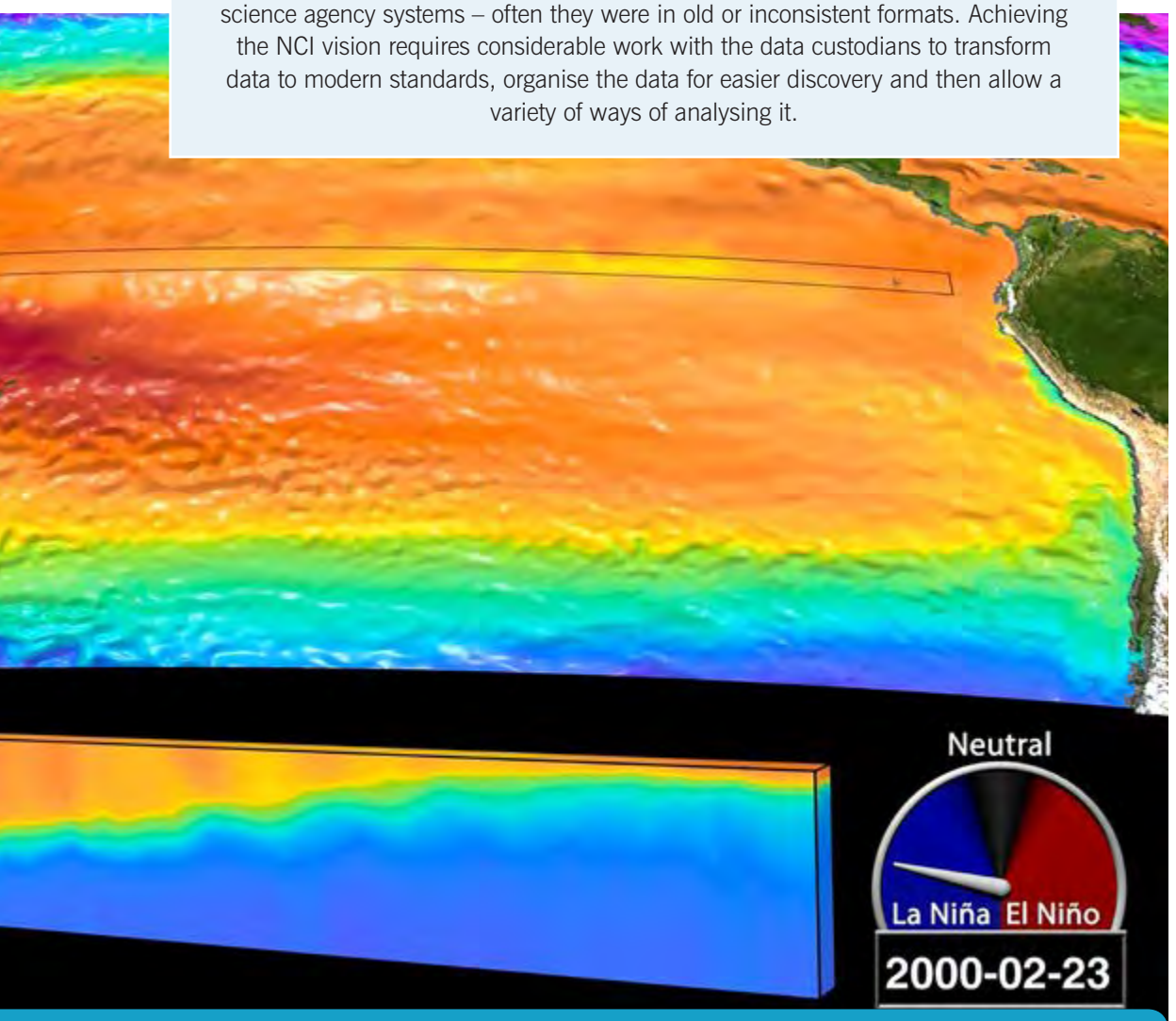
A still from the NCI and ARC Centre of Excellence for Climate System Science visualisation of the El Niño Southern Oscillation.



Many of the activities to improve data access and analytical frameworks are time-consuming and require specialist knowledge beyond any individual research project or research community.

Instead, the Australian Government's investment in national collaborations like NCI reduces the need to replicate data infrastructures and specialist management teams across multiple communities, projects and institutions. It also ensures that this vital work is carried out in ways that improve the quality of the data across domains, as well as for individual domains and internationally.

The Findable, Accessible, Interoperable and Reusable (FAIR) principles of data publishing, developed in 2016 by the FORCE 11 community working to improve research communications and e-scholarship, are increasingly being promoted by major international repositories and research institutions as they provide guidance on the minimum requirements for enabling optimal use of research data across communities. Many of the data collections managed at NCI were previously difficult to find or use because they were held on non-accessible internal-only government science agency systems – often they were in old or inconsistent formats. Achieving the NCI vision requires considerable work with the data custodians to transform data to modern standards, organise the data for easier discovery and then allow a variety of ways of analysing it.



Transferring satellite data across continents

Every day, satellites from the European Space Agency (ESA) and European Meteorological Agency (EUMETSAT) circle the Earth, collecting images and observations from the planet below. Making the data available to a wide community of researchers, emergency services and government agencies in Australia involves the complex technical challenge of moving large volumes of data across the globe.

To provide rapid global access to the data, a number of regional storage hubs have been established. In Australia, the Federal Government through Geoscience Australia and NCI has developed the Australian Regional Copernicus Hub, to manage the data for the South East Asia and Pacific region.

Getting the data here starts when the images and observations are beamed from the satellites to the Copernicus Earth-observation dissemination centre in Frankfurt, Germany, ready for distribution. Then, the data transfer from Frankfurt to Canberra moves 20 terabytes of data every day, the equivalent of streaming around 2,400 movies. The 10,000-kilometre journey takes the data across continents and oceans at the speed of light before reaching NCI's high-performance facility. The data follows a complex network of undersea fibre-optic cables, and links together various National Research and Education Networks in Australia, Europe, Asia and the Americas.

Maintaining the integrity of the data across such a large distance is essential for researchers to be able to trust the accuracy of their datasets. NCI's high-performance data team has developed a data transfer process using specially designed protocols and rigorous quality control methods to guarantee that when data arrives at NCI, it is suitable for use.

To ensure the highest reliability and to handle unexpected network failures, the datasets come to NCI over two geographically separate paths. The first via the USA, crossing the European Géant Network across the Atlantic Ocean from Amsterdam to New York, then transiting the Internet2 network to Seattle where they cross the Pacific Ocean to Sydney, ready for the final leg to Canberra via Australia's Academic and Research Network (AARNet). The second path is via Asia, crossing the Géant network from London, transiting via the Trans-Eurasia Information Network to Singapore and then to Australia via Perth.

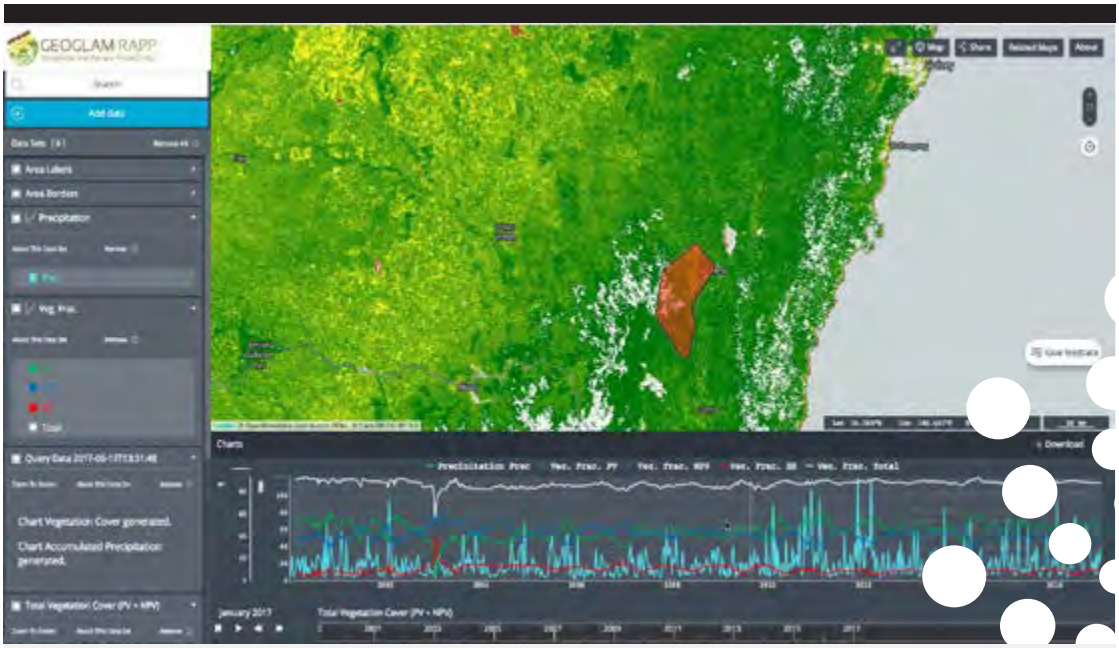
The data managed at NCI is provided by the European Space Agency and EUMETSAT and includes all satellite observations and images covering Australia, New Zealand, Indonesia and many countries in South Asia and the Pacific, as well as Australia's marine reserves and sections of Antarctica.

The measurements include raw and processed datasets like ocean colour, ocean height, ground reflectance and ground moisture. From these datasets, scientists can analyse environmental changes such as the build-up of fuel for bushfires, the

change of flow rates in rivers and how land use is affecting the environment. In addition, advanced radar imaging allows for the determination of ground subsidence with movements down to a few millimetres.

NCI has more than 10 petabytes of curated data collections of reference earth systems datasets, which include environmental data such as satellite imagery and data products, and many years of climate, weather and other geospatial data. These datasets have been organised at NCI in a way that allows for queries, combinations of data and new and innovative research. Working with various research communities, NCI has developed virtual laboratories and a vast software repository integrated together to support researchers to make the best possible use of these data resources.

Wolfe Creek crater in Western Australia, processed by the European Space Agency using modified Copernicus Sentinel data - CC BY-SA IGO 3.0.



A screenshot of the mapping interface in GEOGLAM-RAPP, enabling the visualisation of large and varied environmental datasets.

Making big data easier to handle

Geoscientific data these days comes from a large number of geospatial instruments: from satellites, ground-based radar and seismic sensors, just to name a few. For a long time, researchers have been working with data by downloading datasets that are often comprised of millions of individual files. When working with those datasets and their peculiarities, researchers often have to organise and laboriously work across these files to find the information needed. The sheer complexity means that researchers compromise on the scope of their work, or feel limited in their ability to work with the data.

The question today is how we can more easily do data-intensive research across the many kinds of extremely large and complex datasets that come from these sources. NCI has developed a new online tool that is making the analysis and visualisation of all of this data much easier.

The new data service, called GSKY, makes this old and inefficient way of working with data obsolete. GSKY accesses and analyses the big geospatial data on NCI's cloud and high-performance computing systems, and then delivers it to a user device or website. For example, hundreds of time series and geospatially overlapping data can be seamlessly merged together, allowing researchers to focus on the information rather than dealing with data files. Furthermore, using GSKY's processing capability, that data can be analysed on the fly using user-provided algorithms to extract new information over both space and time.

Behind the scenes, GSKY works out how to manipulate the datasets so that they seamlessly work together. For example, in large-scale environmental analyses, the images from different satellites can be in different shapes and sizes, environmental survey data can come in many different formats, and even urban boundary maps need to be considered. As a user of GSKY, working with data is as easy as choosing from a list of available datasets, specifying a region and time frame, and asking GSKY to analyse the information as harmonised data. GSKY then returns the results of the data required, which can be accessed over the network to the client application or for visualisation in an online map.

One example of such a use is GEOGLAM-RAPP, an interactive online map produced by the Group on Earth Observations and its Global Agricultural Monitoring for tracking Rangeland and Pasture Productivity. GEOGLAM-RAPP takes international satellite data and displays it using GSKY, allowing users to track and analyse the condition of global rangelands used for activities like agriculture and livestock production.

Information that can be displayed using GEOGLAM-RAPP includes:

- vegetation cover
- monthly rainfall
- monthly soil moisture
- global land use and land cover
- livestock density.

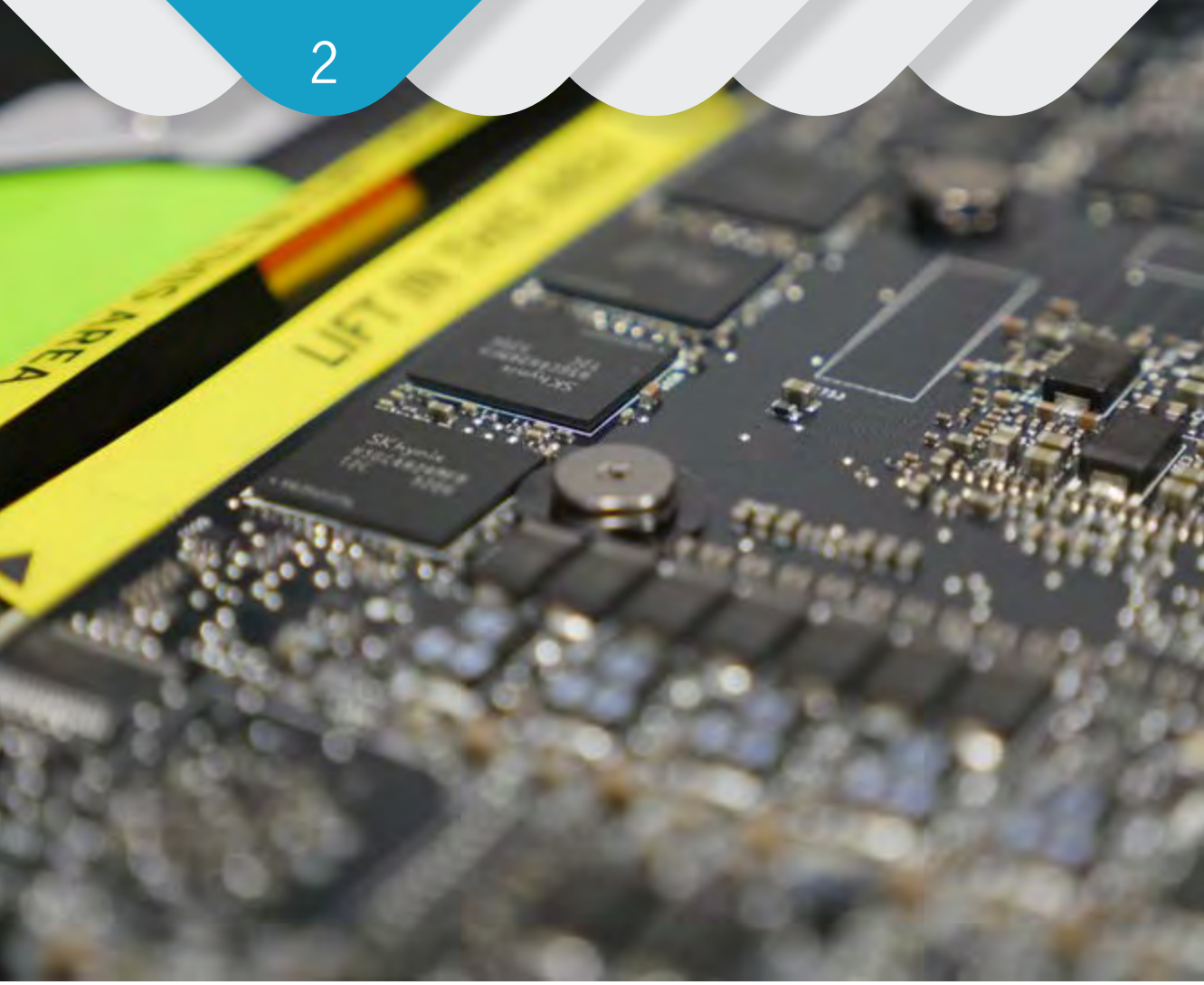
Users accessing GEOGLAM-RAPP are able to view one or more of the above datasets on a local or global scale, with at-a-glance comparisons of multiple datasets. The time-series datasets can be resolved down to a specific week over the course of the last several decades for further investigation, or the entire dataset can be played in its entirety to see changes over time. Using GSKY to access datasets promises to make innovative environmental research even better.

