NCI, The Australian National University
143 Ward Road,
Acton ACT 2601

www.nci.org.au

NCI
NATIONAL COMPUTATIONAL INFRASTRUCTURE

Annual Report 2014/15

World-class high-end computing services for Australian researchers

National Computational Infrastructure
The Australian National University
143 Ward Road
Acton ACT 2601
T +61 2 6125 9800
E enquiries@nci.org.au
W nci.org.au
National Computational Infrastructure
@NCInews
NCINationalFacility

Produced by
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The Australian National University
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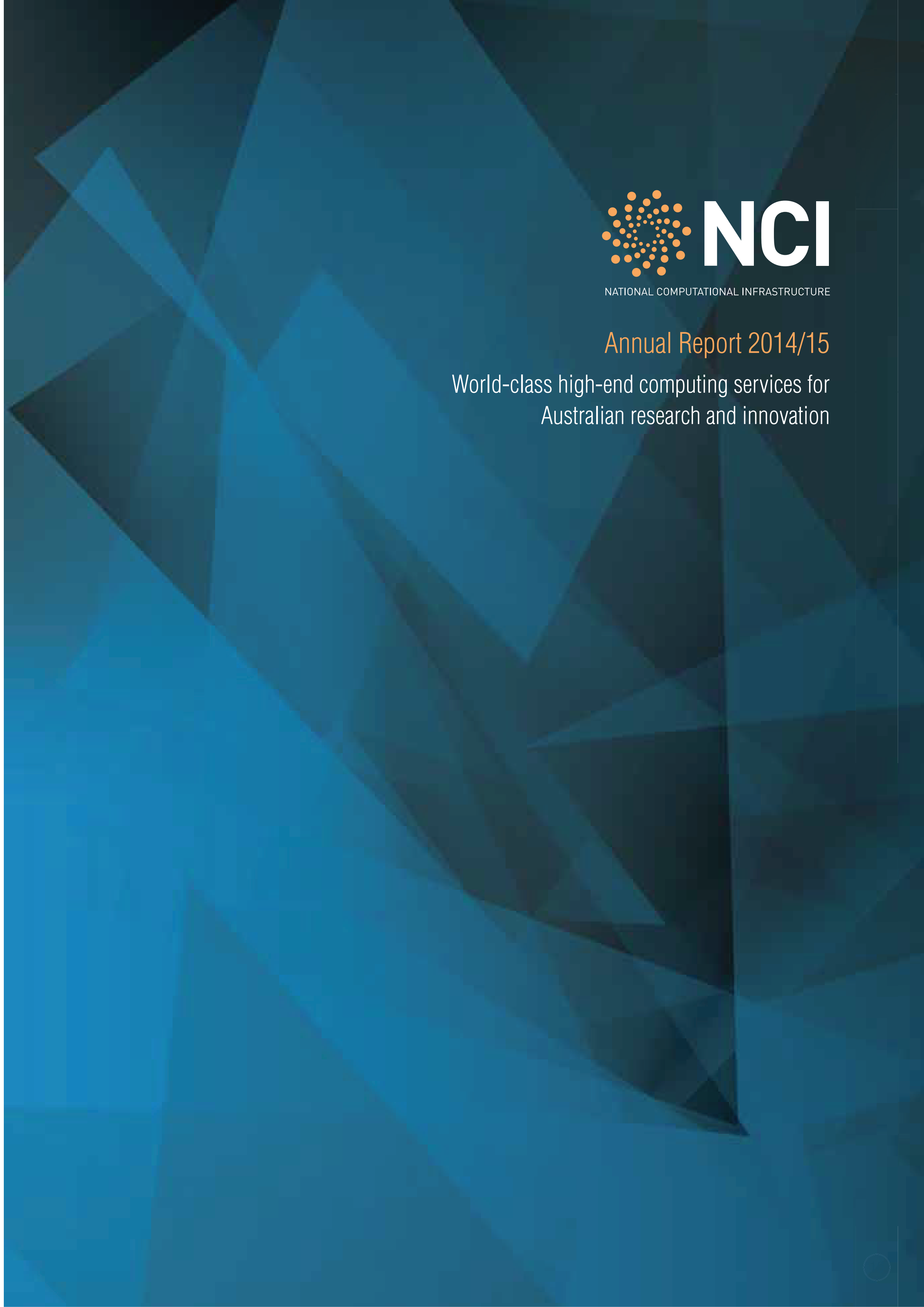
Erica Seccombe, Grow, 2013, (detail), 4D Microcomputed Tomographic X-ray volumetric time-lapse of seeds germinating, single channel projection, formatted for stereoscopic viewing with circular polarized glasses, silver screen, duration: 6min. Visualised and animated using NCI's Drishti software.



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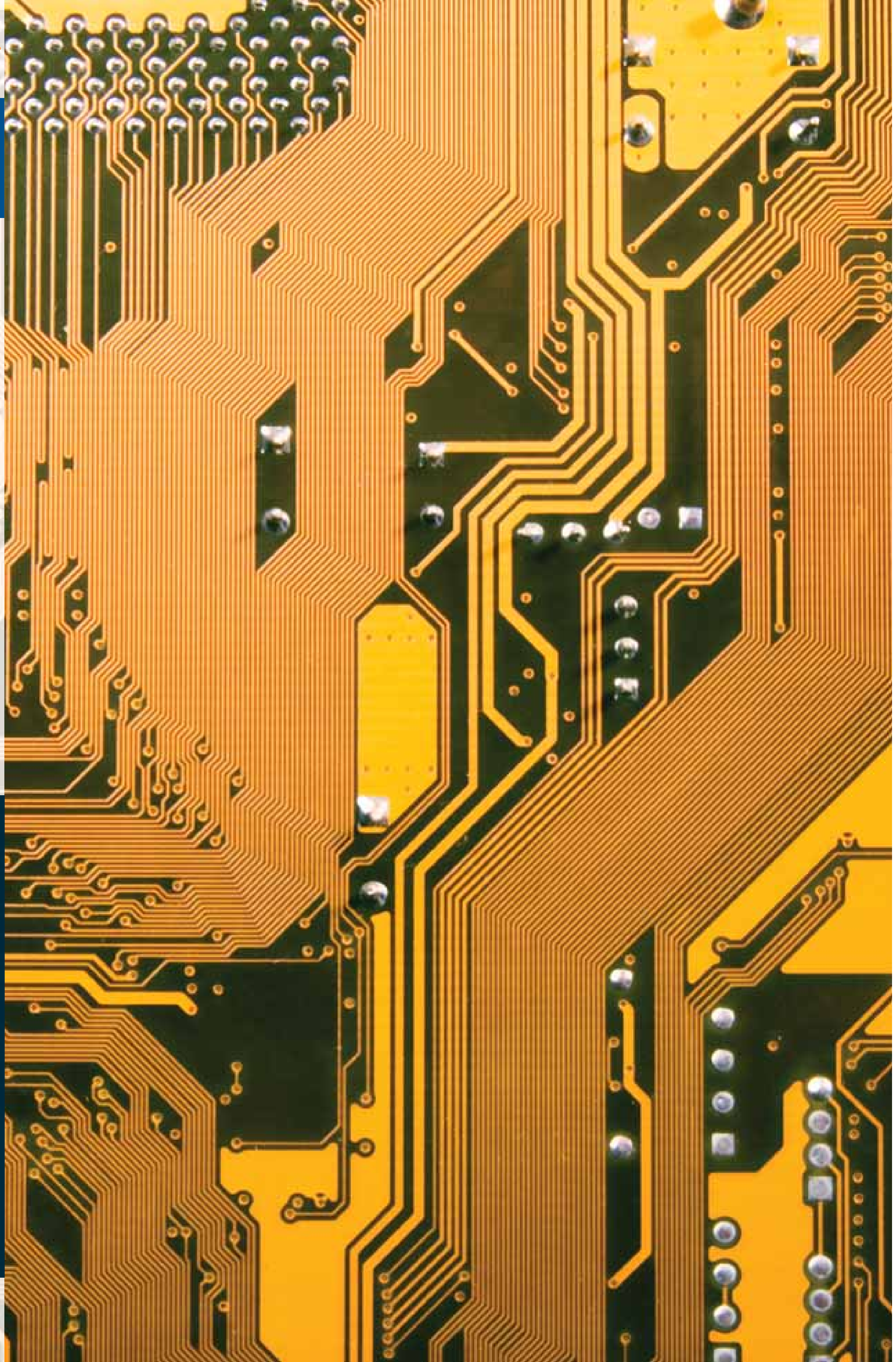
World-class high-end computing services for Australian research and innovation



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Introduction

Who we are

NCI Australia is the nation's most highly-integrated, high-performance research computing environment. NCI has been architected to deliver on national priorities and research excellence. We are driven by our primary objective of raising the ambition, impact, and outcomes of Australian research.

The national and strategic nature of NCI is demonstrated in our funding model, reflecting the shared responsibilities of (a) the Australian Government—through its National Collaborative Research Infrastructure Strategy (NCRIS), for the provision of world-class infrastructure, and (b) the research sector—comprising science agencies, universities, industry and the Australian Research Council, which collectively contribute two-thirds of the recurrent costs.

> "For us, NCI is about as important as a parachute is to someone jumping out of a plane."*

What we do

Based at The Australian National University, we provide high-performance computing (HPC) and high-performance data (HPD) services to a number of the national science agencies, including CSIRO, Geoscience Australia, the Australian Bureau of Meteorology, and a further 2,000+ researchers at 31 Australian universities, five ARC Centres of Excellence, and industry.

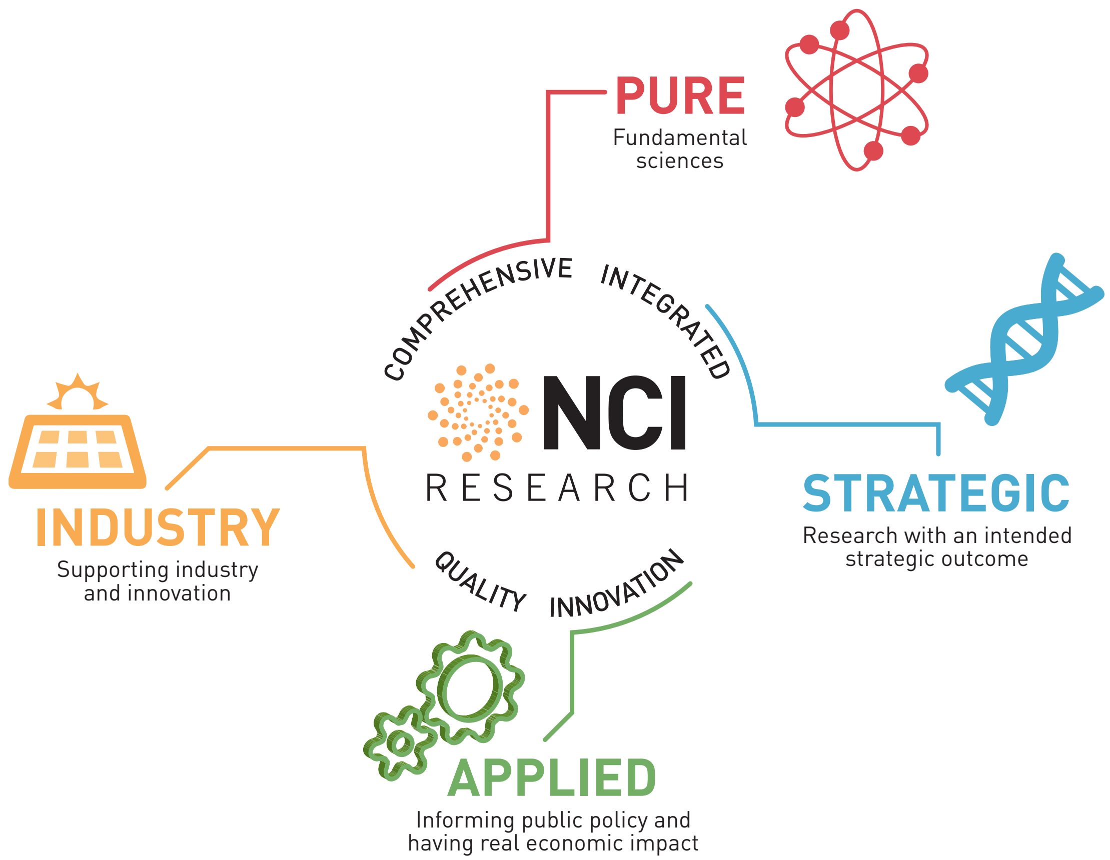
We are home to the nation's first petaflop supercomputer, its highest-performance research cloud, its fastest filesystems and its largest research data repository. Our staff are renowned nationally and internationally for their expertise.

This combination of infrastructure and expertise enables high-impact research and innovation that otherwise would be impossible to undertake, delivers outcomes that inform public policy and national benefits, both in the public sector and in industry, and supports an internationally competitive research environment that attracts and retains world-class researchers for Australia.

Our values

Innovation & quality: NCI is the national leader in the provision of high-performance research computing services and digital laboratories for data-intensive research, all of which is underpinned by our infrastructure and applications support teams, recognised for the quality and innovation of the services they provide.

Comprehensive & integrated: NCI is unique in Australia, and at the forefront of international developments, in that we integrate the nation's first petaflop supercomputer, a supercomputer-class research cloud and the fastest filesystems in Australia—to empower researchers, drive knowledge discovery in fields that are of national priority and at the forefront of international research endeavours, and deliver benefits to the nation by supporting the work of Australia's national science agencies and industry.



> "NCI has been crucial to the success of my research, which has now moved into the commercialisation stage."*

> "We can get our workhorse calculations done without NCI but serious science requires NCI's facilities."*

*Feedback from the 2014 NCI User Survey

Chair's Report

Welcome to the 2014–15 NCI Annual Report. In the following pages you will find many examples of the excellent research and innovation that has been taking place with the support of Australia's national research computing facility over the past year. I am pleased to report that over the past year NCI has grown in strength, with the Collaboration now having three new members, Deakin University, RMIT University and the Antarctic Climate and Ecosystems CRC (through the University of Tasmania). Further, its industry portfolio is growing steadily, directly through services provided by NCI to industry, and indirectly through science agency partner organisations.

The importance of NCI, and its value to the national computational research community is amply recognised by the unanimous decision of our partner organisations to renew their commitment to the NCI Collaboration for a further two years from the end of 2015. The renewal of the Collaboration Agreement (which sustains two-thirds of NCI's recurrent costs), particularly in financially straitened times for government agencies and universities, is a very significant milestone for this year, and on behalf of the Board I thank all organisations for their ongoing support.

This report demonstrates the diversity and the ground-breaking impact of the research and innovation supported by NCI, and I invite you to peruse the Research Highlights throughout this Report. On page 42 you will find Dr Katya Pas from Monash University talking about her revolutionary work on ionic liquids as the industrial solvents of the future. Page 5 highlights NCI's unique capacity as a collaborative platform, while the expertise of NCI staff in optimising and enhancing the scaling of high-performance codes is showcased on page 12.

I take this opportunity to recognise the hard work and dedication of everyone at NCI, including the Director, Professor Lindsay Botten, Associate Directors Allan Williams and Dr Ben Evans, Business Manager Amanda Walker, Deputy Chairman Emeritus Professor Robin Stanton, and the NCI Board. Without their outstanding commitment, the impressive milestones reported herein could not have been achieved.

Emeritus Professor Mark Wainwright AM FTSE
Chair, NCI Board

Director's Report

This past year has seen ongoing strong progress in advancing NCI's mission of world-class, high-end computing services for Australian research and innovation. All aspects of our infrastructure, services development, and operations are driven by the research objectives and priorities of the national research community and our partner organisations. Unique in Australia, we have evolved as a highly integrated research e-infrastructure with a service portfolio that sees high-performance computation and high-performance data-intensive services as natural peers. Grounded by a vision of enabling research that would not otherwise be possible, NCI is delivering solutions for high-impact research that matters, informs public policy, and delivers national benefits.

Today, NCI is truly Australia's national high-performance computing research facility. We service more than 550 projects, the work of 2,000 researchers throughout Australia. Of these projects, more than 190 are ARC-funded activities, which collectively receive $43 million p.a. from the ARC. NCI was acknowledged in more than 1,400 journal articles in the past year, split roughly equally between the university sector and the science agencies. These agencies, the Bureau of Meteorology, CSIRO and Geoscience Australia, undertake R&D using NCI facilities that deliver enormous benefits to Australia including the development of the next-generation weather prediction model, and the implementation of the Australian Geoscience Data Cube. Further, as the Board Chair notes, the portfolio of industry projects exploiting NCI amplifies the importance of a strong national HPC capability for Australia's innovation system.

This year has seen the creation of several new expert service teams at NCI, enhancing the breadth and depth of the ways in which we can support our users. Of particular note is the new HPC Development and Innovations Team who are working closely with our major partners to optimise weather forecasting models of critical national significance. Our data management teams have received international acclamation for the development of the NCI environmental data services interoperability stack, and have also made nation-leading progress in the creation of NCI's Australian Government-funded data repository (see page 13). The operations teams has delivered a year of outstanding service, and has implemented new cloud services, established a new high-performance persistent filesystem, and further enhanced its reputation in the international HPC community with numerous contributions (bug fixes, patches) to Linux and Lustre.

None of this could have been achieved without the expertise and commitment of our staff and I thank sincerely each and every member of the team for their ongoing dedication and innovation. I thank also the Board for its insightful stewardship and the expanding partnership that supports NCI.

Of course, NCI would neither exist nor evolve if it were not for the Australian research community that relies on our infrastructure, whose goals spur us to enhance the quality and innovation of our services, and whose successes reflect well on us. I look forward to working with you all in the future.

Professor Lindsay Botten
Director, NCI

Snap shot –
the year at a glance

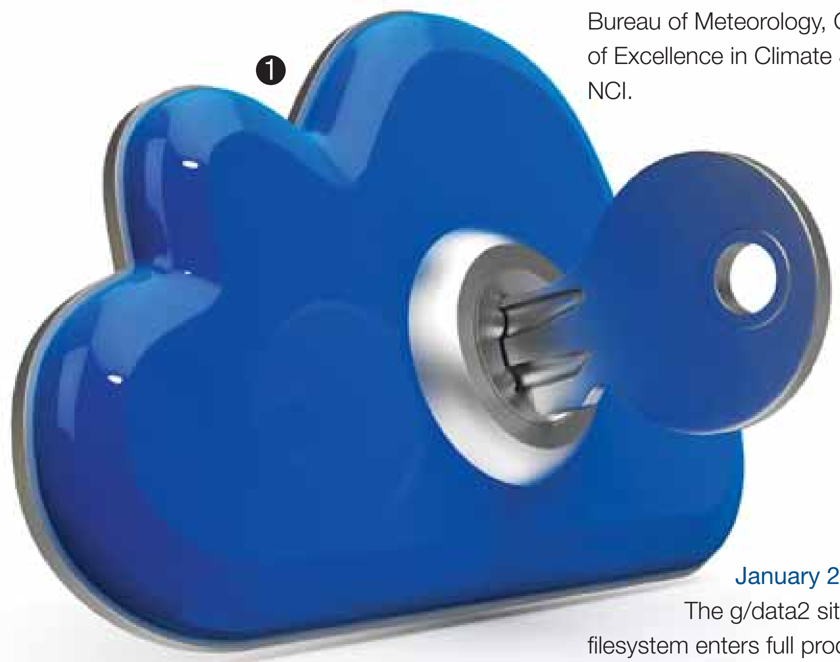
July 2014
Work commences on optimising the functionality of Australia's primary climate and weather modelling suite through a project jointly funded by Fujitsu Limited and NCI, and undertaken in collaboration with BoM and CSIRO (see page 10).