System Enhancements

Early in 2016, NCI was approached by Intel to be part of an international early access program for their Knights Landing (KNL) Xeon Phi accelerators. NCI was the only site in Australia to be selected to participate in this global program, due to the international reputation of staff in benchmarking codes, as well as the heterogeneous research workloads that NCI supports.

In June 2016, NCI took delivery of 32 KNL systems. This provided NCI with 3 months of early access before the product was launched worldwide. As a result, NCI was able to provide guidance to researchers nationally on the applications best suited to take advantage of this new technology. Since their introduction, these servers have seen consistent utilisation with a steadily growing demand from our researchers.

Along with the KNL accelerators, NCI also took delivery of another 64 K80 NVIDIA Graphics Processing Units (GPU) to expand capacity and to meet researcher demand. These GPUs provide a huge number of cores able to work in parallel on computational and data science applications. Demand for these accelerators continues to grow, with demand outstripping supply by as much as 4:1.



In December 2016, with support from the NCRIS Agility Fund and a matching co-contribution from the NCI partners, NCI purchased a significant increase in HPC compute and data storage capacity. This addition to the supercomputer and to NCI's global filesystems provides a significant increase in capacity and capability to Australian researchers.

A total of 814 Lenovo servers were purchased, providing an additional 22,792 Broadwell CPU cores. These newer CPUs are more energy efficient and allow our researchers to collaborate on modern programming efforts nationally and internationally, taking advantage of the more recent instruction sets.

In addition to a boost in raw CPU capacity, the new Agility System uses the latest Mellanox EDR Infiniband Interconnect. This enables the nodes to communicate with each other at 100 Gigabits per second, an almost twofold increase over the FDR Infiniband network used in the rest of the supercomputer. In fact, the Agility System was one of the world's first large deployments of Mellanox's SwitchX2 technology.

In light of the ongoing demand for GPUs, NCI has invested in four P100s, the next generation Nvidia GPU, released in early February 2017. These systems were procured as part of the Agility fund purchase, and are part of the ongoing investigative work that NCI undertakes in assessing and providing access to new technology for Australian researchers.

Understanding the quantum rules of the universe

Inside every atom in the universe, forces are pushing and pulling to keep the atom's fundamental building blocks stuck together, interacting to preserve a delicate energy balance that enables stars to form and life to exist. Right now, we only have an inkling of how those forces work, but that is starting to change. A physics research team from the University of Adelaide is striving to reveal the hidden nature of the theories that make the universe work.

The researchers from the Special Research Centre for the Subatomic Structure of Matter are taking advantage of the new accelerator technologies available at NCI to move their scientific understanding forward. Accelerators, such as Graphics Processing Units (GPUs) and the new Intel Xeon Phi many-core processors, are enabling the team's microscopic simulations. Their work, which involves reconstructing the behaviour of subatomic particles, is impossible to do without calculating all the forces interacting at such a small scale.

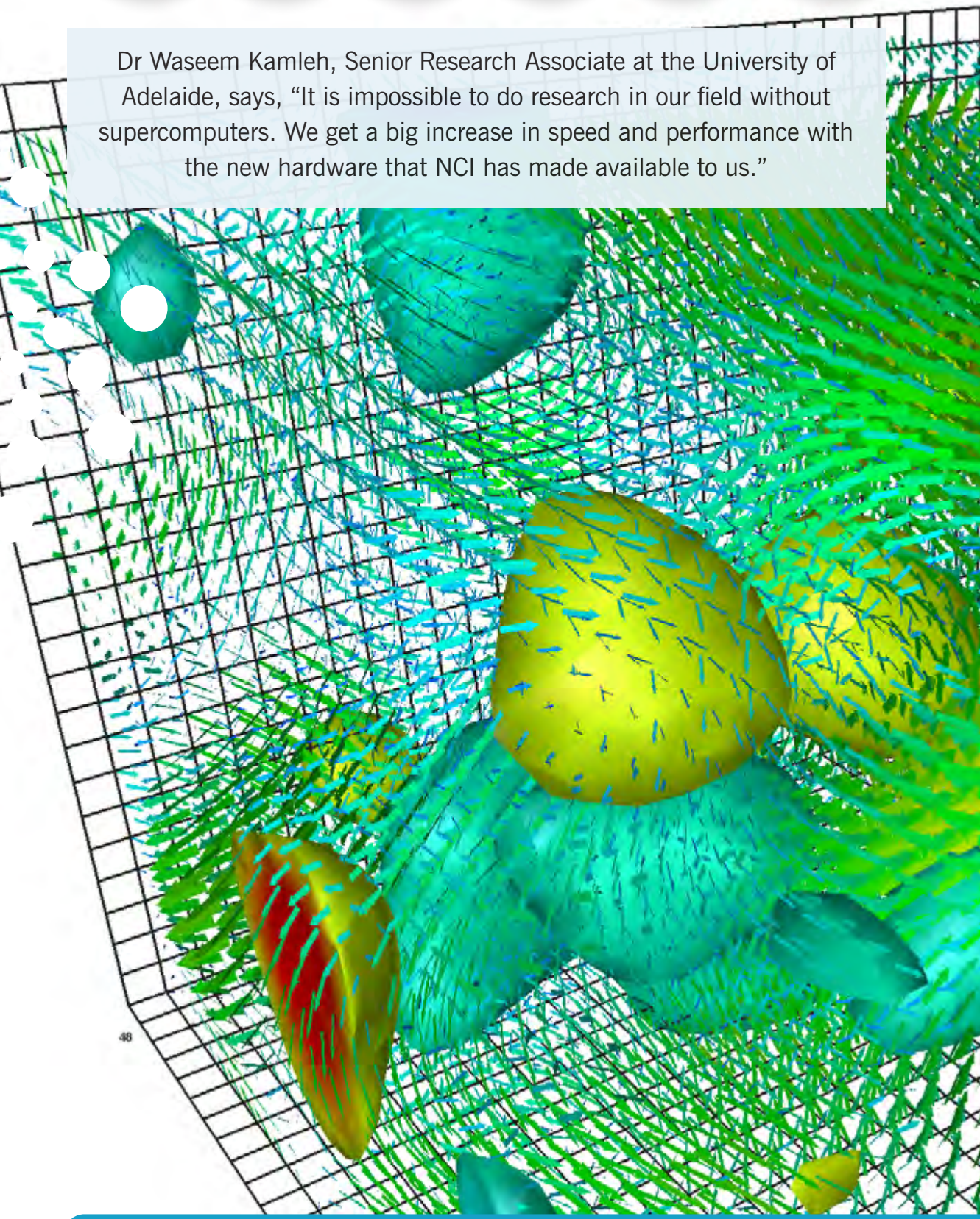
For the simulations, the researchers define a four-dimensional lattice representing space and time in order to compute the effects of the strong force on a particle. The strong force, described by the theory of Quantum Chromodynamics (QCD), binds atomic nuclei together, but due to a phenomenon known as quark confinement, cannot be measured directly in an experiment. For that reason, the researchers turn to supercomputing.

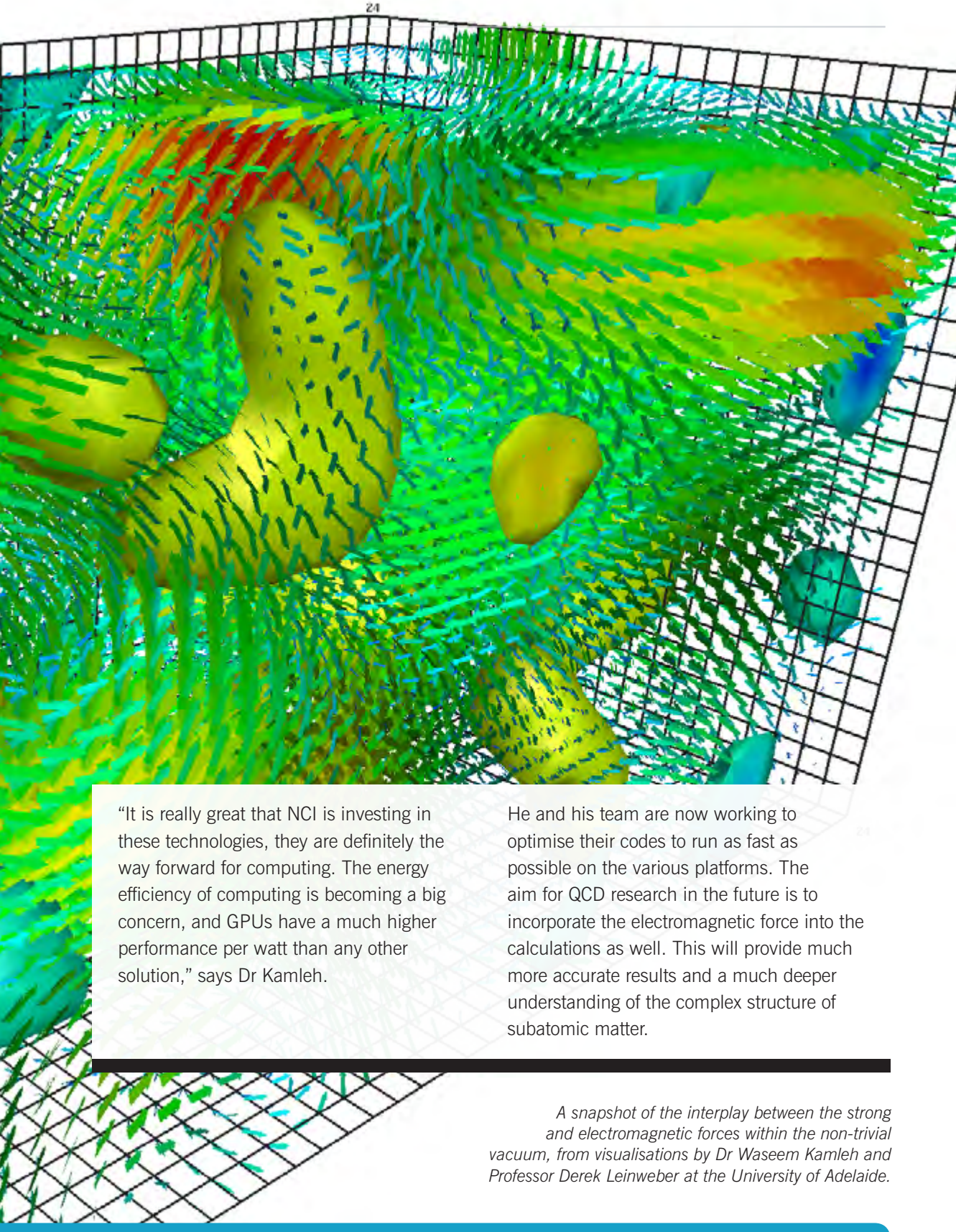
In particular, they use GPUs and many-core processors because of their incredible parallel computing capabilities. The calculations for every point within the QCD lattice come in millions of different variants. They can all run simultaneously, and with the data and calculation speeds provided by accelerated systems, move simulations forward in ways that desktop computers simply cannot.

GPUs were originally designed to process data for the pixels of televisions and computer monitors, so they excel at doing a large number of small, discrete calculations very fast. In high-performance computing, more and more researchers are seeing benefits from these new technologies. QCD researchers are some of NCI's biggest users of these specialised systems, and have been since they first arrived on site. In fact, Dr Kamleh has been using GPUs in his research since the mid-2000s.

Continued on next page

Dr Waseem Kamleh, Senior Research Associate at the University of Adelaide, says, “It is impossible to do research in our field without supercomputers. We get a big increase in speed and performance with the new hardware that NCI has made available to us.”





"It is really great that NCI is investing in these technologies, they are definitely the way forward for computing. The energy efficiency of computing is becoming a big concern, and GPUs have a much higher performance per watt than any other solution," says Dr Kamleh.

He and his team are now working to optimise their codes to run as fast as possible on the various platforms. The aim for QCD research in the future is to incorporate the electromagnetic force into the calculations as well. This will provide much more accurate results and a much deeper understanding of the complex structure of subatomic matter.

A snapshot of the interplay between the strong and electromagnetic forces within the non-trivial vacuum, from visualisations by Dr Waseem Kamleh and Professor Derek Leinweber at the University of Adelaide.

Leadership and Engagements

3

National and International Collaborations

A large part of our work, developing both hardware and software solutions for computational science problems, involves collaborations with national and international organisations. These organisations include a variety of renowned international research bodies such as NASA and the UK Meteorological Office, national bodies such as Collaborative Research Centres and Centres of Excellence, government agencies such as the Bureau of Meteorology, and industry groups such as Fujitsu, with whom we collaborate closely.

Collaboration is especially important when it comes to data collections; the acquisition and distribution of satellite data, climate models and weather observations is an internationally collaborative exercise. NCI participates in these global networks and actively contributes to the development of the data collections and the underlying data management processes, giving NCI an important role on the global research stage.

As an active contributor to these networks, NCI is a key location for researchers wanting to access a large variety of datasets. International

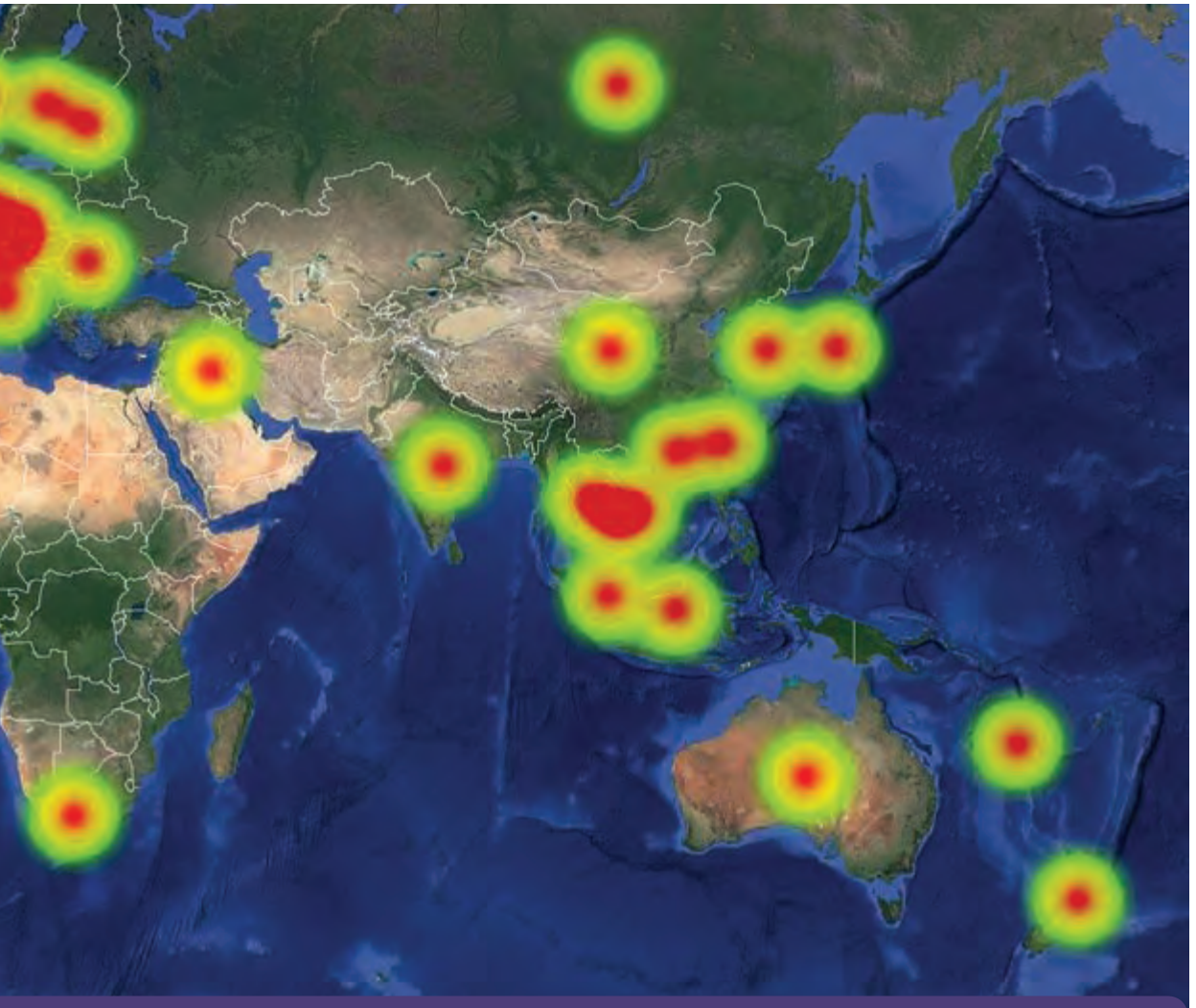
Researchers and facilities all over the world access NCI's data services every year. They download hundreds of terabytes of data from NCI's collection, which shows the high demand for the data we provide. This map shows the most significant locations for international data downloads. A full breakdown of the data is available in the Appendix on page 89.

and national traffic to NCI's data portals shows the level of interest that our earth observation collections in particular are generating.