August 2014
NCI's primary internet connection is upgraded to the latest generation AARNET4 link, moving from a capped to a dedicated full bandwidth 10 Gigabit connection.

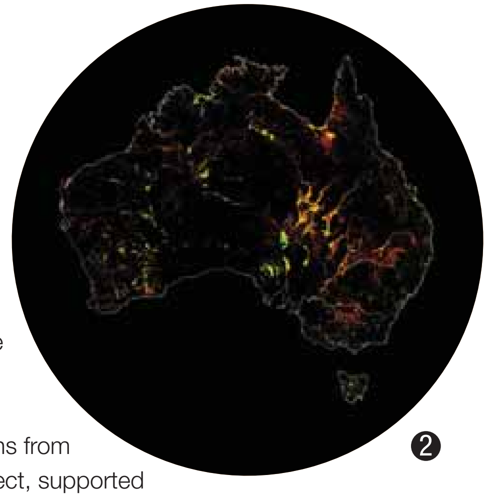
September 2014
Visit to NCI by the then Minister for Communications, the Hon. Malcolm Turnbull, MP.

September 2014 ➊
Tenjin, NCI's supercomputer-grade cloud, becomes available to our partner organisations.

➊



November 2014 ➋
Geoscience Australia's Water Observations from Space project, supported by NCI, wins a Resilient Australia Award (see page 6).



➋

December 2014
NCI is named as the infrastructure partner in the National Agricultural and Environmental Sciences Precinct, funded by the Science and Industry Investment Fund, and announced by the Minister for Industry and Science (see page 18).

December 2014
The NCI-hosted Climate and Weather Science Laboratory is released to the research community (see page 22). The laboratory was built and developed by a partnership of the Bureau of Meteorology, CSIRO, the ARC Centre of Excellence in Climate Systems Science and NCI.

January 2015 ➌
The g/data2 site-wide persistent filesystem enters full production service, expanding from 4.5 PB to 6.7 PB.

➌

February 2015
A new high-speed data transfer system for the international ingest of very large datasets is installed.

April 2015 ➍
NCI signs a $2M deal with Fujitsu to work with NetApp to supply and install the 8 PB g/data3 filesystem, which will be accessible on Raijin and the cloud at up to 140 GB/sec.

➍

May 2015
NCI is allocated $5.3M from the National Collaborative Research Infrastructure Strategy for 2015–16 Project.

May 2015
NCI-supported CSIRO nanotechnologist, Dr Amanda Barnard, wins the Foresight Institute Feynman Prize (see page 31).

June 2015 ➎
NCI's Drishti Prayog visualisation presentation software is displayed at the Emerging Technology Conference in Manchester, UK.

➎

➏

June 2015 ➏
So far more than 7 PB of nationally significant datasets has been ingested into NCI's RDSI-funded data repository and made available to the research community.

> *"NCI has allowed us to revolutionise approaches to the analysis of satellite data."*
>
> Dr Adam Lewis,
> Head of Geoscience Australia's National Earth & Marine Observations branch

System specs at a glance

Raijin:

- Fujitsu Primergy cluster
- 1.2 PFlops peak performance
- 57,472 Intel Xeon cores (Sandy Bridge, 2.6 GHz)
- Mellanox FDR 56 Gb/sec Infiniband full fat-tree interconnect
- 160 TB main memory
- 10 PB disk storage
- 503M core hours/annum
- 300+ software packages
- Access to 20 PB data repository

Fastest filesystems in the Southern Hemisphere (Lustre):

- 7 PB scratch storage on Raijin accessed at 150 GB/sec
- 22 PB active project storage accessed at up to 140 GB/sec
- 12 PB archived data accessed at up to 140 MB/sec
- 49 PB capacity Spectra Logic tape array

Tenjin:

- Australia's highest-performing research cloud
- 33.5 TFlop peak performance
- 1,600 Intel Xeon cores (Sandy Bridge, 2.6 GHz) in 100 nodes
- Mellanox FDR 56 Gb/sec Infiniband full fat-tree interconnect
- 25 TB main memory
- 160 TB Solid State Disk
- Access to 20 PB data repository

Fujin:

- Fujitsu PRIMEHPC FX10 system
- 22 TFlop peak performance
- 1,536 SPARC IXfx cores
- 3 TB memory

Australia's largest research data catalogue:

- 7+ PB of nationally and internationally significant datasets
- Tightly integrated with Raijin and Tenjin

NCI
NATIONAL COMPUTATIONAL INFRASTRUCTURE

Supported by

NCRIS National Research Infrastructure for Australia
An Australian Government Initiative

Collaborating Organisations

Australian National University
CSIRO
Australian Government Bureau of Meteorology
Australian Government Geoscience Australia
RMIT University
Intersect
Deakin University Australia Worldly
qcif
ACE CRC
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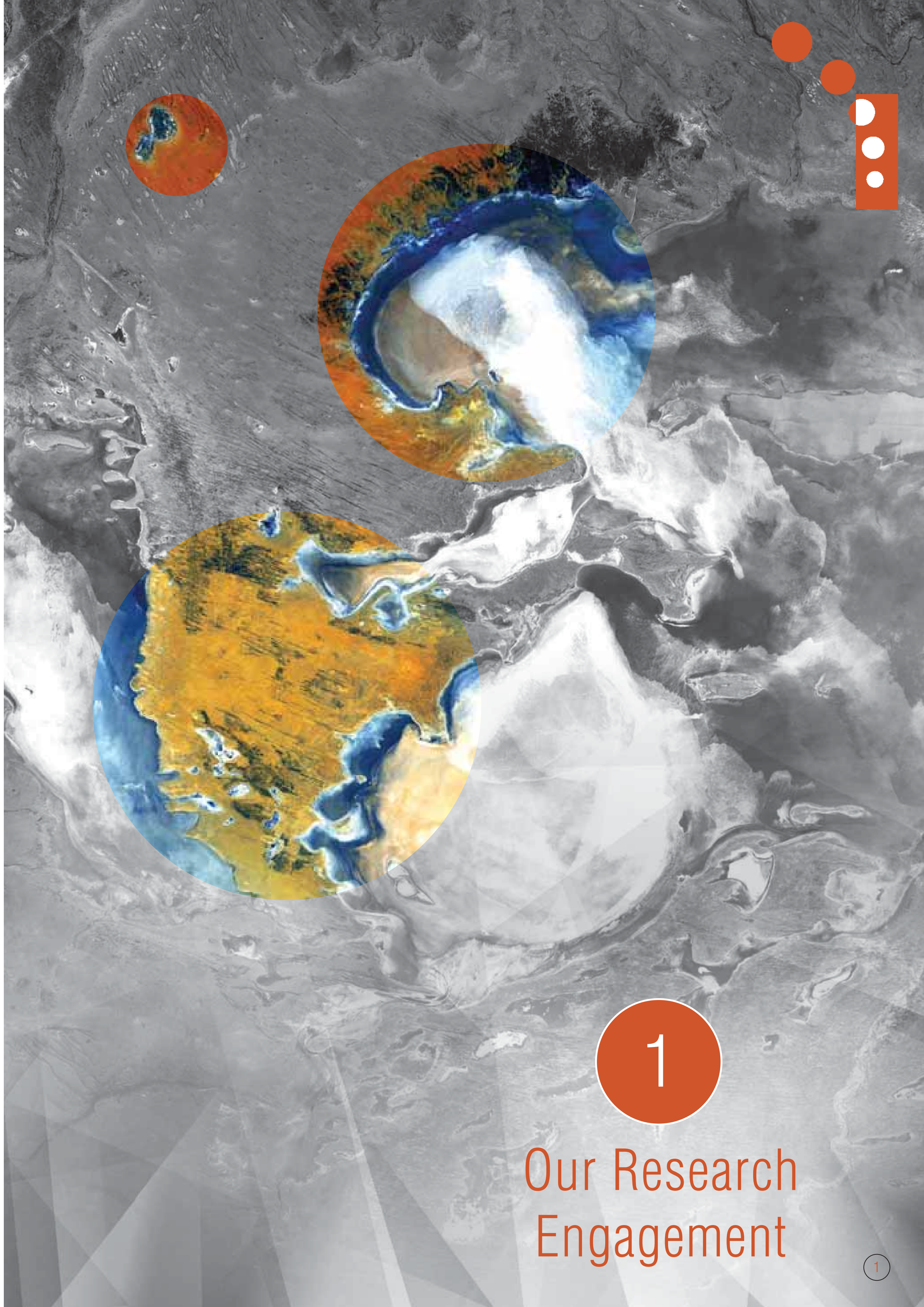


1 Our Research Engagement

Our Research Engagement

Capabilities

NCI is unique in the world, offering Australia's first petaflop supercomputer, Australia's fastest research cloud and Australia's largest research data repository, tightly integrated with the Southern Hemisphere's fastest filesystems.

We offer everything Australian researchers and government agencies need to analyse, access, share, publish and visualise data.

Our services are provided within a tightly integrated infrastructure framework and supported by expert staff who are world leaders in their fields.

Figure 1: NCI's capabilities

CAPABILITY HIGHLIGHT: **HIGHLY PARALLEL COMPUTING**

Scaling massive models

For the past two years, the Australian Bureau of Meteorology (BoM) has been working closely with NCI to test and refine its next-generation national weather prediction models.

"We're trialling our next-generation models on Raijin in preparation for them becoming operational in a year or two," explains Dr Michael Naughton from BoM.

"Every day at NCI we run Australian Community Climate and Earth System Simulator (ACCESS) numerical weather prediction suites, which support research and evaluation of prototype systems, with a special focus on severe and high-impact weather events in the Australian region."

As part of a collaboration with Fujitsu, the NCI code optimisation team have been working with BoM, Fujitsu, CSIRO and the ARC Centre of Excellence for Climate System Science to increase the efficiency of the ACCESS component models. The faster they run, the larger the model that can be supported, and the greater the detail and accuracy provided.

Already collaboration on asynchronous input/output processing has realised a time saving of up to 20% using 2,000 cores.

"The collaborators have worked very effectively together to realise these improvements. The expertise of the NCI team has been essential to solving a number of critical software problems," says Dr Naughton.

NCI's experts have also been collaborating with the ARC Centre of Excellence for Climate System Science to improve the scalability of the US Geophysical Fluid Dynamics Laboratory's Modular Ocean Model, which is critical for BoM's weather prediction models.

The collaboration has already yielded a substantial increase in the scalability of the model, from 2,000 to 20,000 cores, allowing use of more than a third of Raijin's total cores within a single run [read more on page 11].

"Our spectacular Modular Ocean Model work, led by ANU, has benefitted from fantastic support from the NCI team," says Professor Andrew Pitman, Director, ARC Centre of Excellence for Climate System Science.

> *"The expertise of the NCI team has been essential to solving a number of critical software problems."*

Australian Government Bureau of Meteorology

FUJITSU

ARC CENTRE OF EXCELLENCE FOR CLIMATE SYSTEM SCIENCE

CSIRO

CAPABILITY HIGHLIGHT: **CLOUD COMPUTING**

1

Splitting light in the cloud

NCI's supercomputer-grade NeCTAR cloud node is helping researchers design more efficient solar cells.

PhD candidate Björn Sturmberg from the University of Sydney has set up a custom environment on the NCI node of the national research cloud to research a new type of nanostructure for use in 'tandem' solar cells, exploiting theory developed with collaborators at the University of Technology Sydney.

The aim is to use these nanostructures to divert different wavelengths of light towards different types of converters within the cell.

"Silicon solar cells are very good at converting short, visible wavelengths into electricity, but they're not so good at absorbing the longer wavelengths," he says.

"The idea is that you could add a second solar cell made of a different material that absorbs and converts those longer wavelengths more efficiently."

Mr Sturmberg is using the NCI cloud environment to design a nanostructure that uses cleverly placed holes to achieve a clean split of light, efficiently directing different wavelengths to the relevant material.

The process requires substantial computer power, he says.

"Light reacts in really weird and wonderful ways when it interacts with a medium that is structured on the same size scale as it — in ways that you don't normally see in everyday life.

"This means you have to grind out solutions of Maxwell's equations of electromagnetic theory at the nanoscale, and for that you need large computing power."

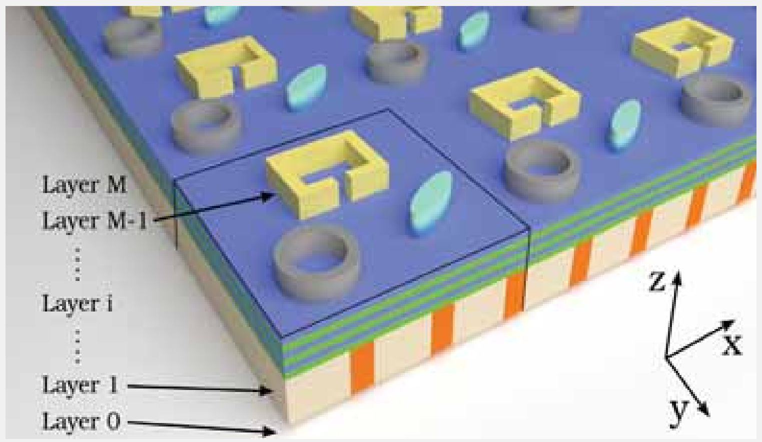
The NCI cloud environment is well-suited to Mr Sturmberg's research because it allows immediate interaction with software outputs.

"I am now able to run simulations that only take a minute, look at them straight away, change something in the model, and run them again," he says.

"The other great thing is that our collaborators at ANU and other students here at the University of Sydney who want to use the same simulation package that I have developed can access it directly without having to worry about operating systems."

Backed by the ARC Centre of Excellence for Ultrahigh bandwidth Devices for Optical Systems, an ARC Discovery Grant, and a PhD scholarship from the Australian Renewable Energy Agency, Mr Sturmberg has been collaborating with Dr Thomas White and Prof Kylie Catchpole at ANU to bring his simulations to life in the lab.

"We use NCI to do the modelling to try and understand what physics is going on in these nanostructures, and then ANU fabricates and tests the structures in the lab," he explains.



CAPABILITY HIGHLIGHT: **COLLABORATION**

Working together to build national datasets

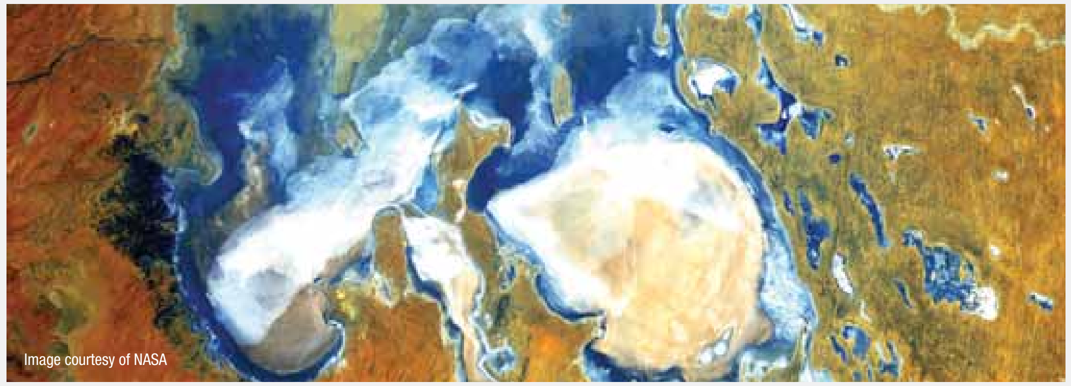


Image courtesy of NASA

NCI is the platform of collaboration between our fellow NCRIS facilities the Integrated Marine Observing System (IMOS) and the Terrestrial Ecosystem Research Network (TERN). Working together, we are building national datasets housed at NCI.

IMOS Remote Sensing Facility Leader Dr Edward King, who is based at CSIRO in Tasmania, says having access to NCI allows his team to easily collaborate with TERN and undertake work that wouldn't be possible otherwise.

"One of my roles is to organise large satellite image datasets, spanning more than ten years, thousands of images and tens of terabytes of data," he says.

"NCI lets us organise these large datasets and collaborate with other institutions, agencies and organisations in a way we can't easily do inside our own organisations."

Acquisition of satellite data has boomed over the past decade and projections for the future are reaching the tens of petabytes scale, presenting a complex computational challenge.

"The growth in satellite data was stretching our compute capabilities at the time TERN and IMOS were coming into being," explains Dr King.

"The high capacity and performance of the NCI were more than equal to the task and made it a natural choice as a platform on which to build our national data collections.

"Even more importantly, TERN and IMOS are multi-institutional endeavours founded on cooperation. In contrast to many of our participating institutions, which have enterprise firewalls with security policies tied to organisation membership, NCI is set up as a collaborative environment."

The collaboration saves both time and money, leading to more efficient and effective outcomes, adds Dr King.

"There's a massive national efficiency that's gained through this work because we can have a single dataset, instead of one dataset for each agency.

"Furthermore, we can make that single dataset comprehensive, meeting the needs of both terrestrial and marine users, whereas previously different institutions would likely have held overlapping subsets of the whole.

"The ability to share resources between not just institutions, but also domains strengthens links within the Australian research sector and enables more integrative science, bringing together complementary expertise to address more complex challenges."

"There's a massive national efficiency that's gained through this work."

CAPABILITY HIGHLIGHT: **BIG DATA**

1

Revolutionising satellite data analysis

Australian Government
Geoscience Australia

NCI is working with our Collaborating Partner Geoscience Australia to unlock more than two petabytes of geoscience data of national policymaking significance.

With support from the Australian Government's Research Data Storage Infrastructure project, experts from NCI and Geoscience Australia have been tackling the mammoth task of migrating this dataset to NCI.

The data represents 11 distinct projects, including 30 years' worth of Australasian earth observation images generated by NASA's Landsat satellites, and the Australian Natural Hazards Data Archive, which includes observational and probabilistic hazard, impact and risk data covering earthquakes, tsunami, floods and tropical cyclones.

Following migration, NCI's Data Management Team collaborates closely with data managers at Geoscience Australia to develop comprehensive data management plans to outline how best to make each dataset accessible, searchable and shareable [see page 15].

The integration of NCI's filesystems with Raijin has enhanced Geoscience Australia's capacity to analyse their datasets, says Dr Adam Lewis, Head of Geoscience Australia's National Earth & Marine Observations branch.

"NCI has allowed us to revolutionise approaches to the analysis of satellite data through the Australian Geoscience Data Cube, producing world-first products such as our Water Observations from Space dataset (WOfS), which maps surface water across Australia," he says.