Our engagement with international partners provides a key service for Australian research by making available new data, new tools and the latest trial hardware from the leading international vendors. This keeps NCI researchers current with trends in the supercomputing space and helps prepare them for developments in the future.

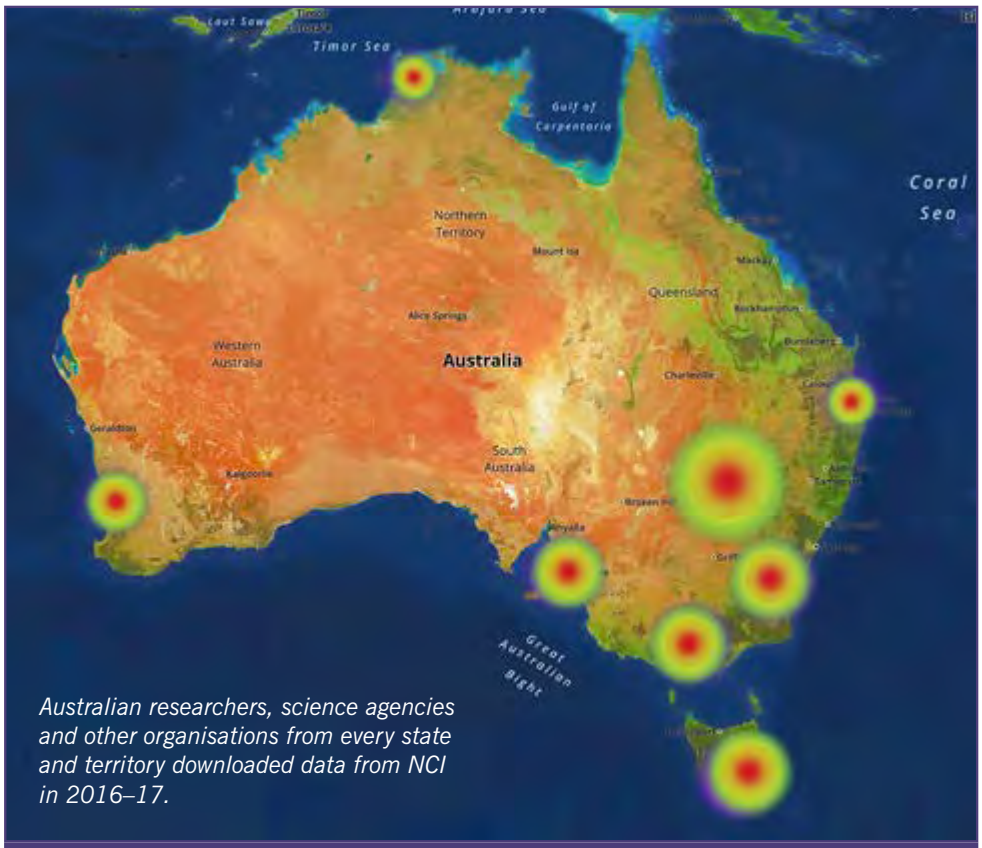
Many organisations and research groups rely on access to the products of our collaborations, such as the ARC Centre of Excellence for Climate System Science making use of the CMIP6 climate dataset, or researchers from the Bureau of Meteorology benefiting from our engagement with Fujitsu around weather model optimisation (see case study on page 30).

Similarly, many researchers are now benefiting from our installation of cutting-edge computing hardware, including the latest P100 NVIDIA Graphics Processing Units (GPUs), Intel Knights Landing processors, and IBM Power8 CPUs. The relationships we maintain with our hardware vendors give us privileged access to their upcoming products, once more positioning NCI as a leading centre for high-performance computing infrastructure and expertise.



Our Users

There were more than 1,800 new users to NCI in 2016–17, continuing the strong growth in demand for these advanced computing resources. Over 6,000 Australian researchers now use NCI to support their scientific projects, including through access to high-performance computing and data resources, access to cutting-edge new technologies, and newly developed data management and analysis portals.



Australian researchers, science agencies and other organisations from every state and territory downloaded data from NCI in 2016–17.

LOCATION	Download (MB)
New South Wales	47,722,548
Tasmania	11,036,555
Australian Capital Territory	9,935,226
Victoria	8,208,668
South Australia	5,842,215
Queensland	1,760,770
Western Australia	1,752,510
Northern Territory	12,749
Total	**86,271,241**

Our Partnerships

The NCI Collaboration

NCI
NATIONAL COMPUTATIONAL INFRASTRUCTURE

Supported by:

NCRIS National Research Infrastructure for Australia
An Australian Government Initiative

Australian Government
Department of Education

Partner Organisations:

Australian National University

CSIRO

Australian Government
Bureau of Meteorology

Australian Government
Geoscience Australia

RMIT UNIVERSITY

INTERSECT

DEAKIN UNIVERSITY AUSTRALIA
Worldly

qcif

ACE
ANTARCTIC CLIMATE & ECOSYSTEMS

UTS
UNIVERSITY OF TECHNOLOGY, SYDNEY

GARVAN INSTITUTE OF MEDICAL RESEARCH

UNIVERSITY OF WOLLONGONG AUSTRALIA

MACQUARIE University

Australian Research Council:

Australian Government
Australian Research Council

THE UNIVERSITY of ADELAIDE

Australian National University

MONASH University

UNSW AUSTRALIA

THE UNIVERSITY OF QUEENSLAND AUSTRALIA

THE UNIVERSITY OF SYDNEY

RMIT UNIVERSITY

A node of:

nectar

RDS Research Data Services

Commercial Partners:

DHI

FEI™

Victor Chang Cardiac Research Institute

Commercial Collaborators:

FUJITSU

DDN STORAGE

intel

NVIDIA

Affiliates:

CAASTRO ALL-SKY ASTROPHYSICS

ARC Centre of Excellence for Climate System Science

ARC Centre of Excellence for Electromaterials Science

BGH

CoEPP ARC Centre of Excellence for Particle Physics at the Terascale

Centre for Nanoscale BioPhotonics ARC Centre of Excellence

cudos An ARC Centre of Excellence

FLEET ARC Centre of Excellence in Future Low-Energy Electronics Technologies

exciton science

ASVO

Virtual Geophysics Laboratory VGL

bccvl

ESGF Earth System Grid Federation

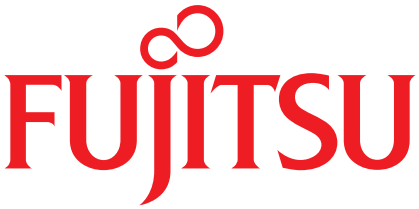
MASSIVE

TERN Terrestrial Ecosystem Research Network

National Committee for Materials Science and Engineering

Natural History Museum

Our Vendors


FUJITSU


Lenovo


XENON
High Performance Computing


DELL


Hewlett Packard
Enterprise


IBM


DDN
STORAGE


NetApp


SPECTRA
SpectraLogic.com


intel


NVIDIA


Mellanox
TECHNOLOGIES


APC
by Schneider Electric


Altair

Outreach

4

Indonesian reporters being shown the NCI facility.

NCI's role as a leader in the advanced computing community in Australia goes beyond the systems and services we provide. We also conduct a large amount of outreach and engagement for community and scientific audiences every year. NCI helps develop the ability of Australian researchers to use our HPC and HPD facilities through workshops and training courses, and fosters community supercomputing knowledge and interest through a variety of public-focused activities throughout the year.

Educational Outreach

From high-school students to scientists in training, NCI regularly welcomes groups keen to learn about the facility and all the things that researchers do with high-performance computing and data. The aim of NCI's outreach to younger generations is to foster an interest in science, technology, engineering and maths and the benefits and future opportunities that supercomputing will provide. Tours of the NCI facility are a great way for them to become excited and curious about a whole new way of doing science. Highlights include the annual visit from the National Youth Science Forum students, Girls

Students from the National Youth Science Forum learning about supercomputer components during their visit to NCI.

in ICT day, National Science Teachers Summer School participants, and the Questacon Science Circus.

Corporate Outreach

NCI attended numerous high-profile science events in 2016–17, including the annual Science Meets Business and Science Meets Parliament events run by Science and Technology Australia. These events are an opportunity to introduce supercomputing to important stakeholders and potential collaborators, including ministers, science leaders and industry representatives.

Training

In 2016–17, NCI ran multiple training sessions and workshops across Australia, the largest being the week-long HPC Summer School held on campus at ANU. Through this, and other training courses held nationwide, new and current users have learnt about how to best make use of the data and compute facilities they have access to. Training sessions such as the Summer School are an important way of developing the skill set of NCI's user community and keeping them up-to-date on the latest technologies they can leverage in their work.

National and International Engagements

As a global leader in the HPC and HPD space, NCI is part of many international working groups, networks and collaborations. NCI staff play important roles in organisations including the Earth System Grid Federation and the American Geophysical Union. Being involved in these key bodies allows NCI to be a part of the development of data management standards and international data sharing activities.

NCI attends many conferences every year to share information about the services available to users.

The 2016 HPC Summer School provided over 50 NCI users with skills to access and use the latest technologies most efficiently.

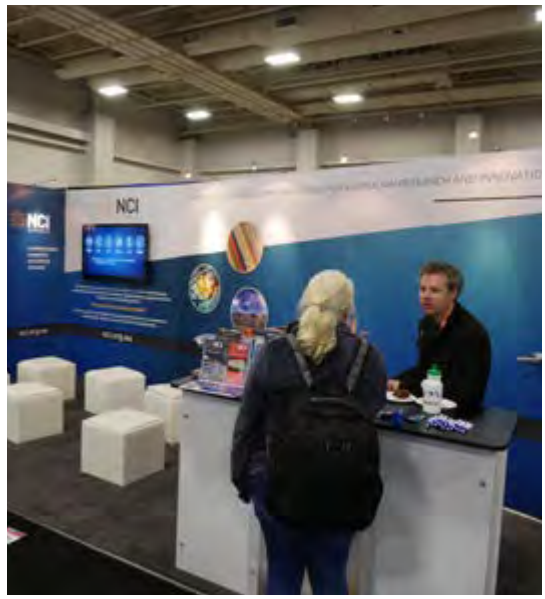
Presentations and Publications

In addition to outreach and engagement with international working groups, NCI is also an active participant in many of the world's biggest open data and supercomputing conferences and journals. Over the course of the year, NCI staff presented talks at more than 40 conferences and published more than a dozen papers. This year, NCI had featured presentations at the American Geophysics Union Fall Meeting in 2016 and at the International Supercomputing Conference (ISC) 2017.

NCI's booth at the International Supercomputing Conference 2017, in Frankfurt, Germany.

NCI attends the Science in ACTion event every year to talk to school students about supercomputing.

HPC Summer School participants were given a tour of the NCI facility during their week-long training course.



At SuperComputing 16 in Salt Lake City, Utah.

Governance

5

The NCI Board

NCI is governed by The Australian National University on the advice of the NCI Board, which comprises:

- an independent Chair appointed by the Board
- the Director, NCI
- one member appointed by each of the Major Collaborators (ANU, CSIRO, BoM and GA)
- additional independent board members appointed for two-year terms by the NCI Board on the basis of their expertise.

The Board is advised by:

- the Nominations Committee
- the Finance, Audit, Risk and Management Committee.

Board Members

Emeritus Professor Michael Barber FAA FTSE
Chair

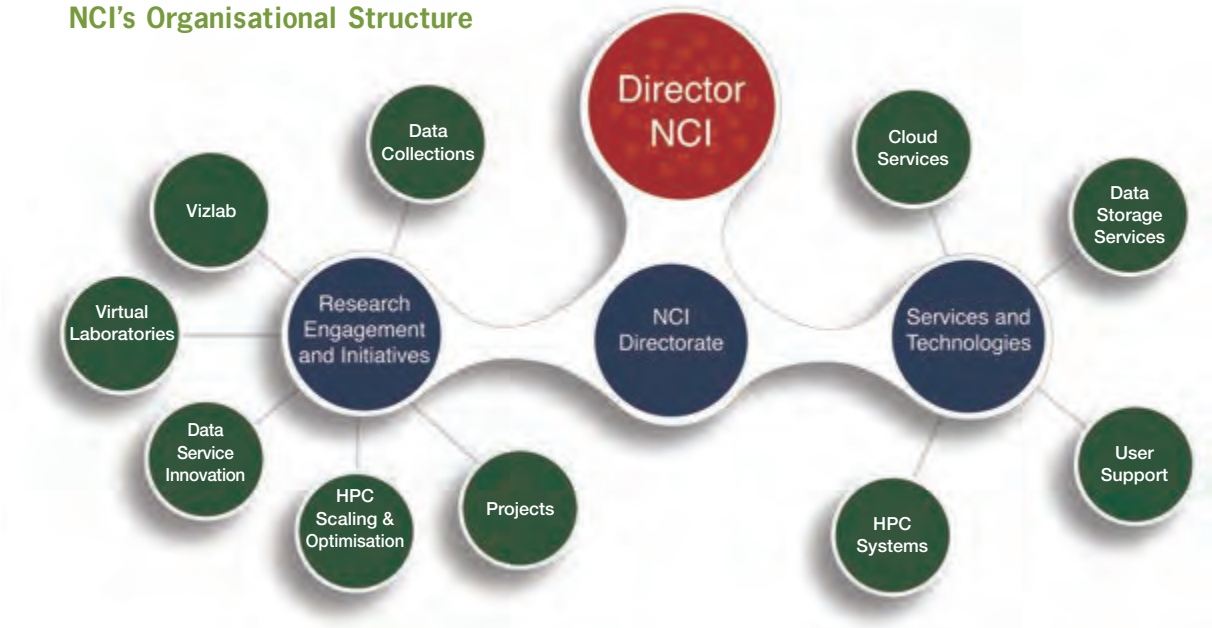
Professor Lindsay Botten
Director, NCI
(Retired May 2017)

Dr Chris Pigram
Chief Executive Officer, Geoscience Australia.
(Retired December 2016)
Interim Director, NCI (From May 2017)

Dr David Williams
Executive Director, National Facilities and Collections, CSIRO

Dr James Johnson
Chief Executive Officer, Geoscience Australia
(From December 2016)

NCI's Organisational Structure



Professor Margaret Harding
Deputy Vice-Chancellor (Research),
Australian National University

Mr Graham Hawke
Deputy Director (Environment & Research),
Bureau of Meteorology

Emeritus Professor Robin Stanton
Independent Member and Deputy Chair

Dr Thomas Barlow
Independent Member
Research Strategist, Barlow Advisory

Financial Report

Preamble

NCI is an organisational unit of The Australian National University. The ANU, as represented by NCI, administers numerous funding contracts that support the operations of NCI. In the interests of providing a comprehensive picture of the NCI operation, a financial report consolidating these funding contracts is presented.

Each funding contract is accounted for in a distinct account within the University ledger, and the University facilitates, and where appropriate acts on, the NCI Board's directions and resolutions on NCI matters insofar as they are consistent with the relevant funding contract and not contrary to University Statutes and policies.

NCI Collaboration Income

The NCI Collaboration Agreement enables many of Australia's leading research intensive universities and science agencies to collectively fund a capability beyond the capacity of any single institution. Together, these institutions (including ANU, CSIRO, BoM, Geoscience Australia, the ARC, and a range of other research intensive universities and consortia) fund a significant proportion of NCI's operating costs. A small, but growing proportion of NCI Collaboration income comes from the commercial sector.

NCI also administers a number of grants and contracts outside of the NCI Collaboration accounts. These special purpose arrangements, fund clearly defined projects, infrastructure and services that provide synergistic benefits to the NCI Collaboration.

NCI received $7 million from the Australian Government's NCRIS Agility Fund in 2016, which is reflected in 'Grant income'.

Expenses

NCI, as Australia's national research computing service, provides world-class, high-end services to Australia's researchers. In order to do this, NCI invests significant amounts of money in its expert team of staff and high-performance computing infrastructure. NCI has been constrained in its capacity to replace infrastructure approaching end-of-life due to the lack of external funding for this purpose. To maintain service quality NCI has, where possible, invested in extending the useful life of its existing infrastructure through the renewal of maintenance contracts. Capital equipment spend includes the procurement of the Agility system as an extension to Raijin and the replacement of data storage infrastructure which reached its operational end of life.

Review/Audit

Each funding contract held by the ANU as represented by NCI has specific financial reporting and auditing requirements, and NCI in conjunction with the University's Finance and Business Services Division and Corporate Governance and Risk Office acquit individual project funds in accordance with these requirements.

This consolidated statement has been reviewed by ANU's Finance and Business Services Division. The Chief Financial Officer certifies that:

The statement accurately summarises the financial records of these grants and that these records have been properly maintained so as to accurately record the Income and Expenditure of these grants.

STATEMENT OF INCOME AND EXPENDITURE

For the period 01 July 2016 to 30 June 2017

For the NCI collaboration and associated project accounts

	2016/17 $
Balance as at 1 July 2016	**16,745,657**
Add	
NCI Collaboration Income	13,838,570
Other grant income	15,492,250
Investment Income	-
Total Income	**29,330,820**
Total Available Funds Before Expenditure	**46,076,477**
Less	
Salaries & Related Costs	6,853,050
Equipment - Capital	13,237,439
Equipment - Non-Capital	177,093
Utilities & Maintenance	5,468,216
Travel, Field & Survey Expenses	427,804
Expendable Research Materials	1,567
Contributions	501,500
Consultancies	309,645
Consumables	383,932
Internal Purchases	112,477
Other Expenses	318,139
Transfers to other	5,000
Total Expenditure	**27,795,860**
Unspent Balance as at 30 June 2017	**18,280,617**

Appendix

6

Infrastructure

Data

Data specs:

- 8 Petabytes scratch filesystem storage on the supercomputer accessed at 150 GB/sec
- 40 Petabytes active Lustre filesystem project storage accessed at up to 140 GB/sec
- 48 Petabytes archived data accessed at up to 140 MB/sec
- 15,000 Fujitsu/Net-App, HPE, DDN hard drives
- 4 global Lustre filesystems accessible by the HPC and cloud systems

HPC and Cloud

HPC specs:

- Hybrid Fujitsu Primergy/Lenovo NeXtScale cluster
- 1.67 Petaflops aggregated peak performance
- 84,656 Intel Xeon cores (2.6 GHz Sandy Bridge, Broadwell, Xeon Phi)
- 4,457 compute nodes

- 120 NVIDIA Tesla K80 GPUs, 8 NVIDIA Tesla P100 GPUs
- Hybrid FDR-EDR Mellanox Infiniband fat-tree interconnect (up to 100 Gb/sec)
- 300 Terabytes of main memory
- 8 Petabytes of operational disk storage
- Over 740 million core hours per year
- 309 software packages

Cloud specs:

- 75 Teraflop peak performance Dell OpenStack cloud offering
- 3,200 Xeon Sandy Bridge cores in 200 nodes
- Mellanox 56 Gb/sec Ethernet – full fat-tree FDR Infiniband
- 50 Terabytes main memory
- 320 Terabytes of disk storage

Usage

Compute projects supported by NCI in 2016–17

Lead CI, Institution	Allocation (KSU)	Project title
Dr Amanda Barnard, CSIRO	55181	Properties and Stability of Nanoparticles for Advanced Applications
Dr Daohua Bi, CSIRO	32419	ACCESS - AOGCM
Dr Michael Naughton, Bureau of Meteorology	28300	BoM ESM research at NCI
Dr Robin Wedd, Bureau of Meteorology	22000	ACCESS-Seasonal
Dr Gary Brassington, Bureau of Meteorology	16100	BLUElink3 - Bureau
Dr Andrew Hogg, Australian National University	15980	The Dynamics of the Southern Ocean
Professor Jill Gready, Australian National University	13500	Simulation and Phylogenetics to decipher Rubisco structure, function and evolution
Prof. Martin Asplund, Australian National University	11920	3D magneto-hydrodynamical stellar modelling and 3D non-equilibrium radiative transfer
Dr Peter Steinle, Bureau of Meteorology	11202	Strategic Radar Enhancement Project
Professor Matthew England, University of NSW	11012	Past, present and future climate variability and change in the Southern Hemisphere
Professor Geoffrey Bicknell, Australian National University	9880	Astrophysical Jets and Winds and their Interactions with the Ambient Medium
Prof Derek Leinweber, University of Adelaide	9551	Electromagnetic Structure of Matter
Dr William Thurston, Bureau of Meteorology	8200	Weather and Environmental Prediction Specialised Forecasting Systems (WEPSFS)
Prof Sean Smith, University of NSW	7538	Computational Nanomaterials Science and Engineering
Professor Malcolm Sambridge, Australian National University	7000	Computational Earth Imaging
Dr Christoph Federrath, Australian National University	6750	Modelling the formation of galaxies, star clusters and binary-star systems
Dr Manolo Per, CSIRO	6571	Development and Application of Quantum Monte Carlo methods
Assoc. Prof. Ben Corry, Australian National University	6500	Simulation studies of biological and synthetic channels
Professor Dietmar Mueller, University of Sydney	6470	Geodynamics and evolution of sedimentary systems
Dr Angus Gray-Weale, Bureau of Meteorology	6200	Data assimilation for seasonal prediction
Prof Carola Vinuesa, Australian National University	5752	Computational identification of medically-relevant, personal genetic variation from the largest volumes of human genome sequences.
Dr Andrew Hogg, Australian National University	5561	Mechanisms and attribution of past and future ocean circulation change
Mr Wenjun Wu, Geoscience Australia	5550	AGDC Operations and code repositories (Public and private)
Prof. Toby Allen, Royal Melbourne Institute of Technology	5493	Mechanisms of membrane-charge transport and ion channel function.
NCI Internal (System, Training, Development)	5389	NCI Internal Projects
Emeritus Professor Ross Griffiths, Australian National University	5100	The role of convection in ocean circulation
Dr Aurel Moise, Bureau of Meteorology	5100	Climate Change Science and Processes
Dr Ravichandar Babarao, CSIRO	5007	CO2 conversion in catalytic MOFs
Dr Emlyn Jones, CSIRO	4926	Coastal Ocean Data Assimilation
Professor Catherine Stampfl, University of Sydney	4874	First-Principles Investigations of Processes and Properties in Catalysis, Coatings, and Devices

Lead CI, Institution	Allocation (KSU)	Project title
Professor Alan Mark, University of Queensland	4832	From molecules to cells Understanding the structural and dynamic properties of cellular components at an atomic level.
Mr Alessio Arena, FEI	4800	Commercial work on Analysis of Sedimentary Rock Material
SITOC Griffith Young, Bureau of Meteorology	4500	Seasonal Prediction Systems and Science
Dr. Rhodri Davies, Australian National University	4100	From Plume Source to Hotspot
Mr Anthony Rafter, CSIRO	4059	Regional-Scale Seasonal Prediction Over Eastern Australia and the Coral Sea
Dr Matthew Chamberlain, CSIRO	4052	ACCSP Dynamical Ocean Downscaling of Climate Change Projections
Assoc. Prof. Ben Corry, Australian National University	4000	Simulation studies of biological and synthetic channels
Dr Megan O'Mara, Australian National University	3850	Investigating membrane and protein dynamics, transport and substrate recognition
Associate Professor Katrin Meissner, University of NSW	3846	Abrupt climate change events in the past, present and future
A/Prof Mike Ford, University of Technology, Sydney	3709	Designing and Building Novel 2D Hybrid Materials
Dr Adam Smith, Bureau of Meteorology	3400	Water Information Services
Professor Michelle Coote, Australian National University	3100	Computer-aided Chemical Design of Catalysts and Control Agents
Dr Andrew Hogg, Australian National University	3000	The Dynamics of the Southern Ocean
NCI Fujitsu Collaboration	3000	NCI-Fujitsu ACCESS Model Optimisation
Professor Christoph Arns, University of NSW	2700	Integration of conventional and digital core analysis
Prof Mark Krumholz, Australian National University	2650	Star Formation and Feedback in a Turbulent Interstellar Medium
A/Prof Serdar Kuyucak, University of Sydney	2650	Molecular Dynamics Simulations of Ion Channels and Transporters
A/Prof. Ekaterina Pas, Monash University	2623	Development and Application of Quantum Chemistry Methods for the prediction of physicochemical properties of ionic materials
Professor Shin-Ho Chung, Australian National University	2500	Action of Toxins from Venomous Animals on Biological Ion Channels Molecular Dynamics Studies
Prof Salvy Russo, Royal Melbourne Institute of Technology	2445	Quantum Modelling of Photo-Electrode Materials
Dr Vincent Wheatley, University of Queensland	2440	Scramjet-based Access-to-Space and Planetary Re-entry
Professor Thomas Huber, Australian National University	2350	protein structure calculation using limited experimental data
Professor Evatt Hawkes, University of NSW	2318	Direct Numerical Simulations of Turbulent Combustion
Prof Justin Borevitz, Australian National University	2296	TraitCapture: An Open Source, High Throughput, Integrative Bioinformatics Pipeline linking Genomics and Phenomics.
Professor Suresh Bhatia, University of Queensland	2292	Interfacial Barriers for the Transport of Nanoconfined Fluids
Dr Shahab Joudaki, Swinburne University of Technology	2252	Testing Gravity on Cosmic Scales with Weak Gravitational Lensing and Redshift Space Distortions
Dr. Ivo Seitenzahl, Australian National University	2180	Hydrodynamical explosion simulations and radiative transfer for thermonuclear and core-collapse supernovae
Dr Abhnil Prasad, University of NSW	2140	The effects of tropical convection on Australia's climate
Professor Michael Ferry, University of NSW	2132	bulk metallic glasses
Dr Terry OKane, CSIRO	2130	The AUStralian community ocean model ReAnalysis project (AURA)
Dr Benjamin Galton-Fenzi, University of Tasmania	2045	Research, development and production computing for Antarctic Climate & Ecosystems CRC under the ACE-CRC/AGP/AAD-NCI partnership

Lead CI, Institution	Allocation (KSU)	Project title
Professor Michelle Coote, Australian National University	2000	Computer-aided Chemical Design of Catalysts and Control Agents
Mr Simon Mortensen, DHI	1986	DHI Lihir Phase 2
Prof Debra Bernhardt, University of Queensland	1983	New materials and fluids for catalysis, battery technologies and sensors.
Dr. Ben Thornber, University of Sydney	1973	Mix in high-acceleration implosions driven by multiple shocks
Professor Evatt Hawkes, University of NSW	1950	Direct Numerical Simulations of Turbulent Combustion
Dr Zhe Liu, Monash University	1948	First-principles computational designs for advanced structural and functional materials
Dr Benjamin Galton-Fenzi, University of Tasmania	1907	Research, development and production computing for the Antarctic Gateway Project under the ACE-CRC/AGP/AAD-NCI partnership
Dr Robert Rees, CSIRO	1904	Molecular Simulations of Ionic Liquids for Energy Storage Applications
Mr Leon Majewski, Bureau of Meteorology	1900	Remotely sensed observations for Earth system modelling
Dr. Hamid Valipour, University of NSW	1865	Atomistic Simulations of Materials in Various Environmental Conditions
Dr Adrian Sheppard, Australian National University	1850	Understanding petrophysical and multiphase flow properties of rock through experiment, 3D imaging and modelling
Prof Brian Smith, La Trobe University	1817	Biomolecular modelling
Prof Allen Rodrigo, Australian National University	1800	Evolutionary analyses using short-read sequences from pooled samples of anonymous, genetically-variable individuals.
Professor Leo Radom, University of Sydney	1752	Structural and Mechanistic Chemistry
Dr Xiaodong Fan, University of NSW	1750	Joint Labour Supply and Retirement of Australian Couples
Professor Julio Soria, Monash University	1740	Investigations of transitional and turbulent shear flows using direct numerical simulations and large eddy simulations
Prof Hugh Blackburn, Monash University	1736	High-Order Methods for Transitional and Turbulent Flows
Dr Marcus Thatcher, CSIRO	1735	High-resolution Downscaled Climate Runs
Prof. Phil Cummins, Geoscience Australia	1700	Geohazard Modelling for the Asia-Pacific Region
Associate Professor Aijun Du, Queensland University of Technology	1700	Nanomaterials for Energy, Nanoelectronics and Environmental Applications: Contribution from Modelling towards Rational Design
Mr Wenjun Wu, Geoscience Australia	1700	AGDC Development and Science (GA internal)
Mr Wenju Cai, CSIRO	1680	Climate Change Impact on Southeast Queensland Water Supply
Dr Kevin Walsh, University of Melbourne	1650	South Pacific High-resolution Climate Model Simulations
Dr Peter Daivis, Royal Melbourne Institute of Technology	1620	Molecular Rheology of Freely Jointed Chain Model Polymer Melts
Dr Callum Smits, Victor Chang Cardiac Research Institute	1610	VC Structural Biology
Assoc Prof Todd Lane, University of Melbourne	1570	Atmospheric and oceanic processes and dynamics
Mr James Goodwin, Geoscience Australia	1550	Geophysics
Professor Mark Ragan, University of Queensland	1506	Comparative Analysis of Completely Sequenced Genomes of Diverse Environments
Professor Nathan Bindoff, University of Tasmania	1500	Turbulence and mixing in the Southern Ocean
Prof Mark Krumholz, Australian National University	1450	The Environmental Dependence of the Stellar Initial Mass Function
Professor Mark Thompson, Monash University	1438	Transition, stability and control of bluff body flows
Prof. Andrew Greentree, Royal Melbourne Institute of Technology	1420	Atom-photon interactions in biologically relevant media
A/Prof. Jason Evans, University of NSW	1418	Precipitation-groundwater interactions over eastern Australia climate change impacts at multiple scales

Lead CI, Institution	Allocation (KSU)	Project title
Associate Professor Michelle Spencer, Royal Melbourne Institute of Technology	1415	Theoretical Investigation of novel materials for industrial and biomedical applications
Professor Orsola De Marco, Macquarie University	1385	Common envelope interaction and stellar outbursts in the era of time-domain Astrophysics
Professor Steven Sherwood, University of NSW	1350	Rethinking atmospheric physics to resolve climate enigmas
Mrs Claire Carouge, University of NSW	1253	Terrestrial modelling within the Centre of Excellence regionalizing land surface processes
Professor David Karoly, University of Melbourne	1170	Mechanisms and attribution of changes in Australian climate extremes
Research Scientist Peter Oke, CSIRO	1141	Bluelink developments
Dr Nikhil Medhekar, Monash University	1134	Atomistic Simulations for Electronic, Chemical amd Mechanical Properties of Nanoscale Materials
Dr Patrick Burr, University of NSW	1124	Energy materials modelling
Associate Professor Gregory Sheard, Monash University	1124	Seeking the ultimate regimes of heat transport in horizontally driven natural convection
Prof Salvy Russo, Royal Melbourne Institute of Technology	1100	CoE Exciton Science
Dr Haibo Yu, University of Wollongong	1096	Molecular Simulations of Enzymatic Catalysis and Computer Aided Molecular Design
Professor Tiffany Walsh, Deakin University	1075	Molecular simulation of carbon fibre composites
Dr Mark Holzer, University of NSW	1062	Decadal Changes in Southern Ocean Ventilation
Prof Alexander Heger, Monash University	1054	Fallback and Mixing in Supernovae from the Early Universe
Professor Aibing Yu, Monash University	1050	Simulation and Modelling of Particulate Systems
Dr Amir Karton, University of Western Australia	1050	High-level quantum chemistry: From theory to thermochemical and biochemical application
Associate Professor Michelle Spencer, Royal Melbourne Institute of Technology	1025	Modelling Nanoscale Materials for Sensing and Device Applications
Dr. Dan Taranu, University of Western Australia	1020	UWA Modelling and simulating the evolution of spiral galaxies
Professor Michael Reeder, Monash University	1017	Predicting and understanding Australia's regional rainfall distribution in a changing climate
Dr Roger Dargaville, University of Melbourne	1015	Atmosphere-Ocean Coupled Chemistry Climate Modelling of Ozone and Aerosols
Dr Benjamin Galton-Fenzi, University of Tasmania	1013	Research, development and production computing for the Australian Antarctic Division under the ACE-CRC/AGP/AAD-NCI partnership
A/Prof. Jason Evans, University of NSW	1000	Regional Climate Modelling in South-east Australia
Dr Benjamin Galton-Fenzi, University of Tasmania	1000	Modelling of the interaction between Antarctica and the Southern Ocean
Prof Susan Clark, Garvan Institute of Medical Research	1000	Cancer Epigenome Computational Analysis
Professor Russell Boyce, UNSW Canberra	992	Physics of the interactions between high-speed craft and their environment
Professor Kerry Hourigan, Monash University	958	Advanced Modelling of Fluid-Structure Interaction and Biofluid Flows
Dr Claudio Cazorla, University of NSW	950	Rational design of novel multiferroic materials for energy harvesting and energy efficiency
Dr Chenghua Sun, Swinburne University of Technology	942	Computer-Aided Materials Design for Clean Energy
Dr Xuebin Zhang, CSIRO	912	Downscaling future climate change from CMIP5 climate models with an eddy-resolving ocean model
Dr Oliver Hofmann, University of Melbourne	912	VCCC Pilot Project
Professor Catherine Stampfl, University of Sydney	910	First-Principles Investigations of Processes and Properties in Catalysis, Coatings, and Devices