The WOfS project received the 2014 nationally significant work award in the Government category at the Resilient Australia Awards.

NCI is an integral part of Geoscience Australia's capability, says Dr Lewis.

"The NCI is benefitting all areas of Geoscience Australia science," he says.

"Through our partnership with NCI we have been able to develop our quantitative science cost effectively, and to increase our collaboration with other organisations such as the CSIRO, the Bureau of Meteorology and ANU, to name a few.

"For example, we've developed a coherent image of the deep geological structure of the Australian continent, which is an essential step toward future minerals prospecting because it helps us to 'see' beneath the regolith that covers much of Australia.

"We see our partnership in NCI as an exemplar of collaboration in Australian government science, which also leverages other government investments, such as the Research Data Services Infrastructure, to maximise value and impact for the taxpayer and the government."

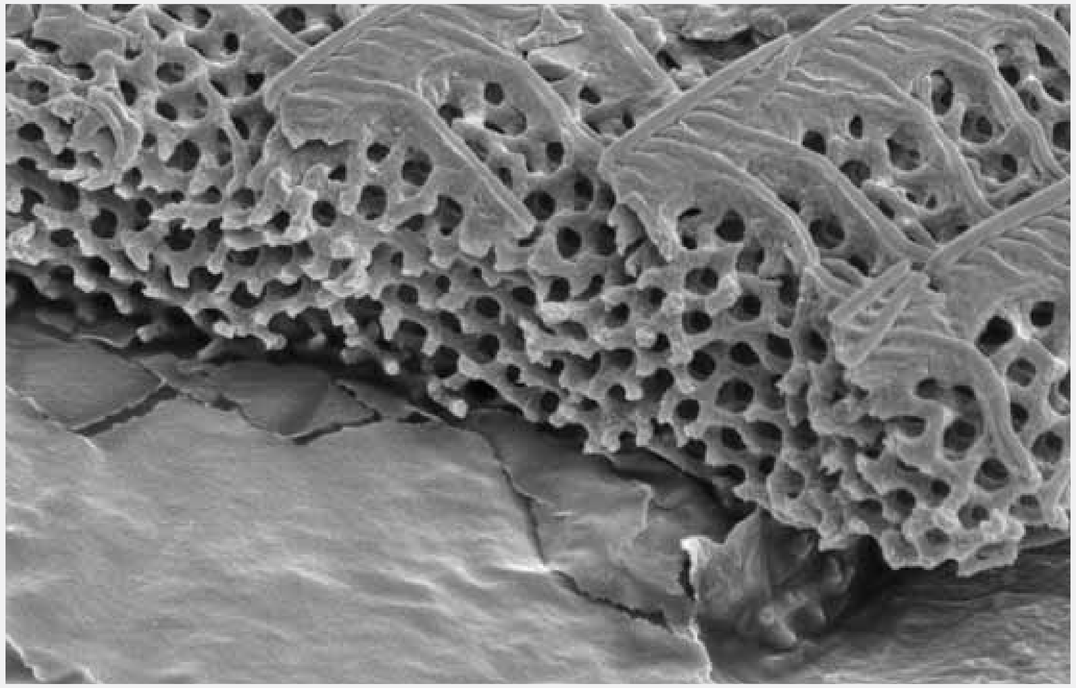
"NCI has allowed us to revolutionise approaches to the analysis of data."


Image courtesy of NASA

CAPABILITY HIGHLIGHT: **VISUALISATION**

Visualising butterfly wings in 3D

Australian National University



Researchers from ANU have used the NCI VizLab's services and expertise to discover that butterfly wings could harbour the blueprint for next-generation supercomputers or slow-release cancer drugs.

Butterfly wings contain some amazing geometrical structures known as photonic crystals. These labyrinthine configurations are responsible for some of nature's most amazing colours.

"The species we looked at has green underwings," says Professor Stephen Hyde from ANU.

"They're green because light comes into the photonic crystals, bounces around, and only the green wavelength is the right size to escape; the rest of the colours get trapped inside.

"If you change the size of the opening, you change which colour can escape."

"Butterfly wings could harbour the blueprint for next-generation supercomputers."

The team made the discovery by employing the power of Raijin to piece together thousands of microscopic images of butterfly wing layers to generate the first 3D reconstruction of butterfly photonic crystals.

The discovery has far-reaching potential applications. Car companies are already using metallic iridescent paint based on butterfly photonic crystals.

VIDEO: http://bit.ly/flyingcol

High-Performance Computation Innovation

The strength of an e-infrastructure capability depends as much on soft infrastructure – skills, software, etc. – as it does on hardware.

The challenges that confront the future use of high-performance computing globally relate not so much to the ability of vendors to provide increasing computational power, but the ability of researchers to utilise these systems effectively.

NCI is addressing this challenge by providing the expertise and services that drive innovation: the development and optimisation of software for simulation and data-intensive computation, along with sophisticated data services, data management, and visualisation services.

> *"The technical developments led by the ARC Centre of Excellence for Climate System Science depend on the high performance computing and data environments provided by NCI."*
>
> Professor Andrew Pitman, Director, ARC Centre of Excellence for Climate System Science

HPC Development and Innovations

This year, NCI has been working with national and international collaborators to optimise a selection of the globe's most important computational models.

FUJITSU COLLABORATION

In April 2014 NCI and Fujitsu signed a formal Collaboration Agreement, supported by a subcontract between NCI and the Australian Bureau of Meteorology (BoM), to undertake:

- Optimisation of the Australian Community Climate and Earth System Simulator model, and
- Research and Development into advanced computational scaling and tools.

This three-year synergistic collaboration draws on the shared strategic goals of Fujitsu and NCI; Fujitsu's expertise in high-performance computing and computational science; and NCI's expertise in the application of high-end computing and data-intensive services to the rich research and development portfolios of our collaborators.

> *NCI: Enabling Government, Researchers and Industry to Innovate.*

RESEARCH HIGHLIGHT

Deep-water ocean modelling for industry

NCI is providing high-performance computational services to global not-for-profit engineering organisation DHI Water and Environment Pty Ltd.

"We specialise in engineering involving water," explains DHI's Head of Marine, Simon Brandi Mortensen.

"Everything from coastal and marine water, like waves and ocean circulation, to ports and ships, and flooding risk and industrial water management.

"We are using Raijin to calculate in great detail how waves and currents around the north-west of Australia are behaving, both in normal conditions and in response to cyclones."

The work is of particular interest to oil and gas companies, which require a thorough understanding of ocean currents to inform design of deep-water infrastructure such as oil rigs, pipelines and moored ships.

"Oil and gas companies want to know what sort of currents they can expect in different parts of Australian waters so they can ensure their infrastructure can withstand a 1-in-10,000-year-chance natural disaster like a major cyclone," explains Mr Brandi Mortensen.

"The challenge is that in order to predict a 10,000-year event you need to describe the predicted cyclone climate over 10,000 years. That requires simulating thousands of storms and taking into account all the variables.

"The processes involved in each cyclone simulation are so complex that you need to use very fine resolution 3D models solving very complex mathematical equations.

"The only way you can feasibly do this is by using a HPC facility where you can run hundreds if not thousands of storm simulations at the same time and thereby deliver results in a matter of a few weeks instead of months."

Mr Brandi Mortensen says the decision to move to NCI was driven by the need to encompass growth in DHI's research.

"We needed to think ahead in terms of the magnitude of our simulations – how many storms we needed to run," he says.

"NCI provides access to 57,000 cores all under one roof, an environment which is unparalleled in Australia.

"We are very happy to be working with NCI and we look forward to working together to move our science in a good direction."

> *"NCI provides an environment which is unparalleled in Australia."*

THE ACCESS OPTIMISATION PROJECT AND THE ADVANCED SCALING AND TOOLS PROJECT

The Australian Community Climate and Earth System Simulator (ACCESS) model is the operational model that BoM uses daily to predict Australia's weather and climate conditions. This vast model, which provides essential information for picnickers to policy-makers, is a conglomeration of six major international models:

- The UK Met Office's **Unified Model** (UM) for atmospheric modelling
- The National Oceanic and Atmospheric Administration (NOAA) Geophysical Fluid Dynamics Laboratory (GFDL)'s **Modular Ocean Model** (MOM) for ocean modelling
- The UK Met Office's **4DVAR Model** for data assimilation
- The US Department of Energy Los Alamos National Laboratory's **CICE model** for sea-ice modelling
- CSIRO's **Community Atmosphere Biosphere Land Exchange model** (CABLE) for land–surface modelling
- The Centre National de la Recherche Scientifique's **OASIS coupler model** to link the other five models together.

This year, the NCI HPC Development and Innovations Team have been working on optimising the individual UM, MOM and 4DVAR models to bring about substantial performance enhancements to the overall ACCESS suite. The Team's expertise has been recognised by adoption of their fixes into the official releases by the custodians of these major international models.

The UK Met Office's Unified Model (UM) for atmospheric modelling

One key achievement of the work so far has been a major improvement to the UM(v8.4) code, which has been adopted into BoM's current operational activities.

Through a combination of better decomposition strategies, alleviating hardware bottlenecks, and MPI communication improvements, BoM has reported that the team's efforts have resulted in an approximately **40% improvement** in the overall performance of the ACCESS model used for the daily weather forecast: the Australian Parallel Suite Global (APSv2-G).

The team have also been working on the latest UM release (v10.2) in preparation for the next-generation BoM operational model. The major outcome of this work has been an approximately **30% gain** in overall UM performance for Numerical Weather Prediction. This was achieved through a major code change to the I/O design which removes a critical inefficiency in the UM design. This improved design for I/O is currently being reviewed by the UK Met Office for inclusion in the next release of the UM (v10.4).

NCI is also assisting CSIRO to adopt the latest version of the UM so it can be used for the International Panel on Climate Change's Coupled Model Intercomparison Project Phase 6 project (see page 15).

NOAA GFDL's Modular Ocean Model for ocean modelling

The NCI HPC Development and Innovations Team has been collaborating with the ARC Centre of Excellence for Climate System Science to implement NOAA's Modular Ocean Model (MOM) on Raijin.

Compared to the previous iteration of MOM, the current 0.1°-resolution model represents a resolution enhancement of 2.5 fold and requires more than 6 times greater computation power per time step. A substantial effort to improve the model's scalability was therefore required for its practical utilisation, resulting in upscaling **from 2,000 to 20,000 cores** — allowing use of more than a third of Raijin's total cores within a single run — as well as a **7.5-fold reduction in computation (wall clock) time.** Furthermore, the project has yielded a **20% reduction in CPU hours** for the 0.25°-resolution version of the model through the introduction of land masking.

The maintainers of MOM, the *National Oceanic and Atmospheric Administration* Geophysical Fluid Dynamics Laboratory, have now verified the NCI changes and demonstrated similar improvements on US computational systems.

NCI staff have also successfully ported MOM onto Fujin, our Fujitsu FX10 cluster, which has a unique SPARC-based architecture shared with Japan's K Computer (the 4th fastest supercomputer worldwide) and is the only FX10 machine outside of Japan. This work has opened up a new computational resource to MOM researchers around the globe.

> *"The NCI team and BoM experts have collaborated very effectively together to realise these improvements."*
> Dr Michael Naughton, Senior Research Scientist, Earth System Modelling Program, Research and Development Branch, Bureau of Meteorology

Fujin, NCI's Fujitsu FX10 cluster.

The UK Met Office's 4DVAR Model for data assimilation

NCI have been working with BoM operators to address keenly sought improvements in the ACCESS model's data assimilation performance. To this end, the adoption of hyper-threading has **reduced data assimilation time by up to 70%.** The team have also achieved a **30% improvement in performance**. These improvements have allowed BoM to exceed its operational goals in time-to-solution and hyper-threading is now available to all NCI users.

Table 1: Code enhancements achieved by NCI in 2014/15

Model	Maintainer	NCI enhancements
Unified Model	UK Met Office	40% improvement in overall performance (APSv2-G); 30% improvement in overall performance (v10.2)
Modular Ocean Model	*National Oceanic and Atmospheric Administration* Geophysical Fluid Dynamics Laboratory	Upscaling from 2,000 to 20,000 cores and 7.5-fold reduction in computation time (0.1°-resolution version); 20% reduction in CPU hours (0.25°-resolution version)
4DVAR Model for data assimilation	UK Met Office	Reduced data assimilation time by up to 70%; 30% improvement in run time

NCI's work on the component parts of the ACCESS suite is already being implemented in BoM's daily operations. This has implications for activities from air-traffic control to natural disaster preparation.

Further work will assist BoM in designing and implementing their next-generation higher-resolution climate simulation suites, which will be world-leading in complexity and resolution.

COMPUTATIONAL CHEMISTRY

For more than 20 years, NCI (and its predecessors) has been collaborating with Fujitsu to ensure key computational chemistry software programs operate effectively and efficiently on Fujitsu's FX10 hardware. NCI staff act as intermediaries between the software developers and Fujitsu's computational chemist market, testing, debugging and optimising software programs including ADF, Amber, GAMESS, VASP, and the current industry standard in computational chemistry – Gaussian.

This last is of particular importance, as Fujitsu has exclusively chosen NCI to port this version for them. Later this year, the team will carry out porting of Gaussian onto Fujitsu's new flagship computer, the FX100.

High-Performance Data Innovation

During the last 15 years, the requirements and expectations of e-infrastructure investments have expanded from solely national supercomputing services in the early years to the rich landscape of today which includes tightly integrated data services, driven by the rapidly developing role of data as a major player in new research.

Enormous advances in the data collection capabilities of genome sequencers, telescopes and satellites have greatly accelerated the requirement for innovative data handling strategies. Research communities are now facing petascale data challenges.

As the home of Australia's largest research data repository, NCI is at the leading edge of developments of data ingest and management techniques. Our aim is to provide a truly high-performance data analysis capability.

Data as a Service

In 2011, the Australian Government initiated the $50 million NCRIS Research Data Storage Infrastructure (RDSI) Project to set up petascale data storage infrastructure, with storage located at six primary and two additional nodes throughout Australia. Of these, NCI's has the largest capacity, with 10 PB of collections storage.

As part of the follow-on Research Data Services (RDS) NCRIS Project established in 2014, NCI is now focussing our RDSI infrastructure into data as a service, in support of research communities with petascale data requirements.

This data as a service delivery operation will:

- Enable projects that are currently challenged by the gap between the infrastructure layer and the 'data science' layer at which research outcomes are realised
- Provide the 'human middleware' bridging between compute and storage services
- Provide operational support that remediates existing service deficiencies, and which, ultimately, can evolve to serve the requirements of future high-impact collections.

"NCI has driven our successful genome and exome informatics through providing access to high performance data storage and computation that has allowed us to scale at the rate of data growth in our exploding field."

Professor Chris Goodnow, Deputy Director, Garvan Institute of Medical Research

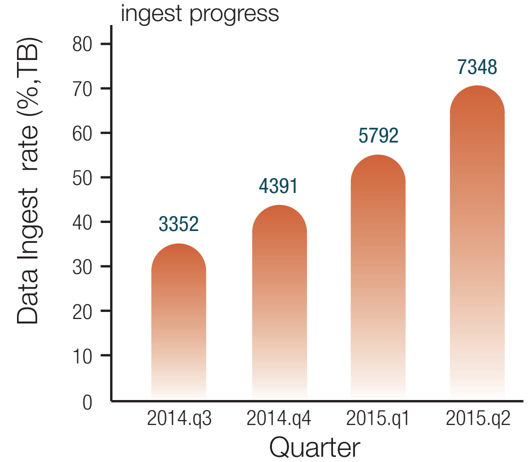
DATA INGEST PROGRESS

Approximately 10 PB of data collections were selected for storage at NCI as part of a formal process under the RDSI scheme (see Table 2). This process identified research data holdings of lasting value and importance to the nation.

The distinctive goals of the NCI Node were:

- Making collections held by national agencies accessible; these collections required either high-performance computational or high-performance data services to unlock their potential
- Co-locating and integrating these collections with other nationally and internationally significant collections to enable interdisciplinary research
- Combining datasets held by research communities into coherent collections, and
- Integrating these collections within a rich environment of high-end computational and data-intensive services.

Figure 2: NCI National Research Data Collection ingest progress



Over the past year, the NCI Data Management Team has overseen the ingestion of an impressive 5 PB of this RDSI-approved data, bringing the total to 7 PB. At an average weekly ingest rate of more than 100 TB, this is both the fastest and largest data ingest among the eight RDSI nodes.

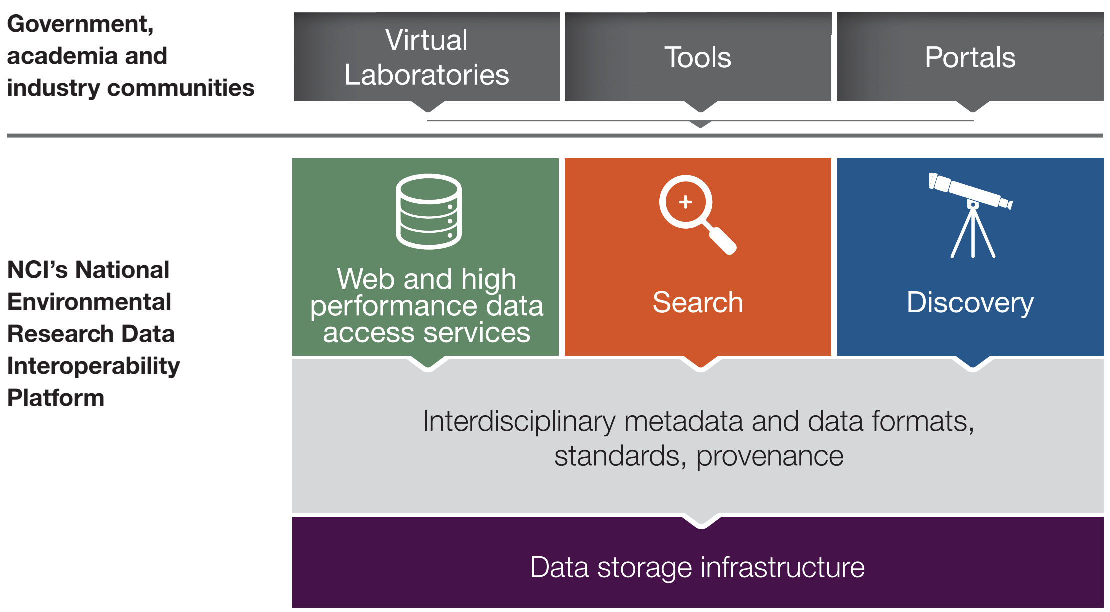
As a result, NCI's RDSI-supported data storage allocation is more than 70% full. All of this data has been made fully accessible for both primary and secondary use: either for direct access on the NCI filesystems for those needing high performance compute resources, or via online data services for access by the broader research community. In addition, all metadata is harvested by Research Data Australia, to be more broadly discoverable through international harvesters and discovery mechanisms, including Google.

Once ingest is complete, NCI will be home to more than 10 PB of nationally and internationally significant datasets. The majority of this data will form the National Environmental Research Data Collection (NERDC), which covers five fields:

- Earth system science, climate and weather observations and models
- Earth and marine observations
- Geoscientific observations and models
- Terrestrial ecosystems observations, and
- Water and hydrology observations.

NCI have created NERDIP, the National Environmental Research Data Interoperability Platform, to provide a unifying, standards-based infrastructure that researchers can access for interdisciplinary research. Having the data assets co-located with the high-performance computing facility at NCI, and harmonised through the use of international standards, means researchers from government, academe and industry now have a platform on which they can trial new mechanisms for high-performance data analysis and modelling on a national, if not global, scale.

Figure 3: NCI's National Environmental Research Data Interoperability Platform



High-speed data transfer

In early 2015 NCI's new High Performance Data Team and the Storage and Infrastructure Team implemented a system to improve data ingest speeds for very large datasets.

Based on the US Department of Energy's Science DMZ model, the Teams installed dedicated data transfer nodes that sit as close as possible to NCI's router connection to the Australian Academic and Research Network (AARNet).

This setup eliminates cumbersome firewalls and checkpoints and has led to increases in data transfer speeds of up to 40%.

The Team has also participated in the International Climate Network Working Group to deploy and tune the University of Chicago's Globus Online service to automate the transfer process, reducing human involvement and increasing system robustness.

Since the new system was implemented, NCI has ingested 1.5 PB of the Coupled Model Intercomparison Project (CMIP) 5 dataset from the Lawrence Livermore National Laboratory in the USA at speeds which can consume almost the entire capacity of the Southern Cross Transport network connection across the Pacific.

This capability paves the way for the next generation of CMIP data, which is anticipated to be in excess of 30 PB and will underpin the next major activities in international climate research.

Using NCI's next generation, high-performance site-wide parallel filesystems, the National Environmental Research Data Collection will be accessible from both Raijin and Tenjin at an unprecedented 140 GB/sec.

Data Management

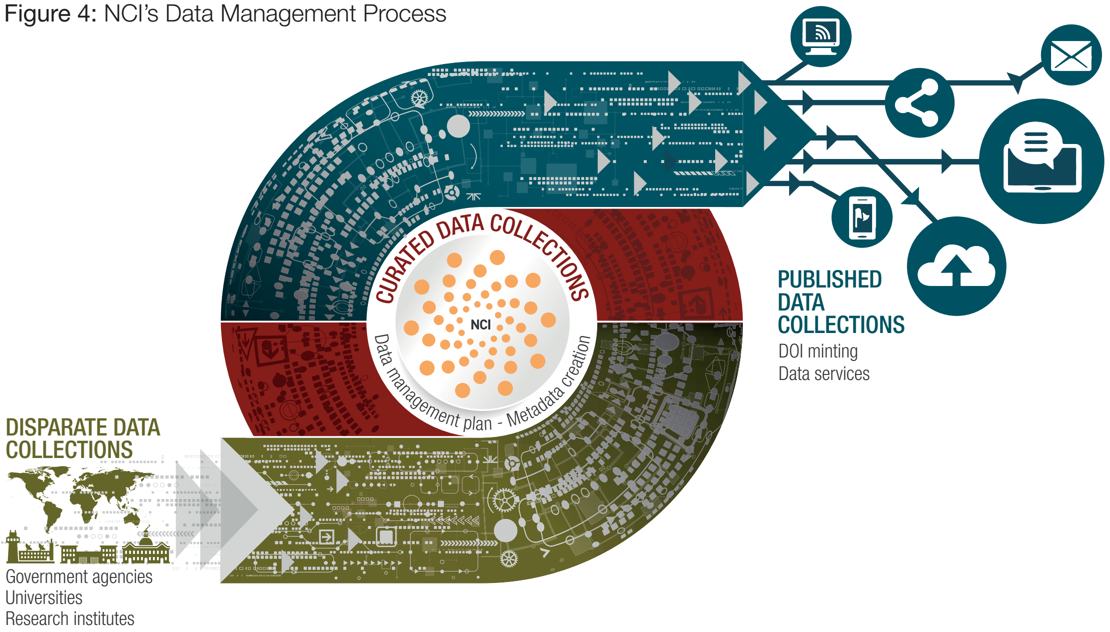
The generation and ingestion of large datasets must be undertaken in a structured and organised manner to ensure the data can be easily accessed, searched, shared and analysed.

NCI is at the forefront of innovative data management processes. Historically, many national datasets have been provided as disparate, heterogeneous data collections that are not formatted to a common grid or data format specification. The same data are then often reformatted for different science domains using an uncoordinated approach. NCI aims to draw together these different uses of the data, and harmonise and simplify their generation.

Over the past year, the NCI Data Management Team have been working with collection custodians to:

- Standardise data formats
- Expose all data attributes for search (i.e., not just collection-level or dataset-level search functions)
- Make all metadata open and discoverable through NCI, ANDS, FIND, data.gov.au and partner data portals (e.g., TERN, IMOS, GA)
- Enable unique and persistent identifiers for provenance and versioning
- Provide programmatic interfaces that link the data to compute resources to enable sophisticated searching and analyses.

Figure 4: NCI's Data Management Process



DATA MANAGEMENT PLANS

The NCI Data Management Team has developed and implemented comprehensive Data Management Plans, working closely with data custodians to maximise the potential utility of each collection.

Data Management Plans record all the information required to organise, publish and share each collection, including workflows, procedures, key contacts and responsibility areas, metadata and licencing information. The Plans' fields have been mapped for straightforward export to the ISO19115 schema and NCI's GeoNetwork catalogue infrastructure.

DATA MANAGEMENT WEB TOOL

In late 2014, NCI delivered an online Data Management Web Tool portal. As well as providing data custodians with access to their Data Management Plan, the Web Tool also provides Digital Objective Identifier (DOI) minting and metadata creation services. These deliverables minimise the workload for record management and data publishing through the NCI GeoNetwork catalogue, and are major milestones funded by The Australian National Data Service.

RESEARCH DATA SERVICES

The newly formed NCI Research Data Services Team has been working to deliver NCI-hosted datasets through the THREDDS Data Server. NCI currently hosts most datasets through THREDDS, but also supports Hyrax, ERDDAP and Geoserver. Over the coming year, the Team will build several other service tools for data users, including a tool that allows NCI-hosted datasets to be displayed, searched and analysed via a web browser.

Earth System Grid Federation node

NCI is the Australian node of the Earth System Grid Federation, the mechanism by which climate data is shared among the global research community. This year, the Research Data Services Team has deployed an updated architecture for the NCI node. Once live, this service will provide all Australian climate model data to the global community for download.

NCI have been engaging with both the modelling and ESGF communities regarding preparation for CMIP6 (see page 15), which is due to start in 2016. To this end, the International Climate Network Working Group has been established to put into place a new set of networking best practices to effectively transport hundreds of petabytes of large-scale climate data such as that generated by CMIP6.

The participating institutions include:

- NCI
- Argonne National Laboratory
- Lawrence Berkeley National Laboratory
- Lawrence Livermore National Laboratory
- Los Alamos National Laboratory
- National Center for Atmospheric Research
- Oak Ridge National Laboratory
- Pacific Marine Environmental Laboratory
- University of Southern California/Information Sciences Institute
- British Atmospheric Data Center
- Earth System Curator
- Geophysical Fluid Dynamics Laboratory
- German Climate Computing Centre
- Jet Propulsion Laboratory
- University of Tokyo Center for Climate System Research

The data centers are aiming to achieve consistent disk-to-disk data transfer rates range from 0.5 to 1 gigabyte per second. This can be thought of as transferring up to 1 PB a fortnight.

RESEARCH HIGHLIGHT

New agricultural precinct supported by NCI

In December 2014, Minister for Industry, the Hon Ian Macfarlane MP, announced the partnership of ANU, CSIRO and NCI in the new Agricultural and Environmental Sciences Precinct.

The Precinct will bring together the brightest minds from CSIRO and ANU with support from NCI to foster research and innovation essential to food security and environmental challenges.

CSIRO researcher Dr Jen Taylor says the partnership will enable collaboration between the three organisations on large projects such as sequencing the genome of one of the globe's most important crops, wheat.

"I'm interested in how we deal with data around making crops more productive and ecosystems more sustainable," says Dr Taylor.

"We use data to understand how those plant systems work and that translates into informing agricultural producers how best to utilise the systems that they have on hand and how to adopt new solutions to help the nation and the globe respond to food security issues."

The Science and Industry Endowment Fund will provide $18 million to support the program, which includes access to supercomputing and data facilities at NCI, and which will augment NCI's capacity by $1M of new large memory compute nodes.

"We can now measure things at a completely different resolution and volume than we could before. Globally in agricultural science there has been the problem of dealing with this deluge of data," says Dr Taylor.

"The Precinct will allow me to work very closely with people at ANU who have similar problems, and look to develop shared solutions on the foundation of the fantastic NCI facility with its strong computing abilities."

NCI's virtual environment will allow Dr Taylor and her team to work closely with collaborators from across the country and the globe.

"What's been challenging about working with other scientists is that we often live in different computational systems, we use different analytical tools, and it's been quite challenging to find ways to work together and share data.

"In getting this system up, what we are going to incorporate into it is essentially a series of virtual 'rooms' or 'laboratories' where we can come together much more easily and share our problems more efficiently than we have been able to before."

"We use data to… inform agricultural producers how best to… help the nation and the globe respond to food security issues."

Table 2: The NCI National Research Data Collection

Dataset Name	Description	Organisation	Dataset size (TB)	Ingest as at 30 June 2015 (TB)
3D Geological Models of Australia	This collection includes ACCESS NWP data, MTSAT satellite data and radar data.	GA	3	1
ACCESS-CM 0.25 Degree Simulations	Initial spin-up simulations from the new high (ocean) resolution coupled version of ACCESS	ANU, UNSW	30	15
ACCESS Numerical Weather Prediction Models	Meteorological weather analysis and forecast model output from NMOC using the ACCESS Prediction System since 2009; represents BoM's daily weather predictions.	BoM, CSIRO, ARCCSS	2750	2300
ARC Centre of Excellence for Climate System Science Datasets Collection	This collection includes all the datasets produced and published by the ARC Centre of Excellence for Climate System Science (ARCCSS) during its existence (2011-2018), with the exclusion of datasets which are part of cooperation projects (for example CMIP5 experiments).	ARCCSS	166	166
Atmospheric Forcing Products	Atmospheric Forcing Products	BoM	5	4
Atmospheric Re-analysis Products	Atmospheric reanalysis and observation data from local Australian and international sources such as NCEP1, NCEP2, ERA40, ERA40c and gridded observation data sets such as AWAP for weather and climate research.	BoM, ARCCSS	2	2
Australian Bathymetry and Elevation Reference Dataset	Australian landforms and seabed topography and elevation data including the 1, 3 and 9 second Shuttle Radar Topographic Mission (SRTM) datasets and derived products and Laser Inferometry Detection and Ranging (LIDAR) data.	GA, IMOS	113	29
Australian Data Archive (Social Sciences)	2,500 social sciences datasets from a wide variety of academic, government and non-government organisations in Australia and globally.	ANU	4	4
Australian Earth Observation Data (Landsat)	30 years of Australasian earth observation data generated by the Landsat satellites.	BoM	1486	1413
Australian Geophysical Data Collection	The most comprehensive publicly available onshore Australian airborne magnetic, gamma-ray, seismic, electromagnetic and gravity measurements.	GA	175	7
Australian Marine Video and Imagery Collection	Archive of seabed video and stills collected on 21 marine surveys between 2007 and 2013 (including from off Antarctica).	GA, IMOS	7	7

Explore the NCI Catalogue at nci.org.au/data-collections

Dataset Name	Description	Organisation	Dataset size (TB)	Ingest as at 30 June 2015 (TB)
Australian Moderate Resolution Satellite Products (NOAA/ AVHRR, MODIS, VIIRS and AusCover)	Earth observation data generated by NASA and NOAA satellites.	CSIRO	435	286
Australian Natural Hazards Data Archive	Observational and probabilistic hazard, impact and risk data covering earthquakes, tsunami, floods and tropical cyclones.	GA	27	3
Bioplatforms Australia Melanoma Collection	Whole-genome sequences from 130+ melanoma patients.	ANU	186	186
Community Atmosphere Biosphere Land Exchange (CABLE) Model Collection	Global datasets for comparison of the CABLE land surface model against observational data. CABLE is part of the Australian Community Climate Earth Systems Science ACCESS model.	CSIRO, ARCCSS, UNSW	24	3
CORDEX Australasia	Output from the World Climate Research Programme's international project to downscale CMIP5 Global Climate Models with Regional Climate Models.	UNSW	57	1
Coupled Model Intercomparison Project (CMIP5)	Climate modelling data from the World Climate Research Programme.	NCI, CSIRO, BoM	2400	1488
CSIRO Coastal Modelling Products	eReefs Hydrodynamic model data products. Collection of various coastal modelling data. They include output from near-real time and hindcast models of hydrodynamics as well as ecological and sediment processes.	CSIRO	2	1
Digitised Australian Aerial Survey Photography Collection	More than 11,000 film negatives, derivative contract prints and diapositives of the Australian and Antarctic landscape captured c.1928-1993.	GA, ANU, CSIRO	74	74
Ecosystem Modelling and Scaling Infrastructure Facility (eMAST) Data	Data from a variety of sources including TERN facilities AusCover, Eco-Informatics, the MSPN, and OzFlux for testing of ecosystem models.	TERN eMAST, MU	90	25
Global Navigation Satellite System (Geodesy) Data Archive	Archive of Global Navigation Satellite System data from hundreds of GNSS sites throughout the world, including the Global Positioning System, the Global Navigation Satellite System, BeiDou, Galileo and Quazi Zenith Satellite System.	GA	6	4

Dataset Name	Description	Organisation	Dataset size (TB)	Ingest as at 30 June 2015 (TB)
High Altitude Ice Crystals - High Ice Water Content	Collection of meteorological data from the High Altitude Ice Crystal (HAIC) / High Ice Water Content (HIWC) field campaign conducted in the Darwin area in the period January - March 2014.	BoM	2	2
Key Water Assets	Murray Darling Basin Plan Draft Report Rainfall and Runoff data; output from the Australian Water Resources Assessment system Landscape model of catchment systems; Bioregional Assessment data.	CSIRO, BoM, GA	44	18
Models of Land and Water Dynamics from Space Data Collection	Data from the Water Observations from Space sub-project of the National Flood Risk Information Portal project, which has systematically analysed every cloud-free Landsat pixel observed between 1998 and 2012.	GA	22	16
National CT-Lab Tomographic Data Collection	Tomographic data acquired since 2001 at the ANU x-ray micro-CT facility including images of fossils, rock cores, grain packings and biological specimens, notably insects and human and animal bone.	ANU	205	171
National Resource Management data	National Resource Management data (post-processed CMIP5)	CSIRO, BoM	4	2
Ocean and Marine Modelling and Forecast Products	Ocean circulation and marine wave analysis and forecast model output from NMOC, including tsunami wave propagation model output; represents BoM's daily forecasting.	BoM, CSIRO	70	6
Ocean Forecasting Australia Model	An OFAM (Ocean Forecasting Australian Model) experiment simulating 1993 to 2012 of near-global, with a 10-km resolution (eddy-resolving) ocean general circulation model coupled with biogeochemistry.	CSIRO	150	70
Ocean Model for the Earth Simulator Re-analysis Datasets	Output from the high-resolution global Japanese Ocean model For the Earth Simulator (OFES); 30-year time series on 3-day temporal resolution.	ARCCSS	27	27
Phenology Monitoring: Near Surface Remote Sensing	Phenocam images of cyclic and seasonal variation in biological systems.	ANU, TERN, CSIRO	12	1
Plant Phenomics Digital Data Repository	High-resolution plant growth imaging data.	CSIRO	10	2
Remote and In-situ Observations Products for Earth System Modelling	Weather and ocean data from NMOC; represents BoM's daily observations and climate model analysis.	BoM	366	232

Dataset Name	Description	Organisation	Dataset size (TB)	Ingest as at 30 June 2015 (TB)
Satellite Soil Moisture Products	Satellite-derived soil moisture products, from a range of data providers, spanning the last 20-30 years.	CSIRO, TERN eMAST	6	2
Seasonal Climate Prediction Data Collection	Intra-seasonal and inter-seasonal climate analysis and forecast model output from NMOC using the ACCESS Prediction System; represents BoM's daily model runs and output including climate outlooks and hindcasts.	BoM	595	435
Severe Weather Case Studies	NCI research data collection of NWP datasets arising from severe weather case studies undertaken at the Bureau of Meteorology	BoM	50	25
SkyMapper Southern Sky Survey	Output from the SkyMapper telescope survey of the entire southern sky.	ANU	227	172
Synthetic Aperture Radar Data	20 year archive of Synthetic Aperture Radar data covering the Australian continent that can be used to observe cm-scale ground motion and surface texture associated rock type, changes in vegetation or floods.	GA	118	31
TERN eMAST Data Assimilation	Assimilation of collections of land surface observations, pre-formatted for the DART-x system, comprising model inputs and outputs.	TERN eMAST	110	10
Tropical Cyclone Scenarios	Tropical Cyclone Scenarios	BoM	200	160
Year Of Tropical Convection Re-analysis Datasets	Coordinated observing, modelling and forecasting data for tropical convection, including monsoons and cyclones, over a one-year period.	ARCCSS	84	84
		Total	**10344**	**7485**

Digital Laboratories

Digital laboratories are online interfaces tailor-made to provide data and services to suit specific research fields.

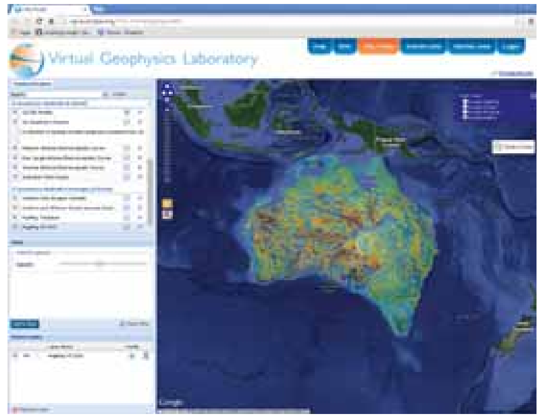
Digital laboratories bring together in a single place everything required for research computing, including easy and fast access to vast data libraries and high performance computing resources, and analysis and visualisation tools.

NCI is a world leader in the design and provision of digital laboratories, backed by our unique integration of a 10 PB data repository with Australia's first petaflop supercomputer and fastest research cloud.

We currently support the Australian Government NeCTAR-funded:

- Climate & Weather Science Laboratory
- All Sky Virtual Observatory, and
- Virtual Geophysics Laboratory.