Lead CI, Institution	Allocation (KSU)	Project title
Dr Andrew Neely, UNSW Canberra	904	Fluid-thermal-structural interactions for high-speed flight and propulsion
Dr Jingming Duan, Geoscience Australia	900	Magnetotelluric and Electrical data inversion
Professor Tiffany Walsh, Deakin University	900	Development and application of bio/nano interfacial simulations
Dr Adrian Pudsey, Royal Melbourne Institute of Technology	900	Aerothermodynamics of Hypersonic Flight and Enabling Technology
Prof Clive McAlpine, University of Queensland	900	The capacity of forests to protect regional climate under global warming: science and policy implications
Dr Ting Liao, Queensland University of Technology	893	Theoretical Design of Carbon Based Materials for Energy Application
Dr Dietmar Dommenget, Monash University	880	Global scale decadal climate variability in a ACCESS hierarchy of climate models
Dr Martin Cope, CSIRO	876	Future Air Quality Projection
Professor Jill Gready, Australian National University	874	Simulation of Enzyme Mechanisms, and Protein Dynamics, Structures and Properties
Prof Benjamin Powell, University of Queensland	867	Computational approaches to organic photonic and electronic materials: from strongly electronics to device engineering
Dr Terry Frankcombe, Australian National University	856	Efficient chemical dynamics in gas phase, solid phase and heterogeneous systems
Prof Margaret Lech, Royal Melbourne Institute of Technology	850	Deep Emotional Intelligence
A/Prof. Jason Sharples, University of NSW	844	Modelling and simulation of dynamic bushifre propagation
Miss Luz Garcia, Swinburne University of Technology	840	Diagnosing Hydrogen Reionization with metal absorption line ratios.
A/Prof Serdar Kuyucak, University of Sydney	833	Free Energy Simulations of Ion Channels and Transporters
Prof Marcela Bilek, University of Sydney	807	Harnessing the bioactivity of protein fragements and peptides
Mr Asger Gronnow, University of Sydney	800	The effect of magnetic fields on the survival of gas clouds in galaxies
A/Prof Craig O'Neill, Macquarie University	800	dfss
Mr Alessio Arena, FEI	800	Lithicon production processing
Professor Simon Ringer, University of Sydney	787	Exploring structure-property correlations in advanced materials: Nexus between computational simulation and atomic resolution microscopy
A/Prof. Jared Cole, Royal Melbourne Institute of Technology	775	The materials science of transport and decoherence in quantum devices.
Dr David Wilson, La Trobe University	772	Computational Study of Novel Molecular Properties
Mr Adam Phipps, Victor Chang Cardiac Research Institute	760	VC Dunwoodie
Dr Adrian Sheppard, Australian National University	750	Computational Mesoscale Physics, Probing Complex and Hierarchical Material Structure
Professor Julian Gale, Curtin University of Technology	750	Atomistic Simulation for Geochemistry and Nanoscience
Professor Sean Li, University of NSW	749	Investigating electronic properties of novel oxide materials for spintronic and energy applications
Mr Simon Mortensen, DHI	740	DHI-005
Professor Geraint Lewis, University of Sydney	725	SSimPL-ACS The Survey Simulation PipeLine - Alternative Cosmologies Study
A/Prof. Valentijn Pauwels, Monash University	722	Bias removal in data assimilation systems for flood forecasting
Dr Trevor Allen, Geoscience Australia	710	EQRM
Prof Salvy Russo, Royal Melbourne Institute of Technology	701	ARC Centre of Excellence in Exciton Science
Prof. emer. Michael Crisp, Australian National University	700	Evolution of Australia's globally unique hotspot of floral diversity: phylogenomic analysis of Myrtaceae
Professor Robert Stranger, Australian National University	700	Computational Studies of the Mn/Ca Cluster in Photosystem II

Lead CI, Institution	Allocation (KSU)	Project title
Mr Craig Arthur, Geoscience Australia	700	Severe Wind and Coastal Inundation Modelling
Dr Daohua Bi, CSIRO	688	ACCESS preparation for IPCC AR5
Prof Richard Sandberg, University of Melbourne	684	High-fidelity simulations of turbomachinery applications
A/Prof Xiao Hua Wang, UNSW Canberra	668	Oceanic Nepheloid Layers and Their Role in Coastal Oceanography
Dr David Huang, University of Adelaide	659	Multi-scale modelling of soft condensed matter in functional materials and biology
Dr Louis Moresi, University of Melbourne	650	Instabilities in the convecting mantle and lithosphere
Prof. David Thomas, Garvan Institute of Medical Research	650	A whole genome study to map heritable risk in sarcoma
Dr. David Lescinsky, Geoscience Australia	650	GA-NCI development collaboration space
Professor Robert Stranger, Australian National University	650	DFT and TD-DFT Studies of Organometallic and Metal Cluster Systems
Associate Professor John Young, UNSW Canberra	646	Low Reynolds Number Aerodynamics of Flapping Wings
Dr Reza Mahjoub, University of NSW	630	Interface control of ferroelectricity in ferroelectric superlattices
Professor Gavin Huttley, Australian National University	626	Statistical modelling of genetic variation
Professor Maria Forsyth, Deakin University	620	Computational investigation of new selective transport materials
Dr Alister Page, University of Newcastle	620	Quantum Chemical Simulation of Interfacial Chemical Phenomena
Dr Hongtao Zhu, University of Wollongong	611	Crystal plasticity FEM simulation of severe plastic deformation techniques
Dr Yan Jiao, University of Adelaide	608	Modeling electrocatalytic energy conversion reactions on precious-metal-free materials by DFT for optimal catalyst design
Dr Junming Ho, University of NSW	607	Anion transporters as novel therapeutic agents
Dr Elizabeth Krenske, University of Queensland	605	Theoretical modelling of protein-inhibitor interactions and chemical reactivity
Professor Shin-Ho Chung, Australian National University	600	Computational Studies of Poplypeptide Toxins from Venomous Animals Targeting Cationic Membrane Channels
Dr Nikhil Medhekar, Monash University	600	CoE FLEET
Professor Peter Rayner, University of Melbourne	600	Assimilation of Trace Atmospheric Constituents for Climate
Prof Andrew Ooi, University of Melbourne	600	Computational Fluid Dynamics Studies of Buoyant Channel and Rough Pipe Flows
Emeritus Professor Ross Griffiths, Australian National University	600	The role of convection in ocean circulation
Mr Adam Phipps, Victor Chang Cardiac Research Institute	600	VC Martinac
Prof Peter Betts, Monash University	591	Subduction disruption - transient modifications to permanent termination of convergent margins
Dr Ming Zhao, University of Western Sydney	587	Accurate prediction of hydrodynamic forces and their variation frequency on inclined offshore cylindrical
Dr Catia Domingues, University of Tasmania	586	Ocean heat uptake processes: implications for global and regional sea level change in the ACCESS model
Prof Hans De Sterck, Monash University	578	Advanced simulation methods for the coupled solar interior and atmosphere
Dr Simon McClusky, Australian National University	575	Environmental Geodesy and Geodynamics
Dr Judy Hart, University of NSW	572	Design and development of new inexpensive materials for efficient hydrogen production
Dr Martin Bell, CSIRO	560	Transients and Variables with the MWA
Prof Salvy Russo, Royal Melbourne Institute of Technology	554	Prediction of the Properties of Materials and Nanomaterials
Dr Jason Monty, University of Melbourne	550	LES of high Reynolds number turbulent wall bounded flows

Lead CI, Institution	Allocation (KSU)	Project title
Dr Marcin Adamski, Australian National University	550	Coral genomics, transcriptomics and epigenomics
Assoc Prof Todd Lane, University of Melbourne	550	Large-eddy simulation of atmospheric turbulence with application to fires, aviation, and clouds
Dr Nicole Kessissoglou, University of NSW	550	Aeroacoustic analysis of a finite wall-mounted airfoil
Dr Thomas Plantard, University of Wollongong	537	Security Analysis of Lattice-based Cryptosystems
Prof Elizabeth Ritchie-Tyo, UNSW Canberra	528	WRF Testing for Tropical Cyclone Studies
Mr Daniel Macdonald, Macquarie University	521	Constraining the circumstellar environment of AGB and post-AGB objects.
Dr Luming Shen, University of Sydney	516	Atomistic simulations of nanoscale liquid flow on solid surface
Dr. Mark Baird, CSIRO	516	Improved estimates of water quality variables for Great Barrier Reef management using a data-assimilating implementation of the eReefs model.
Dr Edoardo Tescari, University of Melbourne	510	The Interplay Between Galaxies and Intergalactic Gas At High Redshift, part III
Prof Craig Moritz, Australian National University	501	Phylogenetic inference using genome-scale data: methods and applications
Dr Diego Molla-Aliod, Macquarie University	500	Deep learning experiments for text summarisation
Dr Daniel Chung, University of Melbourne	500	Direct numerical simulation of wall-bounded and buoyancy-driven turbulent flows
Dr Amanda Barnard, CSIRO	500	Theory and Simulation of Nanomorphology and the Environmental Stability of Nanostructures
A/Prof Peter Strazdins, Australian National University	500	Parallel Systems Course COMP4300
Matthew Bailes, Swinburne University of Technology	500	A search for highly accelerated binary pulsars
Dr Mohammednoor Altarawneh, Murdoch University	500	Fundamental Understanding of the Role of Singlet Molecular Oxygen in Spontaneous fires
Dr Yun Wang, Griffith University	499	Atomic engineering of photoactive MOFs for solar fuel production
Prof Anthony Papenfuss, Peter MacCallum Cancer Centre	498	Towards a Better Understanding of the Evolution of Drug Resistance in Tumours Using Detailed Predictive Computational Models
Professor Nikolai Petrovsky, Flinders University	498	Molecular modelling for design of more effective vaccine adjuvants
Dr Nicholas Williamson, University of Sydney	495	Stratified boundary layers in riverine environments: Modification of flow stability by lateral circulation
Dr. Lars Goerigk, University of Melbourne	483	Theoretical and Computational Quantum Chemistry Including Development of Computational Methods, Computational Materials Science, and Computational Treatment of Biomolecules
Doctor Meredith Jordan, University of Sydney	467	Molecular Interactions
Associate Professor Wouter Schellart, Monash University	464.165	Geodynamic models of episodic mountain building
Mr Dave Penton, CSIRO	452	Australian Water Resource Assessments Calibration Test
Prof Chennupati Jagadish, Australian National University	451	Nanostructured optoelectronic devices: new materials and applications
Dr John Pye, Australian National University	450	Modelling of high-temperature concentrating solar thermal energy systems
Dr Warren Kaplan, Garvan Institute of Medical Research	450	Garvan Genome Pilot
Dr David Gildfind, University of Queensland	443	Simulation of hypersonic flows in expansion tubes
Ass Prof Moninya Roughan, University of NSW	440	Advancing dynamical understanding in the East Australian Current Optimising the ocean observation and prediction effort
Mr Rodrigo Canas, University of Western Australia	430	Intra-Halo Stellar Mass in Simulations
Professor Leo Radom, University of Sydney	430	Structural and Mechanistic Chemistry

Lead CI, Institution	Allocation (KSU)	Project title
Dr Junming Ho, University of NSW	405	Anion transporters as novel therapeutic agents
Dr Marlies Hankel, University of Queensland	400	Nanoporous membranes for energy applications
Dr Warren Kaplan, Garvan Institute of Medical Research	400	Garvan - KCCG Research
Research Fellow Rob Sok, FEI	400	FEI project 2
Dr Iwan Jensen, University of Melbourne	400	Exact Enumerations in Statistical Mechanics and Combinatorics
Dr Warren Kaplan, Garvan Institute of Medical Research	400	Garvan - KCCG MGRB
Dr. Johnathan Kool, Geoscience Australia	400	Marine Operations and Processing
Mr Laurence Davies, Geoscience Australia	400	Tomography Data Processing
Dr Jiabao Yi, University of NSW	400	Mechanism of ferromagnetism in oxide and 2D based diluted magnetic semiconductors (DMSs)
Mr Simon Mortensen, DHI	400	DHI-003
Mr Simon Mortensen, DHI	400	DHI-012 Provision Unlimited
Dr Christoph Rohmann, University of Queensland	400	Computer aided materials design for metal matrix composites reinforcements.
Dr David Chalmers, Monash University	398	The dynamics of drug behaviour in the human body
Dr Cullan Howlett, University of Western Australia	394	SONGS - Simulations Of Non-standard Gravity for Surveys
Dr Alister Page, University of Newcastle	362	Quantum Chemical Modelling of Nanoscale Chemical Processes
Dr Stephen Gould, Australian National University	360	Machine Learning for Computer and Robotic Vision
Dr. Chunguang Tang, University of New South Wales	358	Materials Design for Self-toughening Bulk Metallic Glasses
Dr Tapio Simula, Monash University	356	Quantum Turbulence
Professor Gregory Metha, University of Adelaide	355	Metal Nanoclusters as Catalysts for Photoreduction of CO2
Dr Merlinde Kay, University of NSW	354	Australian Solar Energy Forecasting System (ASEFS) - Phase 1
Dr Rong Chen, Australian National University	350	Animal toxins as novel analgesics and pesticides
Dr Justin Leontini, Swinburne University of Technology	350	Oscillatory flows in complex geometries
Associate Professor Marcel Cardillo, Australian National University	349	Understanding patterns of evolutionary and ecological diversification
Dr Jingxian Yu, University of Adelaide	348	Peptronics: Understanding the Relationship between Structures and Properties
Dr Peter Jones, University of Technology, Sydney	347	Allosteric Control of ATP Hydrolysis in the ABC Transporter Catalytic Cycle.
Dr Michael Fernandez, CSIRO	344	Large Scale Distributed Evolutionary Optimization of Machine Learning Models of Nanomaterials Performance
Professor Ian Dance, University of NSW	343	Computational Bio-inorganic and Supramolecular Chemistry
Prof Lei Wang, University of Wollongong	337	Exploring National Treasure: Automatic Photo Search for the Large Collection of National Archives of Australia
Prof Mark Johnson, Macquarie University	335	Deep Learning for Natural Language Processing
Dr Daniel King, University of NSW	330	Investigation of High Entropy Alloys for use in advanced nuclear applications
A/Prof Mike Ford, University of Technology, Sydney	330	Nanostructured Materials for Energy Efficiency Applications
Mr John Wilford, Geoscience Australia	328	Data mining and geostatistical modelling for geoscience applications
Dr Matthew Perugini, La Trobe University	326	Molecular Dynamics of Protein Targets Linked to Infectious, Diabetic and Age-Related Diseases
Dr Xiaodong Li, Royal Melbourne Institute of Technology	320	Solving real-world large scale black-box optimization problems