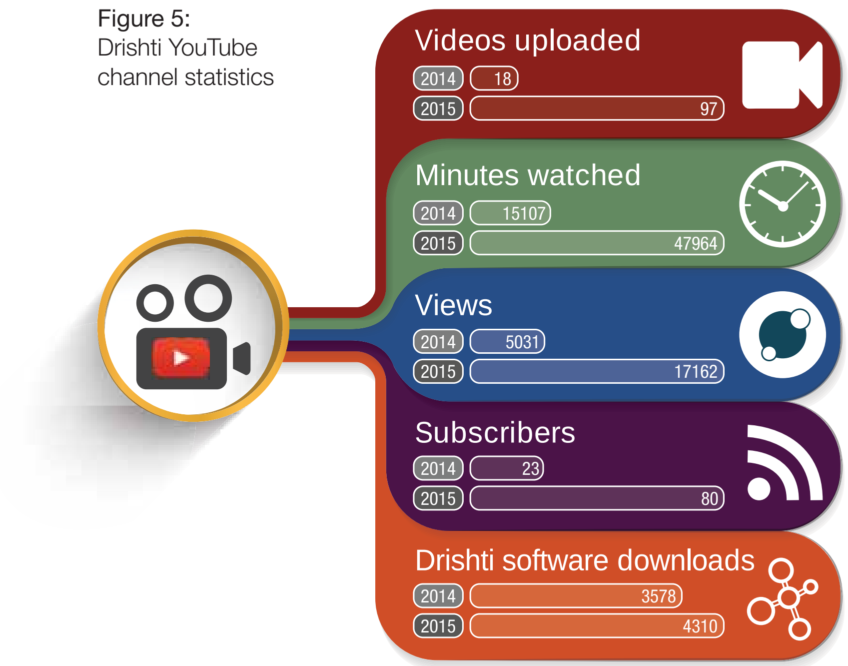
We have also been instrumental in the establishment of the Australian Geosciences Data Cube in partnership with Geoscience Australia and CSIRO.



This year the NCI Digital Laboratories Team have developed a new 'Virtual Desktop Infrastructure' (VDI) technology. The VDI substantially simplifies complicated analysis workflows that span multiple NCI systems by bringing together key data collections, analysis software, and compute systems within a familiar, unified environment which users can access as though from their own computer. So far the VDI has been deployed to the Climate and Weather Science Laboratory, and is due to be expanded for other applications, such as the Australian Geosciences Data Cube and genomics research, later this year.

NCI also provided support to the Geoscience Australia project 'Water Observations from Space' (WOfS), part of the National Flood Risk Information Project. The NCI Team deployed a set of data services to enable Geoscience Australia to effectively access decades of satellite imagery to show the history of surface water across the nation since 1987, providing emergency managers with a new understanding of potential flood impacts. The project won the award for nationally significant work in the government category of the 2014 Resilient Australia Awards. As part of NCI's new data platform (NERDIP; see page 14), the Team provide the data services using Open Geospatial Consortium (OGC) standards-compliant protocols that provide the data to the WOfS portal hosted at Geoscience Australia. By deploying data services which comply with the relevant community interoperability standards, we are enabling researchers to easily utilise internationally available tools and software.

Figure 5:
Drishti YouTube channel statistics



Scientific Visualisation

The value of scientific visualisation lies not in transforming data into pretty pictures, but in exploiting visualisation as a research and investigation tool through which to gain deeper insight into complex datasets. For more than 20 years, NCI VizLab has developed a respected reputation for its expertise in innovating and applying these techniques.

Today this team of specialist programmers works closely with researchers from NCI's partner organisations to help them gain the greatest insights from their data, and present it in clear and appealing ways.

2014/15 has been a particularly productive year for the NCI VizLab, as demonstrated through the various projects in which the team has been involved.

DRISHTI AND DRISHTI PRAYOG

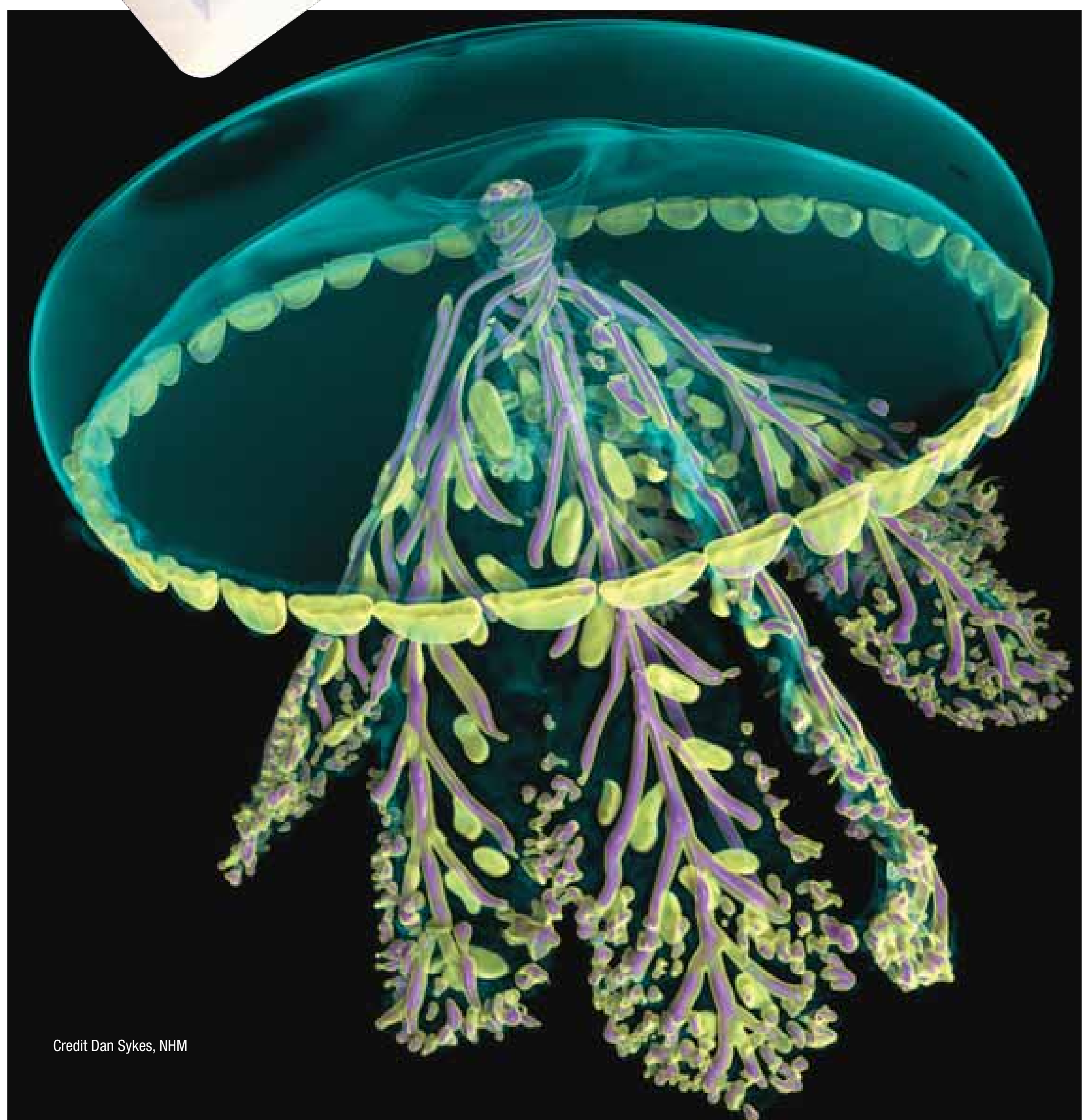
Drishti is a custom, open source software package for visualising volumetric data such as CT scans. It was developed by NCI VizLab's Dr Ajay Limaye more than a decade ago. Used all over the world, including at London's Natural History Museum, Drishti allows researchers to explore objects and specimens in minute detail without cutting them open. Drishti was downloaded 4,310 times in 2014/15.

Supported through development funds from NeCTAR, in the past year Drishti has been enhanced with two updates: landmark-based measurement and semi-automatic data segmentation.

Landmark-based morphometrics is a method used extensively in palaeontology and medical research for comparing size and shape between biological specimens. The technique involves adding digital 'landmarks' to regions such as suture junctions in mammal skulls, where one bone touches another, or the peaks and valleys of eye sockets, and then measuring the distance between two landmarks. The result is a standardised method to compare size and shape between different samples.

Segmentation is a crucial first step in the analysis of volumetric data, whether it be medical, paleontological, material sciences or oil and gas data. Drishti now has a set of tools to semi-automatically extract segments of interest for further analysis. The new version of Drishti also allows the creation of watertight surface mesh for these structures, which can be used for 3D printing.

In its first year of production, the interactive Drishti dataset presentation tool, Drishti Prayog, has been well received. It is already in regular use at the Diamond Synchrotron and Manchester University, in the United Kingdom. In March, The Institute of Marine Biology in Crete held a Drishti Prayog exhibition of marine creatures, and the new technology earned attention at the Touchscreen Developers Day at The University of Reading, UK. Drishti Prayog was also on display at the Emerging Technology Conference in Manchester, UK, in June.



Credit Dan Sykes, NHM

VOLUMINOUS

In 2014, the VizLab team completed development work on the NeCTAR-funded, web-based volume rendering program, Voluminous, which runs on the NCI cloud and exploits GPU technology. Already more than 40 users have uploaded 66 datasets for visualisation.

Voluminous is currently being enhanced to support the rendering and archive of MicroCT data produced by the newly established National CTLab, based at ANU. The system will become the portal for CTLab users to view and download their data as soon as it has been reconstructed using NCI's Raijin supercomputer.

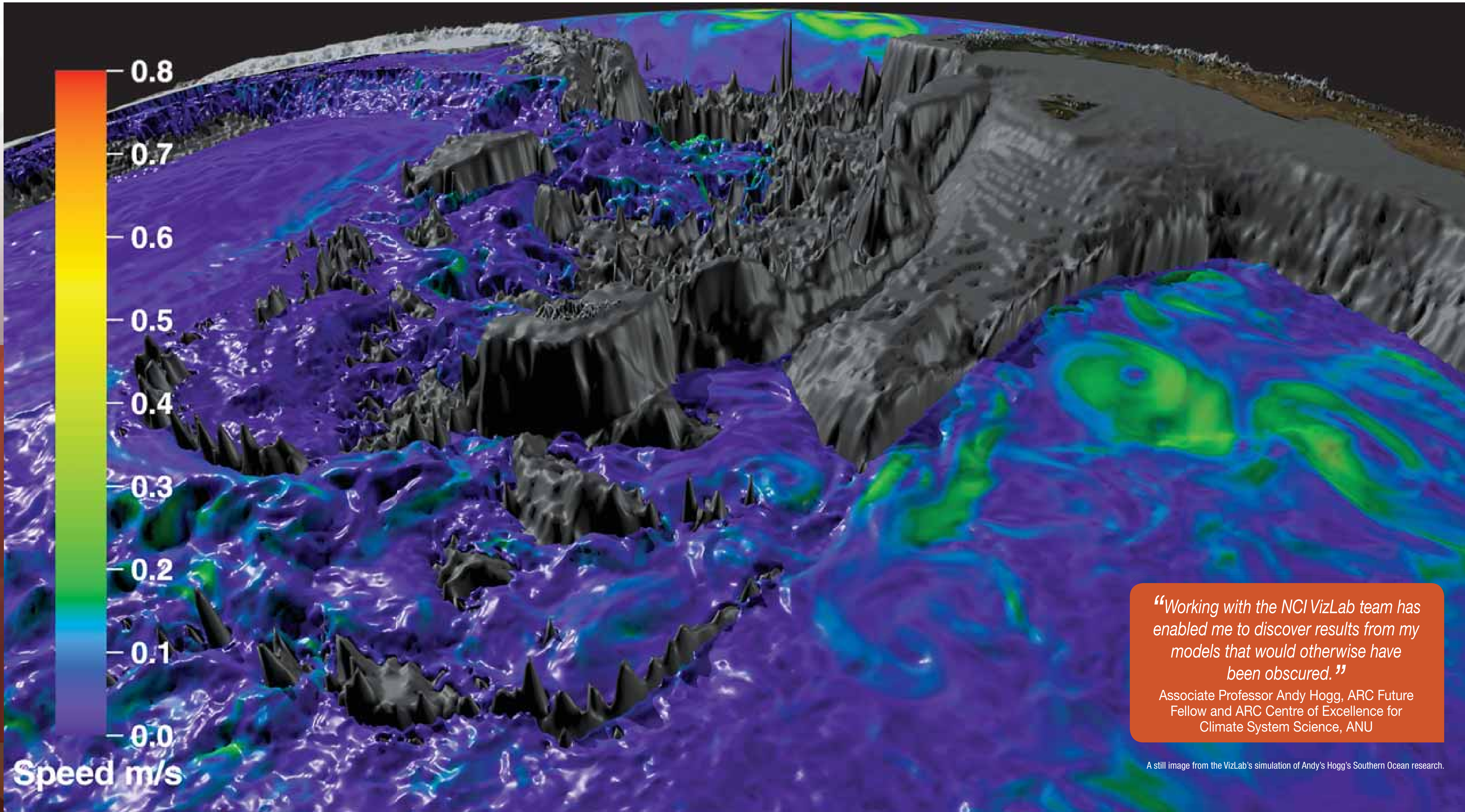
SPECIALIST SERVICES

The VizLab team are experts in applying visualisation as a research and investigation tool to gain deeper insight into complex datasets.

Oceanography

VizLab has continued working with Dr Andy Hogg and his team at ANU to visualise a 1/10th degree model of the global ocean, which is run on Raijin and made possible through NCI's ACCESS scaling activity. The project is a complex one, with more than 4,000 time steps, each at a resolution of 3,600 x 2,700 x 50 with four separate fields: water temperature, salt concentration, current velocity and density. The data is subsampled for prototyping, before the generation of iso-surface geometry and rendering using Houdini volume tools. The result is stunning animations of the global ocean system, revealing the hidden current structures beneath the surface.

VIDEO: bit.ly/VizLab_Hogg



> *"Working with the NCI VizLab team has enabled me to discover results from my models that would otherwise have been obscured."*
>
> Associate Professor Andy Hogg, ARC Future Fellow and ARC Centre of Excellence for Climate System Science, ANU

A still image from the VizLab's simulation of Andy's Hogg's Southern Ocean research.

Meteorology

This year, VizLab has started a project with the Australian Bureau of Meteorology to develop methods for visualising the data produced by the ACCESS weather forecasting model [see page 10]. As a pilot project, data from a forecast of Cyclone Christine, which hit Western Australia on New Year's Eve 2013, is being used as a test case with promising results. The plan is to develop workflows that allow for the automated production of high-quality visualisations after each new regional forecast as it is generated on BoM's production systems. Visualisation of these vast datasets will provide greater insight for policy makers and public safety organisations than can numbers on a page.

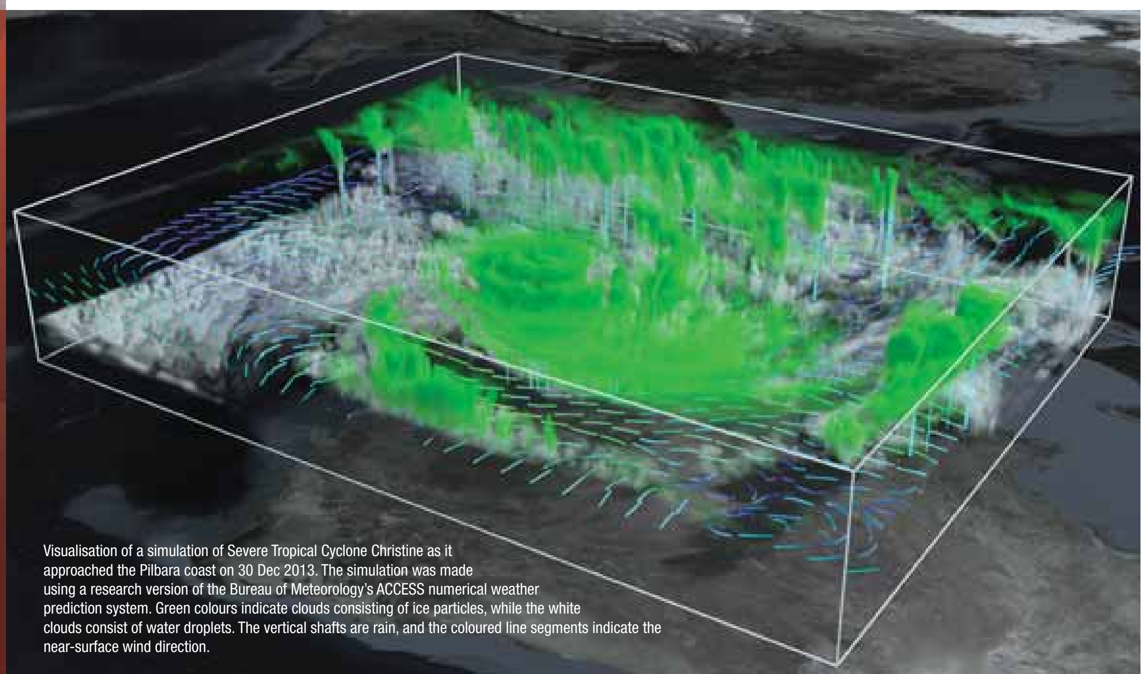
Mathematics

Another ongoing VizLab project is the population of the EPINET (Euclidean Patterns in Non-Euclidean Tilings) database. In collaboration with Professor Stephen Hyde and Dr Vanessa Robins at ANU, VizLab is generating visual models of thousands of crystallographic structures, to be made available as a large online database for chemists, physicists and mathematicians.