Lead CI, Institution	Allocation (KSU)	Project title
Dr Kai Qin, Royal Melbourne Institute of Technology	320	Collaborative Learning and Optimisation
Dr Ailie Gallant, Monash University	312	Mesoscale modelling of urban landscapes for assessing heat adaptation and mitigation strategies with climate change
Dr Felicity Graham, University of Tasmania	310	Improving model simulations of ice sheet dynamic processes that contribute to sea level rise
A/Prof Michael Kirkpatrick, University of Sydney	306	Surface driven mixing of thermally stratified riverine flows
Prof Graham Heinson, University of Adelaide	306	3D Geophysical Imaging for the Australian Lithospheric Architecture Magnetotelluric Project (AusLAMP)
Mr Andrew Driscoll, DHI	300	DHI-019
Research Fellow Rob Sok, FEI	300	FEI project
A/Prof Peter Strazdins, Australian National University	300	Computer Science Undergraduate Course
Professor Duong Do, University of Queensland	300	Novel Characterization of Porous Structure and Surface Chemistry of Carbon by means of Monte Carlo computer simulation
Dr Fang Yuan, Geoscience Australia	300	Copernicus Australia Regional Data Hub - Sentinel Archive
Dr Iwan Cornelius, Australian Commercial Organisation	300	Amentum Production Computing
A/Prof Chris Ling, University of Sydney	292	A combined experimental and computational approach to understanding and developing solid-state ionic conductors
Dr Anh Pham, University of NSW	289	Theoretical study of 2D and 3D topological materials
Dr Aaron McDonough, SGI	286	General Share for User Code Development and Testing
Prof. Albert Van Dijk, Australian National University	282	The next generation of environmental model-data assimilation and forecasting systems
Dr Daniel Rosauer, Australian National University	280	Why are biodiversity hotspots found where they are?
Dr Nicolas Flament, University of Wollongong	277	The geodynamics of past sea level changes
Professor Bijan Samali, University of Western Sydney	272	Intersect adhoc proj 14
Associate Professor Rongkun Zheng, University of Sydney	265	Low dimensional magnetism and supercondcutivity
Prof Andrew Blakers, Australian National University	265	Satisfying 90% of the electricity need in the National Electricity Market with wind, photovoltaics and off-river pumped storage
A/Prof Lexing Xie, Australian National University	263	The Anatomy of Social Media Popularity
Mr Adam Phipps, Victor Chang Cardiac Research Institute	260	VC Suter
Mr Russel Morison, University of NSW	260	Spectral Wind-Wave Model Development
Dr Julian Berengut, University of NSW	260	Electronic spectra of superheavy elements and highly-charged ions
Professor Joseph Lai, UNSW Canberra	257	Disc Brake Squeal
Dr Narjes Gorjizadeh, University of NSW	255	First-principle study of reaction between complex carbon-bearing materials and metallic phase towards a novel approach for recycling waste polymers for sustainable environment
Prof Igor Bray, Curtin University of Technology	250	Atomic Collision Theory
Professor Dougal McCulloch, Royal Melbourne Institute of Technology	250	Electronic structure of boron nitride and other novel coating systems
Dr Timothy Trudgian, UNSW Canberra	250	Verifying the Riemann hypothesis to a new record height
Dr David Gwyther, University of Tasmania	250	Intercomparison models for assessing ice shelf-ocean interaction
Prof Simon Foote, Australian National University	250	Genomic Analysis

Lead CI, Institution	Allocation (KSU)	Project title
Professor Paul Webley, University of Melbourne	250	First-principles computation study of Zeolite for gas separation: novel molecular sieving mechanism and rational design
Professor Lloyd Hollenberg, University of Melbourne	250	Multi-Million Atom Quantum Computer Device Simulations
Dr Brendan Kennedy, University of Western Australia	250	Discovering criteria for blood element differentiation using rigorous simulation
Professor Brian Yates, University of Tasmania	250	Designing Better Catalysts
Dr Luke Barnes, University of Sydney	250	Lyman Alpha and stellar emission from high redshift galaxies
Dr. Alvaro Salazar, University of Queensland	250	The capacity of forests to protect regional climate under global warming
Professor Gleb Beliakov, Deakin University	250	Large scale high accuracy computations for studies of Riemann's zeta function, as part of the 8th Hilbert problem
Professor Christoph Arns, University of NSW	249	Multi-scale multi-physics analysis of porous media
Dr Sergiy Shelyag, Monash University	244	Radiative magneto-hyrdrodynamic modelling of interconnected solar interior and atmosphere
Dr Susanna Guatelli, University of Wollongong	243	Characterisation of novel nanoceramic materials to improve radiotherapy clinical outome in the fight against cancer
Professor Michael Reeder, Monash University	240	The dynamics of subtropical anticyclones and the connection to drought, heatwaves and bushfires in southern Australia
Associate Professor Melih Ozlen, Royal Melbourne Institute of Technology	240	Fuel treatment planning maintaining habitat availability and connectivity for endangered species conservation
Prof Alexander Novikov, University of Technology, Sydney	239	Boundary element methods for goodness-of-fit tests
Prof Kefei Zhang, Royal Melbourne Institute of Technology	235	RMIT SPACE
Dr Joseph Horvat, University of Wollongong	228	Blue shift of terahertz absorption lines for sucrose
Professor Kiet Tieu, University of Wollongong	222	Quantum mechanics and molecular dynamics modelling of triblock copolymers in metal forming applications
Dr Rika Kobayashi, Australian National University	220	Chemistry Porting Project
Dr Mirela Tulbure, University of NSW	211	Surface water dynamics from space
Dr Fangbao Tian, University of NSW	210	Fluid-structure Interactions and Complex Flows in Biological and Biomedical Systems
Dr Quoc Le Gia, University of NSW	210	Simulation of stochastic heat equation on the unit sphere
Dr Evelyne Deplazes, Curtin University of Technology	209	Understanding peptide-membrane interactions at the molecular level
Professor Steven Armfield, University of Sydney	209	Direct simulation of transition for natural convection flow in inclined differentially heated cavities
A/Prof. Jason Evans, University of NSW	206	Will East coast lows change in frequency or intensity in the future?
Dr Christian Wolf, Australian National University	205	SkyMapper and the Southern Sky Survey
Dr Lucy Marshall, University of NSW	205	Bayesian ecohydrological modeling and uncertainty analysis
Dr Jingming Duan, Geoscience Australia	202	GA Workshop
Dr Marcus Doherty, Australian National University	201	First principles innovation of solid-state quantum technologies
Dr Nitin Yadav, Royal Melbourne Institute of Technology	201	Scalability analysis for formal verification techniques
Professor LiangChi Zhang, University of NSW	200	An integral approach for the defect-free fabrication of high-integrity systems
Dr Warren Kaplan, Garvan Institute of Medical Research	200	Garvan - KCCG GenPhen
Dr Marc Schartmann, Swinburne University of Technology	200	The impact of star formation and AGN feedback on circumnuclear discs in nearby active galaxies

Lead CI, Institution	Allocation (KSU)	Project title
A/Prof Michael Kirkpatrick, University of Sydney	200	Surface driven mixing of thermally stratified riverine flows
Dr Fang Yuan, Geoscience Australia	200	Copernicus Partners Testing and Development
Dr Andrew Sims, Commercial	200	Commercial Research
Dr David Wilson, La Trobe University	200	Quantum Chemical Molecular Properties
Dr. Matthew Garthwaite, Geoscience Australia	200	Geodetric research to measure surface deformation of the Australian continent
Professor Andy Pitman, University of NSW	200	Land Surface Science
Mr Simon Mortensen, DHI	200	DHI-013
Researcher Michael Moore, Geoscience Australia	200	Mitigation of Site Specific Errors from Geodetic Time Series
Mr Masoud Abdi, Deakin University	200	Deep learning for Image Classification
Associate Professor Steven Siems, Monash University	196	Simulations of wintertime storms across Southeast Australia, Tasmania and the Southern Ocean
Dr Xiao Liang, University of Sydney	195	Elucidate the fundamental chemistry of biomass hydrothermal liquefaction
Dr Martin Singh, Monash University	192	Idealised convection-resolved modelling of the diurnal cycle and monsoon circulations
Mr Shuai Li, University of Wollongong	188	Automated recognition of daily activities
Dr Xingyong Wang, University of Wollongong	181	Computational study on the molecular mechanisms of UV-induced DNA photodamage and photolyase-catalysed DNA photorepair
Research Scientist Jing Huang, CSIRO	181	Hi-res mapping of renewable energy from meteorological records for Australia
Mr Adam Phipps, Victor Chang Cardiac Research Institute	180	VC HO
Professor Thomas Welberry, Australian National University	180	Computation of X-Ray Diffraction Patterns for 3D Model Systems
Dr Zhimin Ao, University of Technology, Sydney	177	Density functional theory calculation studies on two-dimensional and hybrid materials for a sustainable environment
Dr Yingping Wang, CSIRO	176	Using ACCESS to assess the biophysical consequence of a greening earth
Dr Flora Salim, Royal Melbourne Institute of Technology	175	Multivariate time-series prediction of electricity consumption
Dr Vanessa Haverd, CSIRO	175	The Australian Continental Carbon Budget
Mr Richard Miller, Macquarie University	175	Faculty of Science and Engineering Piloting Environment
Dr Jiangning Song, Monash University	175	Molecular dynamics simulation of the interaction of the antimicrobial peptide polymyxin B with the outer membrane of Pseudomonas aeruginosa
Dr Drew Parsons, Murdoch University	175	Subtle quantum mechanical forces of ions in solution.
Dr Matthew Arnold, University of Technology, Sydney	174	Optimization of plasmonic nanoantennas and metamaterials
Professor Allan Canty, University of Tasmania	174	Catalysis and Organometallic Chemistry
Associate Professor Nicolas Cherbuin, Australian National University	170	Brain structure, cognition, and ageing a magnetic resonance imaging investigation
Dr Michael Breedon, CSIRO	165	The adsorption of molecules onto surfaces found in energy storage devices
Dr Alberto Peruzzo, Royal Melbourne Institute of Technology	163	RMIT Node, ARC Centre of Excellence for Quantum Computation and Communication Technology
Dr Wei Wen, University of NSW	163	Joint Analysis of Imaging and Genomic Data to Study the Structure and Function of Human Brain
Dr Andrew Kiss, UNSW Canberra	161	Nonlinear Dynamics of Ocean Currents
Dr Kasper Kaergaard, DHI	160	DHI-017
Dr Nerilie Abram, Australian National University	160	An ensemble of simulations for Australasian palaeoclimate data-model assessments

Lead CI, Institution	Allocation (KSU)	Project title
Dr Dillon Hunt, University of Queensland	160	DSTO Pilot Project
Prof David Edwards, University of Western Australia	160	Analysis of complex genomes
A/Prof Aaron Oakley, University of Wollongong	156	Dynamics of DNA clamps on DNA
Dr Daniel Edgington-Mitchell, Monash University	152	Investigations into shock-turbulence interaction and its role in sound production for high speed jets.
A/Prof Richard Yang, University of Western Sydney	152	Multiscale modelling of Advanced Engineering Materials and Structures
Dr Jonathan Watmuff, Royal Melbourne Institute of Technology	151	Fundamental physical processes associated with bypass transition
Prof Gary Rosengarten, Royal Melbourne Institute of Technology	151	Simulation of Fluidic Brownian Drift Ratchets
Prof Kefei Zhang, Royal Melbourne Institute of Technology	150	HPC-based data assimilation to forecast ionosphere and thermosphere
Ms Caroline Lai, DHI	150	DHI-018
Dr Stephen Roberts, Australian National University	150	Investigation of techniques to improve the prediction of flood events
A/Prof Craig O'Neill, Macquarie University	150	Tracking mantle slab dewatering using ASPECT
Dr Greg Birkett, University of Queensland	150	Molecular Simulation of Ionic Liquid - Carbon Capacitors
Dr Lawrence Cavedon, Royal Melbourne Institute of Technology	150	Deep Learning for Complex Labeling Tasks
A/Prof Timothy Garoni, Monash University	148	Design, analysis and application of Monte Carlo methods in statistical mechanics
Dr. Ben Thornber, University of Sydney	145	Detached Eddy Simulation of a Generic Road Vehicle
Prof Anatoli Kheifets, Australian National University	145	Theory of multiple atomic ionization
Dr Ashish Sharma, University of NSW	143	Dynamical downscaling hydro-climatic simulations for water resources planning and management in a changing climate
Dr Akbar Khatibi, Royal Melbourne Institute of Technology	140	Numerical Analysis of Scarf Joints
Dr Petra Heil, University of Tasmania	137	(East) Antarctic sea ice: Ice-ocean interactions and ice kinematics in a changing climate.
Dr Anthony Murphy, CSIRO	136	Modelling of the Plasma Production of Nanostructures
A/Prof Adam Trevitt, University of Wollongong	133	Computational Investigation of the Chemistry of Reactive Intermediates
Dr Benjamin Schwessinger, Australian National University	133	The Evolution of stripe rust virulence
Prof John Lattanzio, Monash University	130	Convective nuclear burning in 3D - Fixing the weak link in stellar models
Dr Xiaoke YI, University of Sydney	128	Integrated photonic simulation based on COMSOL
Dr Amr Al Abed, University of NSW	126	Bioelectric multiphysics simulations to optimise the performance of the Bionic Eye
Dr Zheng Liu, University of Wollongong	126	ï¿¼First-principles design and characterisation of topological materials
Dr Angus Gray-Weale, Bureau of Meteorology	125	Defects in hybrid perovskites, and nanoscale hydrodynamic size measurements
Dr Murat Tahtali, UNSW Canberra	125	Imaging Through the Atmosphere, L-SPECT simulation and reconstruction
Mrs Rikki Weber, Geoscience Australia	125	Development of volcanic risk models
Prof Yuantong Gu, Queensland University of Technology	124	Large scale molecular dynamics simulations in biomolecular interactions and material science
Dr Elena Pasternak, University of Western Australia	124	Wave propagation in fragmented materials
Dr Cullan Howlett, University of Western Australia	124	SONGS - Simulations of Non-standard Gravity for Surveys
Dr Lenneke Jong, University of Tasmania	124	Coupled Ice-Ocean modelling using FISOC to investigate the effect of ocean induced basal melt rates on marine ice sheets.