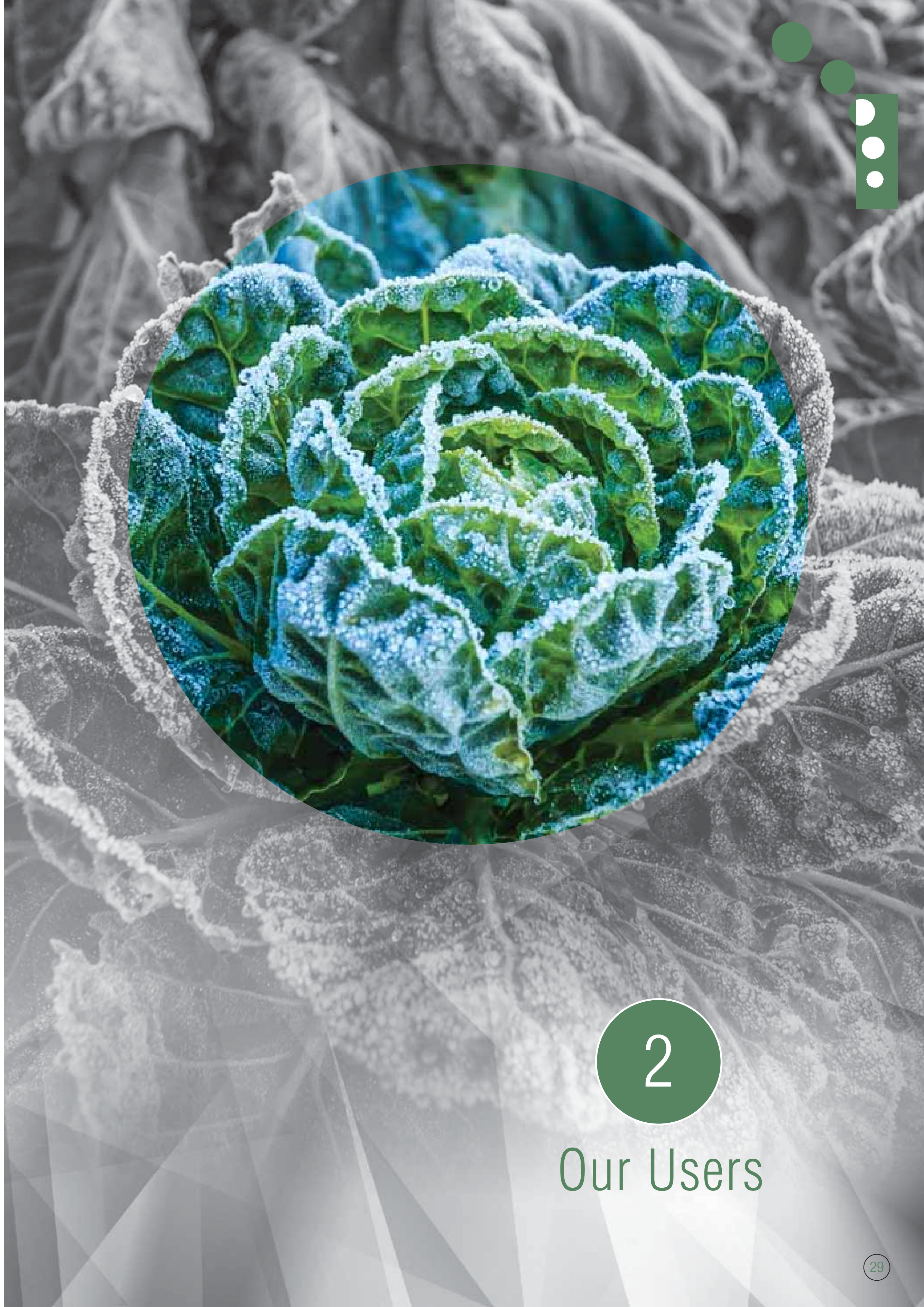
Ecology

Another exciting project, supporting the work of Dr Tim Brown at ANU, involves visualising tree growth at the National Arboretum in Canberra. The aim is to use LIDAR (or 'light radar'), time lapse photography, and environmental and meteorological data to create a digital laboratory that presents the Arboretum's development over the next decade. The project will help researchers understand how weather and climate variability affect tree growth.

Digital representation of trees at the National Arboretum.



Visualisation of a simulation of Severe Tropical Cyclone Christine as it approached the Pilbara coast on 30 Dec 2013. The simulation was made using a research version of the Bureau of Meteorology's ACCESS numerical weather prediction system. Green colours indicate clouds consisting of ice particles, while the white clouds consist of water droplets. The vertical shafts are rain, and the coloured line segments indicate the near-surface wind direction.



2 Our Users

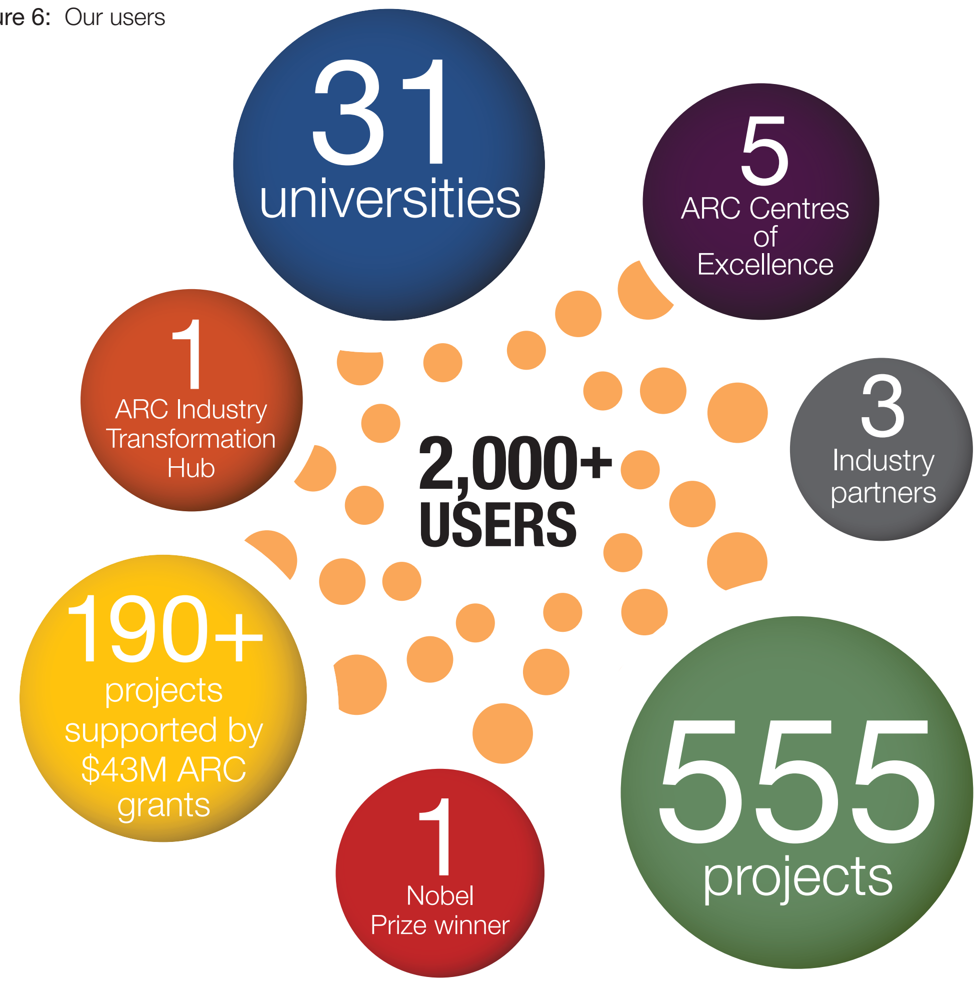
Our Users

NCI is driven by the research goals of our users and partner organisations.

We cater for the full research spectrum, from fundamental investigation to applied, strategic and industry-driven research. We provide integrated compute and data services to three of the nation's government science agencies – CSIRO, Geoscience Australia, the Australian Bureau of Meteorology – as well researchers at 31 Australian universities, five Australian Research Council (ARC) Centres of Excellence, an ARC Industry Transformation Hub, and our industry partners.

In 2014/15 NCI provided support to 555 projects and more than 2,000 research users. Of the National Computational Merit Allocation Scheme university-based projects that NCI supports (see Table 4), more than 85% are funded by the ARC and/or NHMRC and 89% received at least one competitive research grant. A total of 191 NCI projects are supported by $43 million from the ARC through Centres of Excellence, Industry Transformation Hubs, Fellowships and Project Grants.

Figure 6: Our users



RESEARCH HIGHLIGHT

Top prize for NCI user

NCI-supported researcher Amanda Barnard was awarded the prestigious Foresight Institute Feynman Prize in May 2015.

Dr Barnard is both the first Australian and the first woman to receive the award.

"Using entirely theoretical and computational methods, Dr Barnard has spearheaded understanding of the structure and stability of carbon nanostructures," announced the Foresight Institute.

"Although she has made numerous important contributions to the modelling of graphene, nanotubes, and diamond nanowires, it is her work on diamond nanoparticles that has had the greatest impact in the area of molecular nanotechnology."

Using the power of Raijin, Dr Barnard – who leads CSIRO's Virtual Nanoscience Laboratory – has pioneered the investigation of how the structural diversity of nanomaterials impacts their performance in everyday applications.

Dr Barnard's work led to the fundamental discovery that diamond nanoparticles have unique electrostatic properties such that they arrange themselves spontaneously.

The resulting structures could be useful in a number of fields, including self-cleaning surfaces and sustainable fuel cells.

The discovery has already spurred the development of a brain tumour chemotherapy treatment at UCLA.

"In the past the community has focused on simulations of individual nanostructures, which are only representative if experimental samples are perfectly monodispersed," Dr Barnard says.

"Samples of nanostructures cannot be purified, and even the best attempts to make uniform samples still contain distributions of sizes and shapes: some degree of structural diversity is inevitable.

"Although it is tempting to continue to strive for perfect samples, where all the particles are the same, this is not economically sustainable on a large scale, and so manufacturers are more inclined to accept mixtures and develop devices with larger fault tolerances.

"By predicting how imperfections at a molecular level impact on performance, we can design products with less susceptibility to faults from the outset."

A single prediction for just one substance requires hundreds of individual calculations – and each structure requires gigabytes of computer memory. Only the NCI supercomputer can handle such tasks within a reasonable time, says Dr Barnard.

Dr Barnard was also the recipient of the Prime Minister's Prize for the Physical Sciences in 2009.

Amanda Barnard.

"The discovery has already spurred the development of a brain tumour chemotherapy."

Access Schemes

NCI services can be accessed through a number of schemes:

MERIT-BASED

NCMAS

NCI provides secretariat support for the National Computational Merit Allocation Scheme (NCMAS). This is the principal, open access scheme through which researchers at publicly funded research organisations (i.e., universities, and government instrumentalities) are allocated computational resources on the country's five high-performance computing platforms on research merit. In effect, the NCMAS acts as the 'computational complement' to the granting schemes of the national research council, operating with assessment criteria equivalent to that of the ARC and NH&MRC, and determining allocations through an independent, expert panel.

For 2015, NCI provided the largest share of the NCMAS resources, nominally 75 million hours (15% of the facility), with demand exceeding supply by a factor of 2.7. This demonstrates the critical role of high-performance computing in maintaining the international standing of Australian research, particularly in the university sector.

See **ncmas.nci.org.au**

Flagship Scheme

The Flagship Scheme currently supports a number of ARC Centres of Excellence—notably in climate system science, astrophysics, and photonics, ARC Industry Transformation Hubs, and various NCRIS capabilities, notably in the environmental sciences and astronomy.

DEVELOPMENT SHARE

The development share is used to drive industry uptake, in line with the industry, innovation and competitiveness agenda being pursued by the Australian Government. It is also used by NCI to evolve its business model, and its service, reach and impact into the work of universities and government agencies.

PARTNER SHARES

The majority of NCI's HPC resources are provided through partnership contracts. If you represent a university, company or institution that would like to work with NCI, please contact **enquiries@nci.org.au**

"If we didn't have the NCI facilities it could take almost a year just to process our data. We're very grateful to have a resource like NCI." Dr Lexing Xie, ANU

"Our bushfire simulations are extremely computationally demanding and generate very large data sets. If we didn't have access to NCI we wouldn't even attempt it."
Associate Professor Jason Sharples, UNSW

Table 3: Compute allocation profile for 2014/15

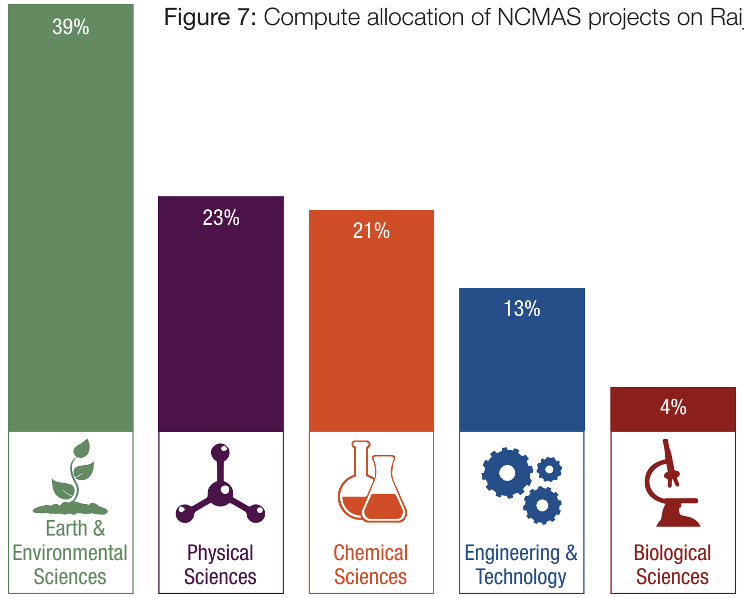
		Stakeholder	Total allocation (kSU)
MERIT ALLOCATION		National Computational Merit Allocation Scheme	88731
	Flagship	ARC Centre of Excellence for Climate System Science	12600
		ARC Centre of Excellence for All-sky Astrophysics	9190
		Astronomy Australia (NCRIS)	2572
		ARC Centre for Nanoscale BioPhotonics	400
		ARC Research Hub for Basin Geodynamics and Evolution of Sedimentary Systems	400
		Terrestrial Ecosystem Research Network (NCRIS)	98
PARTNER SHARE	Collaborators	CSIRO	110367
		Australian Bureau of Meteorology	89016
		The Australian National University	87349
		Intersect Australia*	20367
		Geoscience Australia	15424
		Deakin University	2941
		QCIF	1935
		Antarctic Climate & Ecosystems Cooperative Research Centre / Australian Antarctic Division	1340
	Universities supported by an ARC LIEF Grant	The Australian National University	see above
		University of New South Wales	9282
		Monash University	8742
		University of Adelaide	8377
		University of Queensland	8377
		University of Sydney	7540
		RMIT University	373
		Developmental Share (incl. commercial projects)	6764
		Total	**492186**

*Supported by an ARC LIEF Subscription Grant

Table 4: 2014 Merit Allocation Scheme competitive grant profile

Institution	Total kSU granted	Proportion kSU backed by grant				Grant value			
		ARC	NHMRC	Other	Any	ARC	NHMRC	Other	Any
ANSTO	250	-	-	-	-	$ -	$ -	$ -	$ -
Australian Antarctic Division	1000	-	-	-	-	$ -	$ -	$ -	$ -
CSIRO	1700	6%	-	79%	79%	$77,000	$ -	$4,206,841	$4,283,841
Curtin University	3700	100%	-	84%	100%	$651,079	$ -	$1,593,392	$2,244,471
Deakin University	1400	79%	-	71%	79%	$2,719,405	$ -	$1,633,333	$4,352,738
Flinders University	200	100%	-	-	100%	$203,487	$ -	$ -	$203,487
Griffith University	200	-	-	-	-	$ -	$ -	$ -	$ -
James Cook University	200	-	-	-	-	$ -	$ -	$ -	$ -
La Trobe University	100	100%	-	-	100%	$140,000	$ -	$ -	$140,000
Macquarie University	500	100%	-	100%	100%	$274,173	$ -	$75,000	$349,173
Monash University	15860	98%	4%	48%	98%	$5,555,235	$1,266,162	$5,592,063	$12,413,459
Murdoch University	80	-	-	100%	100%	$ -	$ -	$1,208,750	$1,208,750
NICTA	80	-	-	-	-	$ -	$ -	$ -	$ -
Queensland University of Technology	1240	100%	-	97%	100%	$700,000	$ -	$12,500	$712,500
RMIT University	3300	91%	18%	39%	100%	$4,745,716	$ 601,818	$417,417	$5,764,951
The Australian National University	15300	84%	8%	18%	96%	$8,860,720	$ 481,973	$1,484,897	$10,827,590
University of Adelaide	2000	40%	-	33%	73%	$4,366,245	$ -	$468,250	$4,834,495
University of Melbourne	7840	100%	-	58%	100%	$3,446,717	$ -	$1,246,858	$4,693,575
University of New England	40	100%	-	-	100%	$81,000	$ -	$ -	$81,000
University of New South Wales	14780	75%	-	10%	75%	$2,769,503	$ -	$1,395,750	$4,165,253
University of Newcastle	500	100%	-	50%	100%	$330,000	$ -	$33,938	$363,938
University of Queensland	8600	90%	38%	48%	100%	$2,576,195	$ 750,692		$13,949,477
University of South Australia	40	100%	-	-	100%	$145,000	$ -	$ -	$145,000
University of Sydney	7700	74%	4%	53%	74%	$2,242,663	$ 219,821	$2,143,127	$4,605,611
University of Tasmania	1770	86%	-	14%	100%	$1,249,046	$ -	$22,600	$1,271,646
University of Technology Sydney	600	67%	-	-	67%	$200,000	$ -	$ -	$200,000
University of the Sunshine Coast	80	100%	-	100%	100%	$357,632	$ -	$84,167	$441,799
University of Western Australia	1090	77%	-	73%	77%	$316,740	$ -	$10,000	$326,740
University of Wollongong	1600	50%	13%	-	63%	$136,467	$767,441	$ -	$903,908
UNSW@ADFA	2900	100%	-	76%	100%	$528,500	$ -	$5,860,000	$6,388,500
Total	**94650**	**85%**	**10%**	**40%**	**89%**	**$42,672,522**	**$4,087,907**	**$38,111,473**	**$84,871,901**

Figure 7: Compute allocation of NCMAS projects on Raijin by research field



RESEARCH HIGHLIGHT

NCI researchers awarded AAS Fellowships

Four NCI-supported researchers were announced as Fellows of the Australian Academy of Science in 2015.

Astronomer Professor Martin Asplund and Earth Scientist Professor Malcolm Sambridge from ANU, along with Materials Scientist Professor Maria Forsyth from Deakin University, and Theoretical Chemist Professor Julian Gale from Curtin University, were among the 21 new Fellows.


Professor Martin Asplund. Photo by Stuart Hay.

Professor Asplund, who was recognised for his work on the life and death of stars, said the honour was humbling.

"It's a humbling experience – I never thought I would get to this point so early in my career."

NCI Director Professor Lindsay Botten congratulated all those who were honoured.

"To be elected to the Australian Academy of Science by your peers is a real honour and I congratulate all of the new Fellows," he said.

"All of the Fellows are doing groundbreaking work in their chosen fields and we are proud to support them."

User services

NEW SELF-SERVICE PORTAL

Throughout the year, NCI User Services continued development work on a new self-service registration system, Mancini, which underwent pre-release testing in April–June 2015.

The new system replaces old email-intensive registration and approval workflows with a self-service model that allows users to register and request connections to projects without exchanging email with the NCI Helpdesk. Future releases will allow Lead Chief Investigators and Scheme Administrators to manage more of their projects online.

my.nci.org.au/mancini

TRAINING

A key role of the NCI User Services Team is providing training, both introductory and advanced, to NCI users and partners.

Throughout 2014/15 the NCI User Services Team worked to enhance their suite of training materials. The Team produced a new, intermediate level training course, 'Performance and Parallel Programming on Raijin' which was delivered on-site to three NCI partner organisations: Geoscience Australia, UNSW (ARC Centre of Excellence for Climate System Science) and the University of Queensland.

The Team also updated and revised the general introductory course, introducing information on virtual laboratories and data services. The course was delivered to 11 user groups, compared with 4 in 2013/14.

In February, NCI, in conjunction with CSIRO and NVIDIA, held a one day GPU Accelerated Computing Workshop co-located with the CSIRO CSS conference in Melbourne. This was followed by a day of training in GPU programming techniques, with both days attracting more than 40 attendees.

NCI User Services also collaborated with Mathworks Pty Ltd to host a 'Predictive Analytics and Big Data with MATLAB' seminar for more than 50 ANU and CSIRO researchers in June 2015.

Table 5: NCI training courses

Date	Partner	No. attendees	Name of course
1/5/2014	Deakin University	13	Introduction to NCI
15/7/2014	Monash University	15	Introduction to NCI
9/10/2014	ANU	24	Introduction to NCI
26/2/2015	Garvan Institute for Medical Research	9	Introduction to NCI
2/3/2015	UNSW/ARCCSS	18	Introduction to NCI
3/3/2015	ANU	10	Research Data Management Workshop
11/3/2015	University of Sydney/CAASTRO	13	Introduction to NCI
24/3/2015	Geoscience Australia	10	Introduction to NCI
25/3/2015	Geoscience Australia	10	Performance and Parallel Programming on Raijin
10/4/2015	Monash University	23	Introduction to NCI
12/5/2015	ANU	8	Introduction to NCI
22/5/2015	UNSW	12	Introduction to NCI
25/5/2015	UNSW	12	Performance and Parallel Programming on Raijin
29/6/2015	UQ	35	Introduction to NCI
30/6/2015	UQ	15	Performance and Parallel Programming on Raijin
30/6/2015	ANU/CSIRO	50	Predictive Analytics and Big Data with MATLAB

RESEARCH HIGHLIGHT: **OUR NEW PARTNERS**

Predicting sea level rise

NCI's newest partners, the Antarctic Climate and Ecosystems Cooperative Research Centre (ACE CRC, through the University of Tasmania), are scaling up their models on Raijin to investigate sea level rise.

"The largest uncertainty in predictions of future sea level rise comes from a lack of understanding of how the Antarctic ice sheet will respond to climate change," explains project co-leader Dr Ben Galton-Fenzi from the Australian Antarctic Division.

"The current hypothesis is that the accelerated thinning we've been seeing, for example in the Totten Glacier region, is due to increased basal melting by a warmer ocean."

Initially, the team used time on Raijin allocated through the National Computational Merit Allocation Scheme to develop models to study the processes behind this phenomenon at 2 or 3 km resolution.

However, the time had come to ramp up the models' resolving power.

The team are currently developing an ocean model to cover the entire Antarctic continental ice shelf at 1 km resolution – a step that has substantially increased their requirement for computing resources.

"We'd seen more and more evidence in the literature suggesting that if you're going to do this properly you've got to be running models with at least 1 km resolution," says Dr Galton-Fenzi.

"We were at the stage where we required an order of magnitude increase in CPU hours compared to our regional-scale models.

"The best way to access those resources was to become a formal NCI partner."

The end goal of the work is to collaborate with NCI's expert code optimisation team [see page 10] to couple the ocean model to an ice sheet model to look directly at how changes in the ocean lead to changes in the ice sheet.

The project is a consortium between the Australian Antarctic Division, the Antarctic Gateway Partnership, and ACE CRC.

As the largest reservoir of ice on Earth, melting of the Antarctic ice sheet could have severe implications for the world's major cities, says Dr Galton-Fenzi.

"We're really unsure of how the ice sheet will respond to climate changes and how much potential sea level rise could come from them. There's a big risk to coastal infrastructure, where you have expensive ports and where most of the world's population lives.

"Our research is focused on getting an upper bound prediction of sea level rise for the next hundred or two hundred years."

"We were at the stage where we required an order of magnitude increase in CPU hours."

Totten Glacier, Paul Brown.

Shining new light on the body

RMIT UNIVERSITY · Centre for Nanoscale BioPhotonics

Researchers from the ARC Centre of Excellence for Nanoscale BioPhotonics (CNBP) are using Raijin to design ultrasensitive biosensors for use in research and medical diagnosis.

Led by Professor Andrew Greentree at RMIT University, the team are using computer modelling to design new devices, including ones that incorporate so-called 'Whispering Gallery' resonators.

"In the Whispering Gallery of St Paul's Cathedral in London you can whisper and somebody on the other side of the dome can hear you because the sound travels around the wall," explains Professor Greentree.

"CNBP's Dr Jonathan Hall at the University of Adelaide is designing sensor platforms that do the same thing, but with light instead of sound."

Whispering Gallery resonators provide a highly effective way to trap and measure light signals, says Professor Greentree.

"Light travels so fast that on a scale of a few millimetres it's just going to zip straight past.

"But if you can trap the light in the resonator, it can bounce around inside a few million times, allowing a very small signal to be magnified and measured."

When something comes in contact with the surface of a microbubble, it causes a blip in the resonance signal.

These sensors could be used to detect particular biomolecules of interest to understand how cells work.

The team say NCI allows them to accelerate the experimental development of these useful structures.

"Modifying all the parameters of the system using a supercomputer means experimentalists in the lab don't have to spend time and materials recreating the entire gamut of possibilities," says Professor Greentree.

"We are very excited to have access to NCI because the kind of modelling we are doing is just not possible without supercomputing facilities."

The group is also looking at new types of fluorescent biomarker, such as nano-diamonds and nano-rubies, as well as ways to combine sound and light signals.

"We are also looking at the creation and detection of sound using light, which is something we are very excited about," explains Professor Greentree.

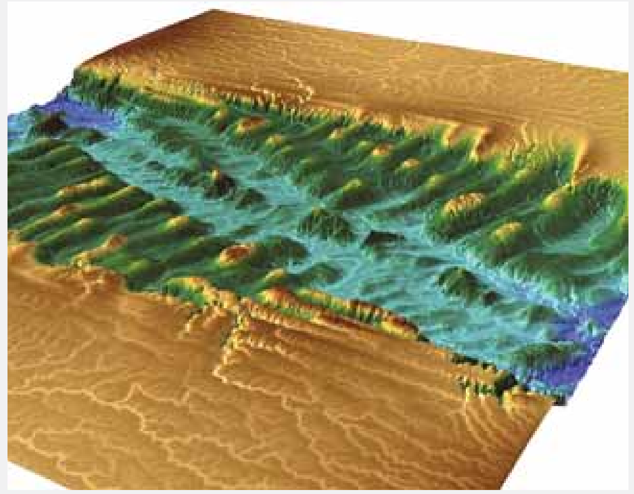
"Conceptually it's the same physics — light and sound kind of behave the same way, but when you try to combine, for example, ultrasound with nanoscale optics there is a big problem because of course there is a huge mismatch between the speed of sound and the speed of light.

"That means that technically it's very hard to work out what's going on; we need very sophisticated, very powerful computer simulations."

> *"The kind of modelling that we are doing is just not possible without supercomputing facilities."*

4D earth modelling supported by industry

BGH · THE UNIVERSITY OF SYDNEY



NCI is the provider of high-performance computing resources for the $5.4M ARC Research Hub for Basin Geodynamics and Evolution of Sedimentary Systems (GENESIS).

The Basin GENESIS Hub will use computer modelling to fine-tune our understanding of the nation's sedimentary basins, which hold many of the natural resources we use in day-to-day life.

The research will be of fundamental importance to the geo-software industry used by exploration and mining companies, explains Hub Director Professor Dietmar Müller from the University of Sydney.

"Sedimentary basins are of interest to us and to industry because they have the potential to provide a range of resources," he says.

"The spaces between the grains of sand within porous sedimentary rocks can contain water or natural gas and could be used for carbon storage."

The Basin Genesis Hub was conceived as a five-year project to develop and refine radical new geoscience software and workflows suited to the needs of industry.

The modelling involved will span entire basins hundreds of kilometres wide down to the individual sediment grain level, going back tens of millions of years.

Only the recent rise in high-performance computing hardware and software capability has made this type of basin modelling possible, says Deputy Hub Director Associate Professor Patrice Rey.

"The software we need to perform this type of modelling can only be run on highly parallelised computing systems," he says.

"That's where NCI comes in; without a computing platform like Raijin, we couldn't execute these models."

As is the case for all the Industry Transformation Hubs, the Basin GENESIS Hub is set up so the ARC funding is balanced with industry contributions.

"We are working directly with international companies such as Chevron and Statoil, as well as local companies 3D-GEO, Oil Search and Intrepid Geophysics to design specific research programs for their basins of interest," Professor Müller says.

Key focus areas are the North-West shelf of Australia – one of the country's richest natural gas resources, Papua New Guinea, and the Atlantic Ocean continental margins.

The Hub has also attracted funding from the New South Wales Government to research the Sydney Basin.

"The Sydney Basin is a good example of where there are competing interests because it provides us with water as well as energy resources," explains Professor Louis Moresi who leads the Melbourne University node of the Hub.

"This complicates the exploration and management of these resources, and calls for advanced integrated basin modelling solutions that provide improved insights into basin dynamics."

> *"The software we need to perform our research can only be run using highly parallelised computing platforms like Raijin."*

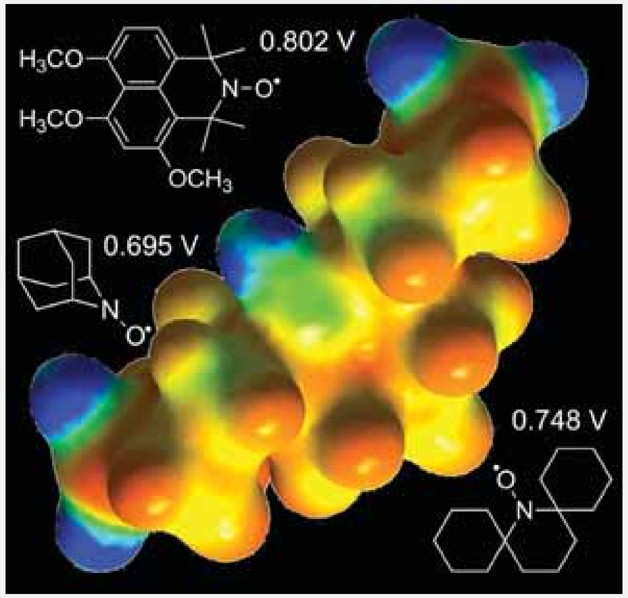
RESEARCH HIGHLIGHT

2

Super-charging solar cell efficiency

Australian National University

ARC Centre of Excellence for Electromaterials Science



ARC Future Fellow Professor Michelle Coote and her team from The Australian National University have used Raijin to double the efficiency of solar cells.

In a dye-sensitised solar cell, the dye absorbs sunlight, causing the dye to change form and release an electron which generates electricity. A second component is then needed to convert the dye back to its starting form so the process can begin again. This component is called a 'redox mediator'.

"Most dye-sensitised solar cells use an iodide molecule as the redox mediator," explains Professor Coote.

"This has a number of disadvantages. Firstly, it is coloured and that cuts down on how much sunlight is available to be absorbed by the dye.

"Secondly, its oxidation potential [its ability to give electrons back to the dye and thus convert it back to its starting form] is not very well matched to the dye, leading to inefficiency."

For several years, researchers had been proposing the use of a nitroxide radical as the redox mediator instead.

"Nitroxide radicals are colourless, and their oxidation potential is much closer to the range needed to get maximum efficiency in the conversion of the dye," explains Professor Coote, who is part of the ARC Centre of Excellence for Electromaterials Science.

The problem was that the researchers who set out to test nitroxide used a molecule that undergoes a number of rearrangements on oxidation.

"That means it's sort of being destroyed in the first round of electron transfer, so it's not around to keep cycling."

Professor Coote and her team saw these results and decided to use computational chemistry to investigate why this particular nitroxide molecule was unstable upon oxidation and what structural changes could be made to stabilise it while keeping its oxidation potential within the ideal range for the dye.

"We used Raijin to investigate many different structures and came up with five predicted compounds that we thought would work," she says.

"Not long afterward, an independent experimental research group manufactured a solar cell using one of our compounds. The new compound doubled the efficiency of the solar cell."

Professor Coote, who is head of the Computer Aided Chemical Design Group at ANU, says using computational quantum chemistry is crucial to her research and provides a much deeper insight into chemical processes than can be provided by experiment.

"We absolutely could not do this work without access to Raijin," she says.

> *"The new compound doubled the efficiency of the solar cell."*

RESEARCH HIGHLIGHT

Better materials for industry

The University of Queensland Australia

Professor Debra Bernhardt from the University of Queensland has been using Raijin and its antecedents for more than 20 years. Her latest work is helping design better materials for industry.

"We use Raijin as an experimental tool to propose and test new materials for applications such as battery technologies, detection of toxic molecules, and conversion of CO_2 into useful chemicals," she says.

Post-doctoral researcher Dr Tanveer Hussain is leading the group's investigation into the design of 'nanosensors' based on nanosheets, which can be used to detect potentially harmful substances in our environment.

"There are many compounds that may not be toxic in everyday life or in low amounts, but they might be undesirable in a particular environment," explains Professor Bernhardt.

"For example, caffeine is fine in your everyday coffee, but you probably wouldn't want to find too much of it in an anaesthetic."

Many biologically relevant molecules, including caffeine, nicotine and ethanol, bind weakly to two-dimensional nanosheets such as graphene.

Upon binding, the electronic properties of the nanosheets change – providing a clear signal that the molecule of interest has been detected.

Nanosheets are ideal for use as sensors because of their extensive surface areas, explains Professor Bernhardt.

"Because these materials are almost entirely made up of surfaces, you can have a very large sensory area that's still compact and light weight," she says.

Key to creating better nanosensors is identifying ways to increase the specificity and strength of the bond between the chemical and the nanosheet, which is where computer modelling comes to the fore.

"At the moment, the exact nature of the binding of some substances and their effect on the electronic properties of the nanosheet is still unknown," says Professor Bernhardt.

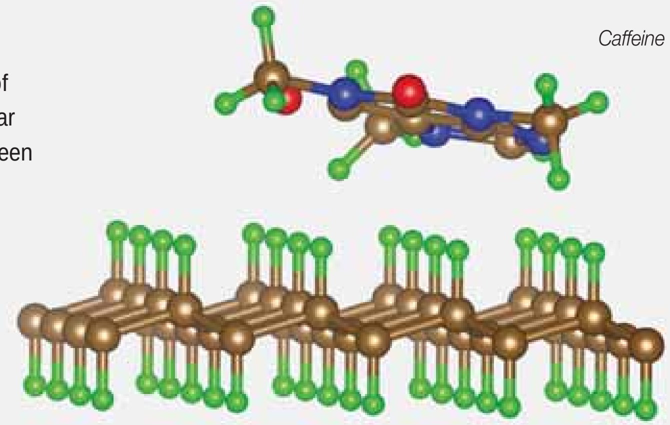
"There's a strong need to study and understand this interaction to design efficient nanosensors."

The group's current projects could never have been performed using the supercomputers of the past, says Professor Bernhardt.

"Back in the 90s, I was working on small alkali metal cations," she says. "They're only found in extreme situations such as fusion reactors or lasers, but we looked at them partly because they were small enough that we could actually perform the necessary calculations.

"Now my students and postdocs are working on more commonplace systems, with large biomolecules or structures; it would have been impossible to study nicotine on graphene back in those early days."

Caffeine



> *"Caffeine is fine in your everyday coffee, but you probably wouldn't want to find too much of it in an anaesthetic."*

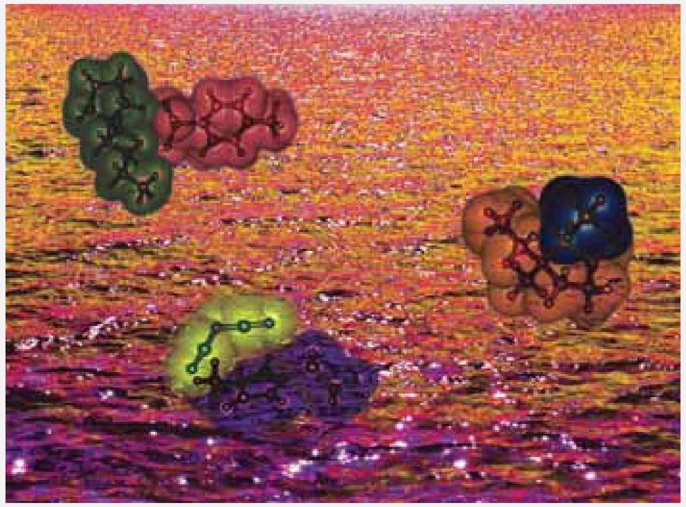
RESEARCH HIGHLIGHT

2

Solvents of the future

ARC Future Fellow Dr Katya Pas from Monash University is using Raijin to pioneer the potentially industry-revolutionising field of ionic liquids.

Current industry processes, such as making paper from cellulose, use toxic organic solvents that break down and evaporate at high temperatures.



"Ionic liquids are considered the solvents of the future," explains Dr Pas.

"They have beneficial properties such as high conductivity and being liquid at room temperature, but they do not evaporate, and the majority of them are chemically stable at higher temperatures.

"That means when organic solvents will start to decompose, ionic liquids will actually stay intact which is fantastic because it means that you don't have to constantly replenish your solvent, plus you will not have the toxic products associated with organic solvents."

Ionic liquids are generated by weakening the interactions in ionic compounds to reduce their melting temperature.

"Basically ionic materials consist entirely of ions; for example, table salt consists of only sodium and chloride ions. Because the main attraction is ionic, it means that the strength is so high that these compounds have a high melting temperature.

"The idea behind ionic liquids is to introduce chemical groups that either 'shield' or draw charge away from the centre charge and the result is a conductive salt that has a low melting point."

Ionic liquids are already being used by industry in Europe to dissolve cellulose at just 80°C, leading to a huge reduction in energy costs. The only downside is the cost of production, says Dr Pas.

"Unfortunately ionic liquids are much more expensive than organic solvents," she says.

She and her group are using Raijin to develop low-cost methods to predict the properties of ionic liquids for screening.

"There are about one trillion possible ionic liquids," she says.

"You'd have to spend a century in the lab to be able to go through all the possible combinations. That's just not sensible in terms of energy and we need ionic solutions soon."

Dr Pas is also collaborating with Singaporean company H2SG Energy to look at developing ionic hydrogels for use as membranes in energy devices such as fuel cells.

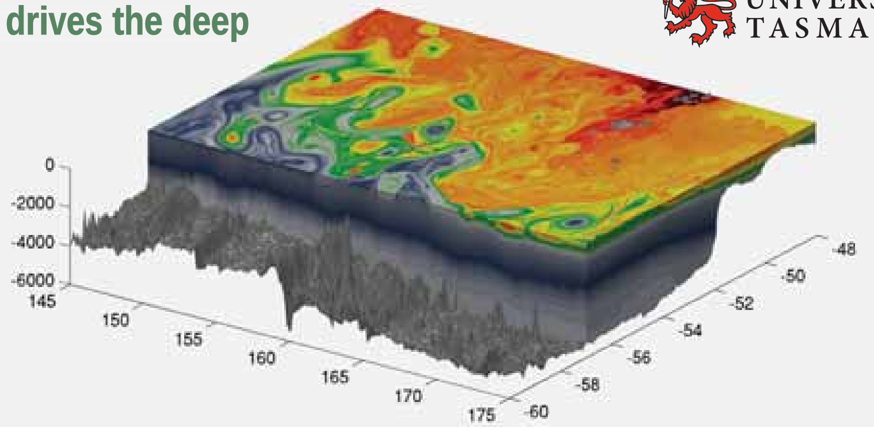
"Honestly I do believe that ionic liquids will be the solvents of the future," says Dr Pas.