Lead CI, Institution	Allocation (KSU)	Project title
Dr Charlotte Welker, University of Western Australia	124	Playing on the E-STRINGS: Effects of STReam INfall on Galactic Structure
Dr James Bull, University of Melbourne	124	Molecular photoswitching: Combining ion mobility mass spectrometry and computational chemistry
Dr Kazuya Kusahara, University of Tasmania	124	Modelling the intimate links between sea ice, landfast ice, water mass formation and ice shelf melt around East Antarctica
Pascal Elahi, University of Western Australia	124	Building Synthetic UniveRses for Surveys
Dr Tiannan Guo, Children's Medical Research Institute	124	Intelligent data mining of 70,000 human cancer proteomes from the ACRF ProCan
Dr Asaph Widmer-Cooper, University of Sydney	122	Interactions and self-assembly of colloidal nanorods: Establishing design rules for creating new nano-structured materials
Dr Torsten Thomas, University of NSW	121	Assembly of next-generation sequencing data for microbial metagenomes
Dr Tony Vo, Monash University	120	From Saturn's hexagon to Earth's polar vortex; elucidating shear-layer instability in rotating flows
Dr Pauline Ding, Australian National University	120	Bootstrapping F-test for Random Effects in Linear Mixed Models
Dr Leo Lymburner, Geoscience Australia	120	AGDC Experimental (External)
Mr Richard Miller, Macquarie University	120	Novel Microwave Antennas and EM Structures
Dr Shahram Karami, Monash University	120	DNS of supersonic jet
Dr Craig Harrison, Geoscience Australia	120	Least-squares adjustment of the national geodetic network
Mr David Kent, Bureau of Meteorology	120	Extended Hydrological Prediction modelling
Associate Professor Melih Ozlen, Royal Melbourne Institute of Technology	119	Energy Store Optimisation
Dr Ryan Armstrong, University of NSW	117	MUTRIS: Unconventional Rescources
Dr Ian Harman, CSIRO	115	Constructing a Coupled Economic-Climate System Model
Dr. David Lescinsky, Geoscience Australia	115	Assessing geothermal energy potential for the Australian Continent
Professor Qing-Hua Qin, Australian National University	113	Piezoelectric bone remodeling analysis by finite element method
Dr David Henry, Murdoch University	110	Nanoscale materials and Nanoscale Interactions - From Catalysts through to Hydrophobic Soils
Dr. Jenny Fisher, University of Wollongong	109	The use of state-of-the-art 3-D chemical transport modelling to unravel the effects of atmospheric chemistry on climate
Dr Edward King, CSIRO	108	National Remote Sensing Processing Facility
Dr Timothy Churches, University of NSW	106	General practice network discovery and surgical billing practices variation discovery using linked 10% sample MBS and PBS (Medicare) data
Dr Naomi Haworth, Australian National University	106	How does insulin work?
Dr Junfang Zhang, CSIRO	106	Molecular Dynamics Study of Gas Storage and Transport in Coals
Mr Dale Kerper, DHI	105	DHI-016
Prof Lan Wang, Royal Melbourne Institute of Technology	104	novel transport effects and phase transitions in topological semimetals
Professor LiangChi Zhang, University of NSW	104	Multiscale mechanics of metal/semi-conductor/bulk metallic glass (BMG) systems, mixed lubrication and fibre-reinforced composites
Dr Shahram Karami, Monash University	104	Direct numerical simulation of free circular and rectangular jets
Dr Jong-Leng Liow, UNSW Canberra	102	Study of xanthan gum behaviour through computational fluid dynamics and molecular simulation
A/Prof Balazs Csaba, Monash University	102	Dark Matter Discovery

Lead CI, Institution	Allocation (KSU)	Project title
Dr Andrew Hung, Royal Melbourne Institute of Technology	102	Conotoxins as Potential New Treatments for Nervous System Disorders
Professor Evatt Hawkes, University of NSW	101	Direct Numerical Simulations of Turbulent Combustion - Ancillary project
Mrs Chenoa Tremblay, Curtin University of Technology	101	Searching for Molecular Transitions with the MWA
Dr Arif Khan, Charles Sturt University	101	GA Computation for VANETs
Dr Louis Ranjard, Australian National University	101	Modelling dispersal and ecological parameters in Bayesian phylogeography
Dr Michael Hewson, Central Queensland University	100	ARC Linkage Wind Generation Project - WRF Wind Climatology
Professor Anthony Hill, Australian National University	100	DFT: in probing the uncharted areas of organometallic chemistry
Dr David McGuinness, University of Tasmania	100	Production of Linear Alpha Olefins Mechanistic and Applied Investigations
Professor Ian Dance, University of NSW	100	Computational Bio-inorganic and Supramolecular Chemistry
Dr Charlotte Welker, University of Western Australia	100	Playing on the E-STRINGS: the dwarf regime
Miss Sara Hamouda, Australian National University	100	Supporting User-Level Fault Tolerance in Extreme Scale Runtime Systems
Mr Siqi Liu, University of Sydney	100	Automatic 3D Neuron Reconstruction from Microscopic Images
Dr. Deidre Cleland, CSIRO	100	Stochastic optimisation of molecular geometries
Professor Andrew Rohl, Curtin University of Technology	100	Realistic Modelling of the Effects of Solvent and Additives on Crystallisation
Dr Tianfang Wang, University of the Sunshine Coast	100	Bioinformatics, molecular dynamic simulation of biofunctional proteins and mass spectrometric fragmentation mechanisms
Mr Azam Ahmad Bakir, University of NSW	100	Multiphysics biventricular model of the heart
Professor Brendan McKay, Australian National University	100	Extremal graph theory and Ramsey theory
Dr Joseph Antony, Australian National University	100	HPD on Raijin & Tenjin - Accelerating End-User Science Objectives using existing NCI HPD Assets
Barry Ninham Chair Stephen Hyde, Australian National University	100	Self-assembly of Polyphiles via Espresso Simulations
Dr Eva Cheng, Royal Melbourne Institute of Technology	100	Investigation of the mechanism of wind-induced acoustic noise
Prof Lin Padgham, Royal Melbourne Institute of Technology	100	Simulation experimentation
Mr Andre Minoche, Garvan Institute of Medical Research	99	Resolve complex clinical relevant structural variation and haplotypesÂ using novel linked short reads
Dr Alejandro Montoya, University of Sydney	95	Modelling of the Lithium Extraction from Aluminosilicates
Professor Tony Vassallo, University of Sydney	95	Modelling the interactions and influences of organic compounds in zinc-bromine redox flow battery systems
PhD Luis Azofra, Monash University	92	Electrochemical CO2 Conversion into Hydrocarbon Green Fuels. In-Silico Design for the Prediction of Novel and Efficient Catalysts
Dr. Mark Baird, CSIRO	90	eReefs Marine Modelling GBR1
Assoc. Prof. Wenyi Yan, Monash University	90	Optimization and structural analysis for additive manufacturing and maintenance
Dr Dandan Cui, University of Queensland	90	Understanding nanoscale adhesion and friction with the aid of molecular dynamics simulaition
Prof Peter Gill, Australian National University	90	Development and application of new quantum chemistry algorithms
Professor Iain Prentice, Macquarie University	82	Primary production in space and time

Lead CI, Institution	Allocation (KSU)	Project title
Dr Varghese Swamy, Monash University	80	First-Principles Modeling of Functional Titanium Dioxides and Hybrid Metalorganic Perovskites
Mrs Sarah Chapman, University of Queensland	80	The effect of climate change and urban growth on the urban heat island in Australian Cities
Prof Vanessa Hayes, Garvan Institute of Medical Research	80	Garvan - Human Comparative and Prostate Cancer Genomics - Vanessa Hayes
Prof Susan Clark, Garvan Institute of Medical Research	80	Garvan - Epigenetics Research - Susan Clark
Ms Tracy Bailey, ARPANSA	80	ARPANSA Pilot Project
Mr Derrick Lin, Garvan Institute of Medical Research	80	Garvan - Garvan DICE - Derrick Lin
Dr. David Lescinsky, Geoscience Australia	80	Virtual Laboratories development environment
Prof Ismet Canbulat, University of NSW	80	Coalburst prediction based on the energy approach methods
Mr Aaron Sedgmen, Geoscience Australia	80	EODS Web Services Delivery
Dr Ralf Haese, Geoscience Australia	80	Multiphase fluid flow and heat transport modelling with Tough2-MP
Dr Ross Brodie, Geoscience Australia	80	Potential Field Modelling in Cartesian Coordinates
A/Prof Aaron Oakley, University of Wollongong	80	Dynamics of DNA Clamps and Clamp Loaders
Prof Andreas Ernst, Monash University	80	Mine Planning Optimisation
Dr Merlinde Kay, University of NSW	80	Forecasting generation of distributed PV systems
Professor William Foley, Australian National University	78	Whole genome analysis of Eucalyptus - Australia's foundation tree
Professor Ravi Jagadeeshan, Monash University	77	The Mechanical Properties of Bio-Macromolecules
Dr Pierre Loos, Australian National University	76	Spherical geometry in chemistry and physics
Dr David Humphreys, Victor Chang Cardiac Research Institute	76	Decoding cardiac transcriptional complexity by utilizing high performance computing to analyse sequencing data sets
A/Prof. Matthew Hole, Australian National University	76	Computational Applications in Equilibrium and Instabilities of Advanced Plasma Confinement Geometries
Dr Wisam Hussam, Monash University	75	Rotating horizontal convection at high Rayleigh number
Dr Cagri Kumru, Australian National University	75	The road to efficiency
Dr Paul Slade, Australian National University	75	Efficient model choice for measurably evolving populations
Dr. Anoop Cherian, Australian National University	75	Deep Learning for Human Activity Recognition Using Computer Vision
Professor Timothy Baldwin, University of Melbourne	74	Deep Language Understanding
Dr Jeffrey Chan, Royal Melbourne Institute of Technology	71	Developing robust, distributed and efficient optimisation approaches using machine learning
Prof Matt Duckham, Royal Melbourne Institute of Technology	71	Open Spatial Analytics
Dr Zongyan Zhou, Monash University	70	Multiscale modelIng of Flow and Heat Transfer in Particulate Systems
Dr Citsabehsan Devendran, Monash University	70	Piezoelectric-Acoustic Interactions within Acoustofluidic systems
Associate Professor Tracie Barber, University of NSW	70	CFDMECH
Dr Jay Larson, Australian National University	68	Unified Model porting
Professor Paul Cally, Monash University	68	Numerical modelling of MHD effects and sunspot interior structure and dynamics
Prof Belinda Medlyn, University of Western Sydney	66	Development of an Australian terrestrial vegetation model
Dr Mario Mongiardini, University of NSW	63	Australian Naturalistic Driving Study (ANDS)
Dr Jorg Schluter, Deakin University	61	Computational Fluid Dynamics

Lead CI, Institution	Allocation (KSU)	Project title
Mr Michael Whimpey, Bureau of Meteorology	60	Radar Science and Nowcasting
Dr Leonard Hamey, Macquarie University	60	Affect Recognition from Video
A/Prof Peter Strazdins, Australian National University	60	Performance Analysis and Optimization of Large-scale Scientific Simulations
Mr Timothy Womersley, DHI	60	DHI-006
Dr Michael Ireland, Australian National University	60	Discovering and dating nearby young stellar associations with orbital traceback
Dr Cormac Corr, Australian National University	60	Modelling a linear plasma device for material studies
Dr Kei-Wai Kevin Cheung, Macquarie University	60	Studies on High-impact Weather, Climate Variability and Systems Dynamics
Dr Ki Wook Kim, University of NSW	60	Characterisation of the virome in children with and without islet autoimmunity.
Dr Daniel Cocks, Australian National University	60	How antimatter and matter solvate in liquids
Prof Saeid Nahavandi, Deakin University	60	A Deep Feature-based Medical Image Classification Framework
Prof Alan Chaffee, Monash University	60	Computational Quantum Chemistry
Professor Curt Wentrup, University of Queensland	59	Theoretical calculations on reactive molecules, intermediates and prebiotic chemistry pathways
Miss Nerida Wilson, Geoscience Australia	59	SRTM DEM processing
Dr Sebastian Kurscheid, Australian National University	58	Systematic optimization of parameters for ChIP-Seq peak calling algorithms using simulated short-read sequencing data
Dr Antonio Tricoli, Australian National University	58	Simulation of Nanoparticle Films Self-Assembly for Breath Analysis and Non-Invasive Medical Diagnosis
Dr Alejandro Montoya, University of Sydney	57	Molecular Modelling of Reactive Materials
Mr Leighton Alcock, University of Wollongong	56	Metal complexes of expanded cavity cage ligands
Dr Deanna D'Alessandro, University of Sydney	56	Towards conducting nanoporous framework materials
Dr Hui Zhang, Monash University	55	Interface in Mg Alloys
Dr Colin Jackson, Australian National University	55	Computational Structural Biology and Protein Engineering
Dr Thomas Poulet, University of NSW	55	Multiphyisics geological simulations using MOOSE
Dr Patrick Burr, University of NSW	54	Understanding the precipitation of Zr hydrides: a path integral molecular dynamics study.
Professor Peter Harrowell, University of Sydney	54	Soft Modes, Amorphous Defects and the Mechanical Properties of Metallic Glasses
Dr Gregory Wilson, CSIRO	53	Electronic Structure of Organic/Inorganic Dyes for Photovoltaic Applications
Dr Jason Wong, University of NSW	53	Annotation of non-coding mutations in whole cancer genomes
Professor Jeffrey Reimers, University of Sydney	53	Application of quantum electronic-structure methods to protein crystallography and photosynthetic function
Prof Michael Banner, University of NSW	52	Computational study of 3D breaking deep water, shallow water and shoaling water waves
Dr Alan Blair, University of NSW	52	Spiking Networks and Deep Learning for Speech, Language, Images and Games
Dr Alexander Swarbrick, Garvan Institute of Medical Research	50	Molecular characterisation of metastatic breast cancers
Mr Neil Symington, Geoscience Australia	50	High-performance Computational Groundwater Science
Professor Alistair Rendell, Australian National University	50	Large scale online learning with a mixed regularization model
Prof. Albert Van Dijk, Australian National University	50	OzEWEX
Assoc Prof Uta Wille, University of Melbourne	50	Free radicals in organic chemistry: Mechanistic insight into radical and non-radical processes using computational methods
Prof Tom Gedeon, Australian National University	50	Deep learning from psychophysiological data
Prof Simon Easteal, Australian National University	50	The National Centre for Indigenous Genomics

Lead CI, Institution	Allocation (KSU)	Project title
Dr Hardip Patel, Australian National University	50	Analysis of genome scale data to understand systems biology
Dr. Eugenia Kuo, ANSTO	50	Modelling mixed cation sodalites for radioactive iodine-129 capture and disposal in the nuclear fuel cycle
Dr Neshev Dragomir, Australian National University	50	Nonlinear and tunable dielectric metasurfaces
Dr Feng Wang, Swinburne University of Technology	50	Computational studies of ferrocene and its derivatives
Doctor Sebastien Allgeyer, Australian National University	50	Development of a better physics behind the tsunami modelling and coastal infrastructure behaviour.
Dr Robert Bursill, University of NSW	50	Lattice Models of Condensed Matter and Lattice Gauge Theory
Dr Scott Morrison, Australian National University	50	Subfactors and planar algebras
Dr Daniel Murtagh, Australian National University	50	Field ionization of Rydberg State anti-hydrogen
Associate Professor Nigel Marks, Curtin University of Technology	50	Atomistic Modelling of Carbon Nanostructures
Associate Professor Elena Ostrovskaya, Australian National University	50	Polariton Bose-Einstein Condensation in Optically-Induced and Microstructured Potentials
Dr Nicholas Matzke, Australian National University	50	Massive parallel analysis: Reconstructing the role of distance and seed traits in the global history of flowering plant dispersal
Dr Damian Moran, Macquarie University	50	Innovative Molecular Scaffolds by Design
Dr Vinuthaa Murthy, Charles Darwin University	50	Theoretical Investigations of Surface Reactions on Chromium Carbide and Mixed-Metal Carbides
Dr Tim Gould, Griffith University	50	Ab-initio calculation of high-temperature superconducting properties of palladium hydride
Professor Geoffrey Webb, Monash University	50	Learning from big data with generative and discriminative strategies
Dr Louise Olsen-Kettle, University of Queensland	50	Fractures and Earthquakes: modelling extreme events and instabilities
Dr Basura Fernando, Australian National University	50	Anticipating Human Activities in Real-time from Video Streams
Dr Brendan Malone, University of Sydney	49	Multiscale Digital Soil Mapping
Dr Christopher McAvaney, Deakin University	48	Deakin eResearch kick start project
Dr Courtney Ennis, La Trobe University	47	DFT and ab initio calculations of nitrile clusters and surfaces.
Dr Robert Woodcock, CSIRO	47	Earth Observation and Informatics
Dr Edward Simpson, Australian National University	45	Nuclear reactions and structure
Professor Terry Bossomaier, Charles Sturt University	45	Information flow in Vicsek Models
Professor Eric Kennedy, University of Newcastle	43	Non-equilibrium plasma conversion of toxic halogenated compounds and waste halogenated refrigerants to value added polymers - continuing
Dr Leonard Hamey, Macquarie University	42	Data Analytics for Malware Using Machine Learning
Dr Joseph Antony, Australian National University	41	Copernicus QA
Mr Matt Paget, CSIRO	41	Data Cube Rangelands and Crop Mapping Applications
Dr Gareth Vio, University of Sydney	41	Analysis of Fluid Structure Interaction Problems
Dr Akram Hourani, Royal Melbourne Institute of Technology	41	Autonomous Distributed Simultaneous Localization and Mapping
Dr Joseph Antony, Australian National University	40	NCI REI Demonstration Workspace
Dr Ross Brodie, Geoscience Australia	40	Potential Field Modelling in Spherical Coordinates
Dr Joshua Machacek, Australian National University	40	Positrons in Dust Grains
Dr Peter Milligan, Geoscience Australia	40	External Geophysics Users

Lead CI, Institution	Allocation (KSU)	Project title
Dr Andrew Fowlie, Monash University	40	Analysing Beyond the Standard Model physics with NCI computing time
Dr Daniel Lester, Royal Melbourne Institute of Technology	40	The Tensorial Rheology of Strong Colloidal Gels
Dr Graham Ball, University of NSW	40	DFT and Ab Initio Studies of Inorganic and Organometallic Complexes and Drug DNA complexes
Dr Amanda Karakas, Australian National University	40	The heavy element composition of post-AGB stars and planetary nebulae
Dr Leonardo Hardtke, University of Technology, Sydney	40	Himawari-8 EVI development in support of TERN Phenology product and forecasting.
Dr Atsushi Sekimoto, Monash University	40	Direct numerical simulations of Couette turbulence with adverse pressure gradient
Dr. Riyan Cheng, Australian National University	37	A powerful mixed effect model approach for novel genetic discoveries using joint analysis of multiple complex traits
Dr Lan Du, Monash University	37	Scalable Probabilistic Models for learning complex relational data with rich side information
Dr Gareth Vio, University of Sydney	36	Fluid-Structure Interaction using higher Order CFD
Dr Sophie Calabretto, Macquarie University	35	Absolute versus convective instabilites in three-dimensional boundary layers
Dr Alireza Valizadeh, Monash University	35	Modelling Porous Breakwaters using SPH method
Dr Joachim Mai, Intersect	34	Intersect commercial 01
Professor Eric Kennedy, University of Newcastle	34	Solid Oxide Fuel Cells
Dr Rose Andrew, University of New England	33	Woodland Eucalyptus Genomics
Dr Chuang Feng, Royal Melbourne Institute of Technology	31	Electro-mechanical behaviours of carbon nanotube composite structures
Prof. Jie Yang, Royal Melbourne Institute of Technology	31	Buckling of Functionally Graded Multilayer Graphene Nanocomposites
Dr Tania Vodenitcharova, University of Sydney	31	Numerical modelling of cutting of soft materials
Mr Johannes Pottas, Australian National University	31	Structural modelling of components in solar thermal energy systems
Dr Farzad Alavi Fard, Royal Melbourne Institute of Technology	31	Dynamic Programing for Australian Retirees
Dr Haydar Demirhan, Royal Melbourne Institute of Technology	31	Statistical Performance of Cryptographic Randomness Tests
Professor Malin Premaratne, Monash University	30	Computational framework for an Ab-initio Computer Model of SPASER
Dr Joseph Horvat, University of Wollongong	30	GaAs 1-x-y P y Bi x mixed crystals with tunable bandgap, ab initio calculations and experiment
Dr Tao Zou, Australian National University	30	On the Statistical Inference for Large Precision Matrices with Dependent Data
Dr Callum Atkinson, Monash University	30	Extending numerical simulation of turbulent flows via assimilation with experimental data
Professor Peter Karuso, Macquarie University	30	understanding fluorescence using DFT and ab initio methods
Dr Yu Lin, Australian National University	30	Large-Scale Genome Assembly and Analysis
Associate Prof. Nicholas Robins, Australian National University	30	Higher order interactions and lattice dynamics of Bose-Einstein condensates
Dr Snjezana Tomljenovic-Hanic, University of Melbourne	29	Diamond-based quantum devices
Dr Cedric Simenel, Australian National University	28	Microscopic and Macroscopic Studies for Nuclear Reactions
Dr Jeremy Davis, University of Wollongong	27	Microdosimetry for quality assurance of radiotherapy treatments and radioprotection applications
Dr Kylie Catchpole, Australian National University	26	Nanoplasmonic Solar Cells

Lead CI, Institution	Allocation (KSU)	Project title
Dr DukYong Choi, Australian National University	26	Simulation of Photonic Nanostructures
Dr Kris Ryan, Monash University	26	The evolution and stability of vortex rings and synthetic jets moving parallel to a flat plate
Mr Wei Liu, Griffith University	25	Force calculation of POSCARs for phonon calculation of real and postulated Zr3Fe and LaNi5 hydrides
Dr Victor Ciesielski, Royal Melbourne Institute of Technology	25	Genetic programming with expensive fitness evaluation
Dr. Francis Hui, Australian National University	25	Resampling-based hypothesis testing on the FLC test
Dr Anil Kumar Gorle, Griffith University	25	Binding of antiangiogenic platinum with glycasaminoglycans(GAGs): A study of structure and dynamics of Platinum bound GAG fragments
Mr Shea Andrews, Australian National University	25	Association of Alzheimer's disease genetic variants with cognitive performance
Dr Deborah Apthorp, Australian National University	25	Using machine learning to track disease progression in Parkinson's disease
Dr Megan McDonald, Australian National University	25	Resequencing fungal plant pathogen genomes with the Oxford Nanopore MinIon
Dr Justin Bruner, Australian National University	25	The evolution of the status quo bias
Principal Research S Tim McVicar, CSIRO	24	Developing an Australian Landsat-MODIS Blending Infrastructure (ALMBI)
Dr Denis O'Meally, University of Sydney	23	Koala genome project, genome annotation
Prof Andrew Eberhard, Royal Melbourne Institute of Technology	23	Decomposition and Duality: New Approaches to Integer and Stochastic Integer Programming
Mr Aaron Scott, University of Newcastle	22	University of Newcastle - IT Services - Development and Test Project
Prof. Markus Hegland, Australian National University	22	Sparse grid combination technique for quantities of interest
Mr Adam Phipps, Victor Chang Cardiac Research Institute	22	VC Harvey
Dr Dean Cutajar, University of Wollongong	22	Monte Carlo based treatment planning for brachytherapy
Dr Shane Culpepper, Royal Melbourne Institute of Technology	22	Discovery - Geospatial Search
Prof Jennifer Beck, University of Wollongong	22	Quadruplex MXB
Dr Stephen Davis, Royal Melbourne Institute of Technology	21	Disease emergence and dynamics on biologically motivated contact networks
Mr Grant Sayer, Macquarie University	20	Macquarie University Pilot Project
Dr Kiao Inthavong, Royal Melbourne Institute of Technology	20	Detailed analysis of fluid particle flows in the respiratory airway
Mr Pawan Parajuli, Australian National University	20	Study of Bacteriophage acquired virulence in Shigella flexneri strains
Dr Xingyong Wang, University of Wollongong	20	Theoretical exploration into the mechanism of UV-induced DNA damage
Dr Junfang Zhang, CSIRO	20	Adsorption Behavior of Hydrocarbon on Illite
Dr Timothy Trudgian, UNSW Canberra	20	Verifying the Riemann hypothesis to a new record height
Dr Shankar Kalyanasundaram, Australian National University	20	Finite Element Modelling of Engineering Systems
Mr James Slaughter, University of Wollongong	20	UoW FSAE Full Car Straight Line/Cornering and Yaw Models
Prof Michael Collins, Australian National University	20	Molecular Potential Energy Surfaces and Properties of Large Molecules
Prof Hans De Sterck, Monash University	20	test
Various Researchers	1311	Small Allocations - not specified

International Data Access in 2016-17

Europe	Hits	Download (MB)
Switzerland	50,077	21,560,688
Germany	316,543	10,296,699
France	78,966	5,047,480
Italy	253,931	4,952,038
United Kingdom	106,278	1,349,002
Spain	271,495	385,474
Norway	1,245	232,786
Sweden	212,096	1,562
Netherlands	14,114	1,310
Russia	6,355	23
Ireland	3,181	19
Romania	7,647	16
Portugal	2,148	7
Czech Republic	2,044	4
Estonia	2,474	4
Austria	1,185	2
Total	**1,329,779**	**43,827,114**

Asia	Hits	Download (MB)
China	744,589	861,695
Japan	14,906	775,836
Taiwan	8,976	303,879
India	16,979	67,097
Singapore	31,468	1,572
South Korea	5,853	26
Indonesia	10,435	22
Hong Kong	6,223	17
Vietnam	3,321	12
Iraq	6,516	11
Cambodia	1,531	3
Thailand	988	2
Total	**851,785**	**2,010,172**

North America	Hits	Download (MB)
United States	407,585	5,203,033
Canada	157,494	76,068
Mexico	14,523	67
Total	**579,602**	**5,279,167**

Africa	Hits	Download (MB)
South Africa	5,731	5,848
Morocco	4,173	7
Total	**9,904**	**5,855**

Oceania	Hits	Download (MB)
Australia	106,425,552	86,271,240
New Caledonia	1,046	94,552
New Zealand	9,214	1,778
Total	**106,435,812**	**86,367,569**

	Hits	Download (MB)
Grand Total	**109,238,126**	**137,525,022**

NCI Links to Government Portfolios

Government Department Impacted	Programme/Agency	Activities/Projects supported by NC
Education and Training	Australian Research Council (ARC)	Dependencies from more than 300 projects funded by the ARC's National Competitive Grant Programs (NCGP)
	NCRIS	Support for services provided by eight other NCRIS Capabilities
Industry, Innovation and Science	CSIRO	Australian Community Climate and Earth System Simulator (ACCESS)
		Earth Systems and Climate Change (ESCC) Hub of the NESP
	CSIRO and the Australian Institute of Marine Science (AIMS)	eReefs
	Geoscience Australia (GA)	Australian Geoscience Data Cube (AGDC)
		Copernicus Data Hub
		Uncover Initiative
		National Reference Grid
		Exploring For The Future Initiative
		Water Observations from Space (WOfS)
		Australian Natural Hazards Data Archive
Environment and Energy	National Environmental Science Programme (NESP)	Earth Systems and Climate Science Hub
	Environmental policy development	eReefs
	Bureau of Meteorology (BoM)	ACCESS
	BoM	ESCC Hub of the NESP
	Australian Antarctic Division	Antarctic Climate and Environment CRC (ACE-CRC)
Health	National Health and Medical Research Council	Dependencies from more than 20 NHMRC funded projects and fellowships
Agriculture and Water Resources	Policy development for the agricultural industry and water resources	ACCESS development with BoM/CSIRO; Development and hosting of the AGDC with GA and CSIRO, and WOfS with GA
	Murray-Darling Basin Authority	Exploitation of AGDC data

Government Department Impacted	Programme/Agency	Activities/Projects supported by NC
Resources and Northern Australia	Geoscience Australia	Exploring for the Future Initiative
Defence	Australian Geospatial Intelligence Organisation (AGIO)	Onshore topographic data and products provided by GA
	Australian Hydrographic Service (AHS)	Raw and processed bathymetric data collections provided by GA
Foreign Affairs and Trade	Policy development for, and by, the tourism sector	eReefs (through CSIRO)
Infrastructure and Regional Development	Australian Marine Safety Authority (AMSA)	Managing risks to marine vessels in Australian waters (undertaken with consultant DHI)
	Aviation Programs	Weather reports for the aviation industry
	Transport Infrastructure Programs	National Reference Grid

Outreach

Tours and Events

Group	Date
Science in ACTion: National Science Week event	12-13 August 2016
Visit from Chinese delegation	5 September 2016
IBM EXITE Camp	6 October 2016
Data Intensive Workshops	3-4 and 10-11 November 2016
Visit from Argentinian delegation	8 November 2016
Visit from Indonesian Reporters and Students Group	30 November 2016
Visit from OzEWEX Summer Institute Students	6 December 2016
Presentation and Tour with UNSW Canberra group	7 December 2016
Visit from National Youth Science Forum Session A	11 January 2017
Visit from National Science Teachers Summer School	12 January 2017
Visit from National Youth Science Forum Session C	25 January 2017
HPC Summer School	6-10 February 2017
Visit from College of Engineering and Computer Science students	20 March 2017
Science Meets Parliament	21-22 March 2017
Intel Xeon Phi (Knights Landing) Workshop	23-24 March 2017
Visit for Girls in ICT day	6 April 2017
Visit from ANU computer science students	16 May 2017
Allinea software training	17-18 May 2017
Visit from Science Circus students	26 May 2017

Presentations and Publications

Date	Event/Conference/Meeting	Location
July 2016	Australian Genomics Health Alliance	Canberra, Australia
July 2016	Preparing for your data future	Canberra, Australia
July 2016	QUESTnet	Gold Coast, Australia
August 2016	ANU GIS Forum	Canberra, Australia
August 2016	FOSS4G	Bonn, Germany
September 2016	Tomography for Scientific Advancement Conference	Bath, United Kingdom
September 2016	Geological Society of America	Denver, USA
September 2016	Lustre User Group Australia	Canberra, Australia
September 2016	Lustre Admins & Developers Conference	Paris, France
September 2016	2016 International Industrial Supercomputing Workshop	Barcelona, Spain
September 2016	NetApp InSight	Las Vegas, USA
September 2016	Geological Society of America	Denver, USA
September 2016	SciDataCon 2016: Advancing the Frontiers of Data in Research	Denver, USA
September 2016	RepScience 2016: First International Workshop on Reproducible Open Science	Hannover, Germany
September 2016	Prime Minister and Cabinet Open Data Forum	Canberra, Australia
October 2016	Australian Coastal and Oceans Modelling and Observations Workshop (ACOMO)	Canberra, Australia
October 2016	eResearch Australasia 2016	Melbourne, Australia
November 2016	Gov Innovate 2016	Canberra, Australia
November 2016	Data Intensive Workshop (x2)	Canberra, Australia
November 2016	Super Computing 2016	Salt Lake City, USA
December 2016	OzViz Conference	Sunshine Coast, Australia
December 2016	Bureau of Meteorology R & D Annual Workshop 2016	Melbourne, Australia
December 2016	ESGF Annual Meeting	Washington, D.C., USA
December 2016	2016 IEEE International Big Data Conference	Washington, D.C., USA
December 2016	American Geophysical Union: Fall Meeting	San Francisco, USA
January 2017	Earth Science Information Partners Winter Meeting	Bethesda, USA
January 2017	19th International Conference on Ecological Informatics and Ecosystems Conservation	Sydney, Australia
February 2017	Australian Meteorological and Oceanographic Society (AMOS) Conference	Canberra, Australia
February 2017	Australian Science Communicators Conference 2017	Adelaide, Australia

Date	Event/Conference/Meeting	Location
March 2017	CSIRO Earth Observations Conference	Canberra, Australia
March 2017	CSIRO Postdoctoral Fellow Conference	Melbourne, Australia
March 2017	Coupled Model Workshop 2017	Princeton. USA
March 2017	NeCTAR Science Clouds All-hands meeting	Melbourne, Australia
March 2017	7th Ocean Data Interoperability Platform Workshop	Hobart, Australia
March 2017	Intergovernmental Science Policy Platform on Biodiversity and Ecosystem Services Plenary	Bonn, Germany
March 2017	Open Geospatial Consortium Technical Meeting	Delft, Netherlands
March 2017	International Oceanographic Data and Information Exchange Meeting	Kuala Lumpur, Malaysia
April 2017	19th International Conference on Semantic Web and Natural Language Processing	Paris, France
April 2017	6th International Conference on Informatics, Environment, Energy and Applications	Jeju Island, South Korea
April 2017	GeoNetwork Forum	Canberra, Australia
April 2017	Digital Earth and the Locate 17 Conference	Sydney, Australia
April 2017	43rd Meeting of the Working Group on Information Systems & Services	Annapolis, USA
April 2017	WWW Conference 2017	Perth, Australia
April 2017	9th Research Data Alliance Plenary	Barcelona, Spain
April 2017	Target 2017	Perth, Australia
April 2017	European Geophysical Union (EGU) General Assembly 2017	Vienna, Austria
April 2017	Belmont Forum digital skills curriculum development workshop	Vienna, Austria
May 2017	International Symposium on Environmental Software Systems	Zadar, Croatia
May 2017	American Geophysical Union: Fall Meeting Program Committee	Washington D.C., USA
May 2017	Fujitsu-NCI collaboration meeting	Tokyo, Japan
May 2017	1st EU Environmental Research Infrastructures-Industry Joint Innovation Partnering Forum	Grenoble, France
May 2017	Japan Geoscience Union/American Geophysical Union Joint Meeting 2017	Chiba, Japan
May-June 2017	3rd Blue Planet Symposium	Bethesda, USA
May - June 2017	CSIRO Linked Data Symposium	Canberra, Australia
May-June 2017	Nordic e-Infrastructures Conferences	Umea, Sweden
June 2017	Invited Drishti workshop at Chinese Academy of Sciences	Beijing, China
June 2017	UN Conference on Oceans and Seas	New York, USA

Date	Event/Conference/Meeting	Location
June 2017	2017 All-Hands EarthCube Meeting	Seattle, USA
June 2017	Rodinia 2017: Supercontinent Cycles and Global Geodynamics	Townsville, Australia
June 2017	ANDS Drones and Big Spatial Data Workshop	Canberra, Australia
June 2017	International Council for Science Committee on Data for Science and Technology	Paris, France
June 2017	Open Repositories	Brisbane, Australia
June 2017	Open Geospatial Consortium Technical Meeting	St John's, Canada
June 2017	International Super Computing (ISC) 2017	Frankfurt, Germany

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