"They are so fantastic in terms of reducing energy that there will probably be no alternative but to go for them, as long as we can reduce the cost of their production."

"You'd have to spend a century in the lab to be able to go through all the possible combinations."

RESEARCH HIGHLIGHT

What drives the deep



Professor Nathan Bindoff and his team at the University of Tasmania are using Raijin to investigate how the Southern Ocean drives the Earth's climate systems.

"The Earth's poles are actually warmer than you would expect, and the equator is colder than you would expect, on the basis of the way the sun shines on the Earth," says Professor Bindoff.

"This is because the oceans are circulating heat from the equator to the poles."

Oceans are not just static bodies of water; constant movement and mixing in all directions results in a continuous shifting of energy, nutrients and heat.

These fine-scale motions have big impacts on the Earth's climate equilibrium.

"In the atmosphere, we talk about highs and lows," explains Professor Bindoff.

"The ocean has precisely the same thing occurring: weather systems that blow in, blow out. We call these eddies. Eddies shift energy around in the water column and that energy balance is part of what sets the movement of heat from the equator to the poles."

The team, including key researchers Max Nikurashin and Andreas Klocker, is using complex 3D computer simulations to work out the different factors at play in eddy behaviour.

Their work, which is supported by three grants from the Australian Research Council, is informing multi-million dollar ship-based observational work.

"The only way we can do some aspects of ocean research is through computer simulation," says Professor Bindoff.

"We are creating models to discover the role of different factors, such as ocean floor topography in the presence of really strong currents like the Antarctic Circumpolar Current.

"Using the results of these simulations, we have proposed observational experiments to go out and measure the same things to validate our models.

"So this is a great example of how theoretical simulations to some extent can drive observational science."

The team's simulations require millions of compute hours, hundreds of processors, and produce tens of terabytes of data – logistics that have only been made possible by recent advances in computational facilities such as NCI.

"Ten years ago you couldn't have done this work," says Professor Bindoff. "Now that computers are capable of these simulations, there's been a renaissance in oceanography.

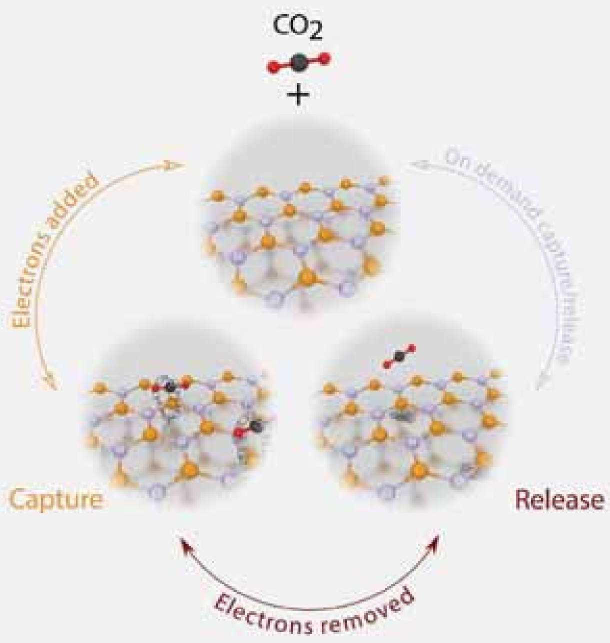
"The project's results will guide the development of state-of-the-art global ocean and climate models and improve our ability to predict and respond more effectively to climate change."

"This is a great example of how theoretical simulations to some extent can drive observational science."

RESEARCH HIGHLIGHT

Carbon capture's 'Goldilocks problem'

Researchers from UNSW are using NCI's supercomputer to pinpoint the 'sweet spot' of new carbon capture materials.



Current materials for capturing carbon from power plant exhaust tend to bind CO_2 too effectively. This causes problems when the carbon needs to be released again for sequestration or recycling.

"If the material binds to CO_2 too strongly, which is the basic problem with current materials, then you have to heat them up to a high temperature to pull the CO_2 off, and that costs money," explains chief investigator Professor Sean Smith.

"It's a 'Goldilocks problem'."

Professor Smith and his team are taking a novel approach to the search for new materials. They have identified several materials that adopt altered binding behaviour when exposed to electrical charge.

"Normally, if you put CO_2 in contact with these materials there is very weak binding – they won't capture CO_2 at all. But if you put an electrical charge on the material, suddenly it binds CO_2 quite effectively," says Professor Smith. "And if you then remove the charge, it lets the CO_2 go."

The result is a material that can be 'switched' on and off with an electrical charge, side-stepping the expensive heating requirements of current industry materials.

However, these new charge-responsive materials come with a hurdle of their own.

"One of the materials we're looking at now, for example, is boron nitride, which is a semiconductor with a very large bandgap. That means it takes a lot of voltage to put enough charge on, and there is a cost to that," says Professor Smith.

"What we're using NCI to do is search for materials that have a similar capacity to bind CO_2 but with a much smaller bandgap."

The team is running first principles and electronic structure calculations on Raijin to work out exactly how each new material interacts with CO_2, predicting the binding strength and voltage response profile to pinpoint a material with ideally balanced properties.

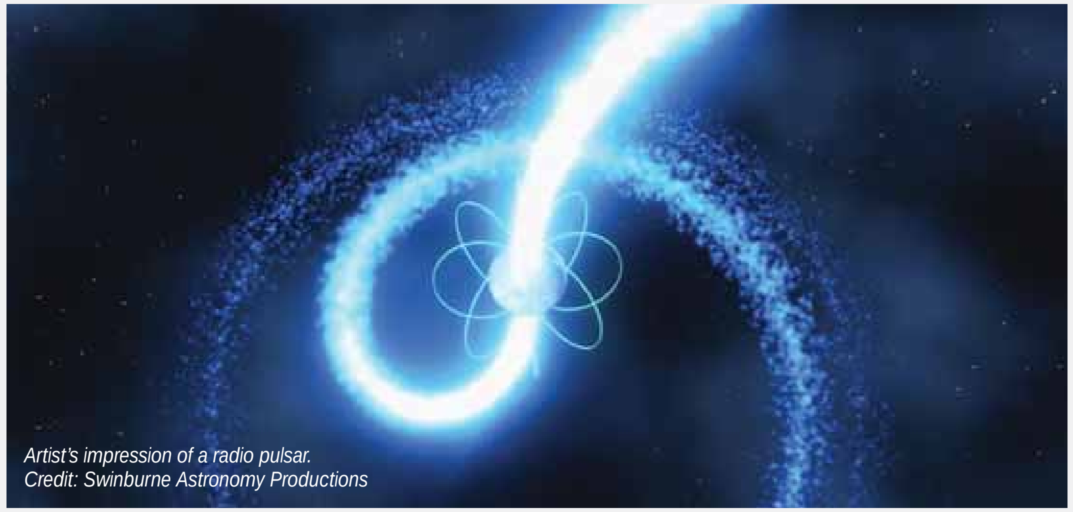
"These are very numerically intensive calculations, which demands that we have access to a facility of the order of capability that the NCI has," explains Professor Smith.

"There is no other way you can do this work."

> *"Current materials for capturing carbon tend to bind CO_2 too effectively."*

RESEARCH HIGHLIGHT

Searching for super-dense neutron stars



Artist's impression of a radio pulsar.
Credit: Swinburne Astronomy Productions

Researchers are using Raijin to perform the deepest ever search of our galaxy for neutron stars. The discoveries will help test Einstein's theory of general relativity.

"It's not possible to test Einstein's general theory of relativity easily in our solar system because our stars are just not heavy enough to sufficiently bend space–time," explains Pro Vice Chancellor (Research) at Swinburne University of Technology and the dynamic theme leader of the ARC Centre of Excellence for All-Sky Astrophysics, Professor Matthew Bailes.

"We are searching for neutron stars, which have a gravitational field about two hundred billion times stronger than Earth's, and which will enable us to test aspects of general relativity much more easily than we can here in the laboratory."

Neutron stars are the super-dense collapsed cores of once-massive stars some 10 times bigger than our sun.

"The density of neutron stars is typically one billion tonnes per cubic centimetre," says Professor Bailes.

"They are also highly magnetised and spin very rapidly. That combination leads to emission of a beam that sweeps through the galaxy and impacts our telescope after travelling up to thousands of years."

Neutron stars display a very characteristic signal, says Professor Bailes.

"When a neutron star pulse hits our telescope it first appears in the high frequency radio stations and then it sort of sweeps down to the lower frequency radio stations afterwards.

"We use Raijin to search for these characteristic delays between our 1,024 regularly-spaced radio stations to find our neutron stars."

So far, the project, which is a collaboration with CSIRO, the Max Planck Institute, the University of Cagliari and Manchester University, has led to the discovery of more than 50 neutron stars.

The undertaking is highly compute-intensive, says Professor Bailes.

"Our dataset is around half a petabyte in size," he says.

"We're looking at 16 million consecutive time samples, and we need Raijin's large memory and processing power to search that data for all the potential neutron stars."

> *"Our dataset is around half a petabyte in size."*

RESEARCH HIGHLIGHT

More frosts to hit WA crops

New research performed on Raijin suggests south-western Australia will become even drier, with severe implications for the region's $4.5 billion agricultural industry.

Professor Tom Lyons and his team at Murdoch University are using the high-performance computing facilities at NCI to predict the future climate in the region – information that is critical for informing crop management strategies.

"Current global climate models give estimates of changes in rainfall at a resolution of about 250 square kilometres, which isn't that much use for farmers," explains Professor Lyons.

"What we have been attempting to do is to take global climate models and downscale them to a farm-relevant scale of fewer than five square kilometres."

After several rounds of model validation, the team is starting to predict the climate over the years 2029 to 2060.

This mammoth task requires a lot of computing power, says Professor Lyons, who is supported by funding from the Grains Research and Development Council.

"To give you an example, it takes us about eight hours real time to model a single month. We run these studies over 30 years, so you can imagine it tends to tie up a lot of resources, and produce large amounts of data."

One of the most striking findings of the future climate modelling so far is that south-west Western Australia is set to see more intense and frequent frosts.

"Frost is a particular problem for broad-acre agriculture, where you're looking at thousands of acres," says Professor Lyons. "You can't take action against that."

The only way for broad-acre farmers to avoid frost damage is to know the timing of frosts so they can adjust their planting decisions, says Professor Lyons.

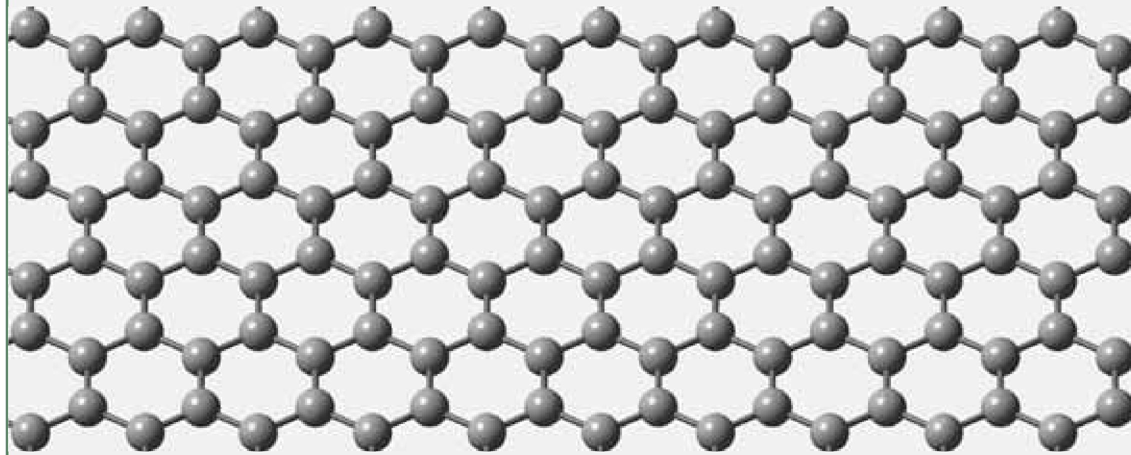
"The problem is if you plant too early or late you've also got to worry about whether there is going to be enough soil moisture around when you need it," he says.

"So it's quite a nifty balance. We are basically trying to solve that problem with farm-scale meteorology."

> *"It takes us about eight hours real time to model a single month."*

RESEARCH HIGHLIGHT

New function for Nobel compound



Researchers have used Raijin to discover that nano-sized fragments of graphene can speed up the rate of chemical reactions.

Assistant Professor Amir Karton from the University of Western Australia says the finding suggests graphene – sheets of pure carbon – might have potential applications in catalysing chemical reactions of industrial and medical importance.

"Graphene is one of the most exciting materials to work with in nanotechnology because its 2D structure and unique chemical properties make it a promising candidate for new applications like nanodevices that can be used in mobile phones, health care devices and renewable energy," says Professor Karton.

"Ever since the discovery of graphene in 2004, scientists have been searching for applications.

"Our team has discovered a new catalytic activity of graphene nanoflakes, which is very exciting."

Graphene is remarkably strong for its weight – about 100 times stronger than steel – and conducts heat and electricity with great efficiency.

The global market for graphene is reported to have reached US$9 million per year with most sales concentrated in the semiconductor, electronics, battery energy and composites.

"Graphene is a very hot topic at the moment," says Professor Karton.

"Its discoverers earned a Nobel prize in 2010 just six years after its discovery. Most compounds of historical significance have been recognised with a Nobel Prize 20 or even 30 years after discovery. That's how amazing this material is."

Assistant Professor Karton and his team used Raijin to show, for the first time, that graphene nanoflakes could efficiently catalyse a range of chemical reactions.

The sophisticated computational modelling they used had enormous compute and data requirements.

"Graphene nanoflakes are relatively large, as far as molecules go, which meant the compute requirements of the modelling increased exponentially with the size of the system.

"We required really large-scale calculations that we couldn't do on any other cluster in Australia but Raijin.

"The two things that were really crucial for this project were very large memory, and very large and fast disks. We couldn't have done it without the NCI facilities."

> *"Our team has discovered a new catalytic activity of graphene nanoflakes."*

RESEARCH HIGHLIGHT

Tracking the Sun's history

Raijin is helping researchers to track variations in the Sun's activity over recent millennia.

Dr Andrew Smith at the Australian Nuclear Science and Technology Organisation (ANSTO) has been making trips to Antarctica for almost two decades, bringing back ice cores for analysis.

He is searching for beryllium-10, a radioactive atom that holds the secret to the story of our Sun's recent history.

"Beryllium-10 is produced when cosmic rays smash into the Earth's atmosphere and collide with the nuclei of atmospheric gases," explains Dr Smith.

Dr Andrew Smith holds an ice core for analysis

"Beryllium-10 is then rained or snowed out of the atmosphere down to the Earth's surface, where it is deposited in layers of Antarctic ice."

Not all of the cosmic rays bombarding Earth make it to our atmosphere; many are deflected by the Sun's magnetic field as they travel through the Solar System. This affects how much beryllium-10 reaches the ground.

"When the Sun is more active, its magnetic field is stronger so there is a greater degree of deflection of the cosmic rays," explains Dr Smith.

"That means the production rate of beryllium-10 decreases. And so, in principle, by measuring the concentration of beryllium-10 in successive layers of the Earth's polar ice you can reconstruct the activity of the Sun in past times."

Understanding patterns of variation in the Sun's intensity is critical to understanding future climate change, says Dr Smith, whose expeditions are funded by the Australian Antarctic Division.

Of course, nothing is ever as simple as it seems. There are a whole range of factors, such as the Earth's dipolar magnetic field, that affect the levels of beryllium-10 found on Earth's surface.

Dr Smith's colleague, Dr Ulla Heikkilä, has been using Raijin to model some of these processes.

"There is a seasonal variation in beryllium-10 at the site at which we collect our ice cores," says Dr Smith.

"We have a maximum in summer and a minimum in winter.

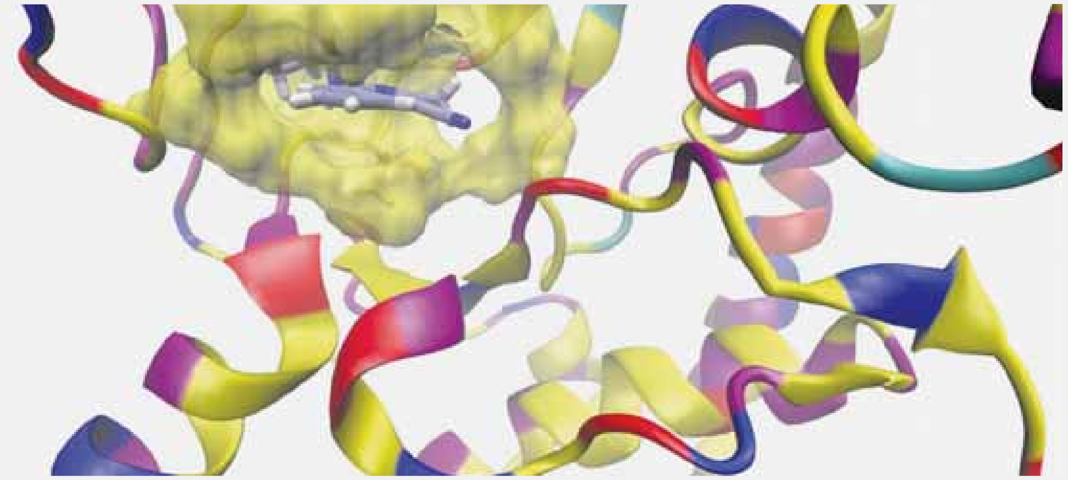
"If you didn't know any better you might interpret that increased concentration as being a decrease in solar activity, but it's not.

"The modelling on Raijin revealed that it is actually caused by a change in the weather systems, allowing stratospheric stratospheric air, which has more beryllium-10 in it than tropospheric air, to descend down to the site."

> *"Understanding patterns of variation in the Sun's intensity is critical to understanding future climate change."*

RESEARCH HIGHLIGHT

Computer-aided drug design



Dr David Wilson from La Trobe University is using Raijin to design new drugs for diseases such as cancer and Alzheimer's.

"We're looking at kinases – a group of proteins that are involved in the signalling pathways of a whole bunch of different diseases," explains Dr Wilson.

"If we could stop these kinases working, we could target those disease states."

Dr Wilson and his team are using molecular modelling programs on Raijin to design small molecules that block the kinases' active sites.

"By understanding the structure of these kinases we can begin to define small molecules that could bind to and block up the active sites of these proteins and stop them from functioning," he says.

The team is working with experimental biologists to test their computer-designed drugs in the lab.

"We model lots of different molecules and then choose the best 10 to synthesise and perform biological assays with," explains Dr Wilson.

"Then, on the basis of those experiments we go back and modify the models to refine the best target molecules.

"We've been making some good progress and have several lead compounds that look promising."

The process is complex and compute-intensive, says Dr Wilson.

"These molecules and proteins are very dynamic, moving, flexible systems," he says.

"Traditionally scientists thought of molecules binding to active sites like a 'key in a lock'.

"But the reason the lock and key at home on your front door works is because the components don't move – they're inflexible.

"If both your key and lock are flexible and can move and change shape, that makes it a whole lot harder.

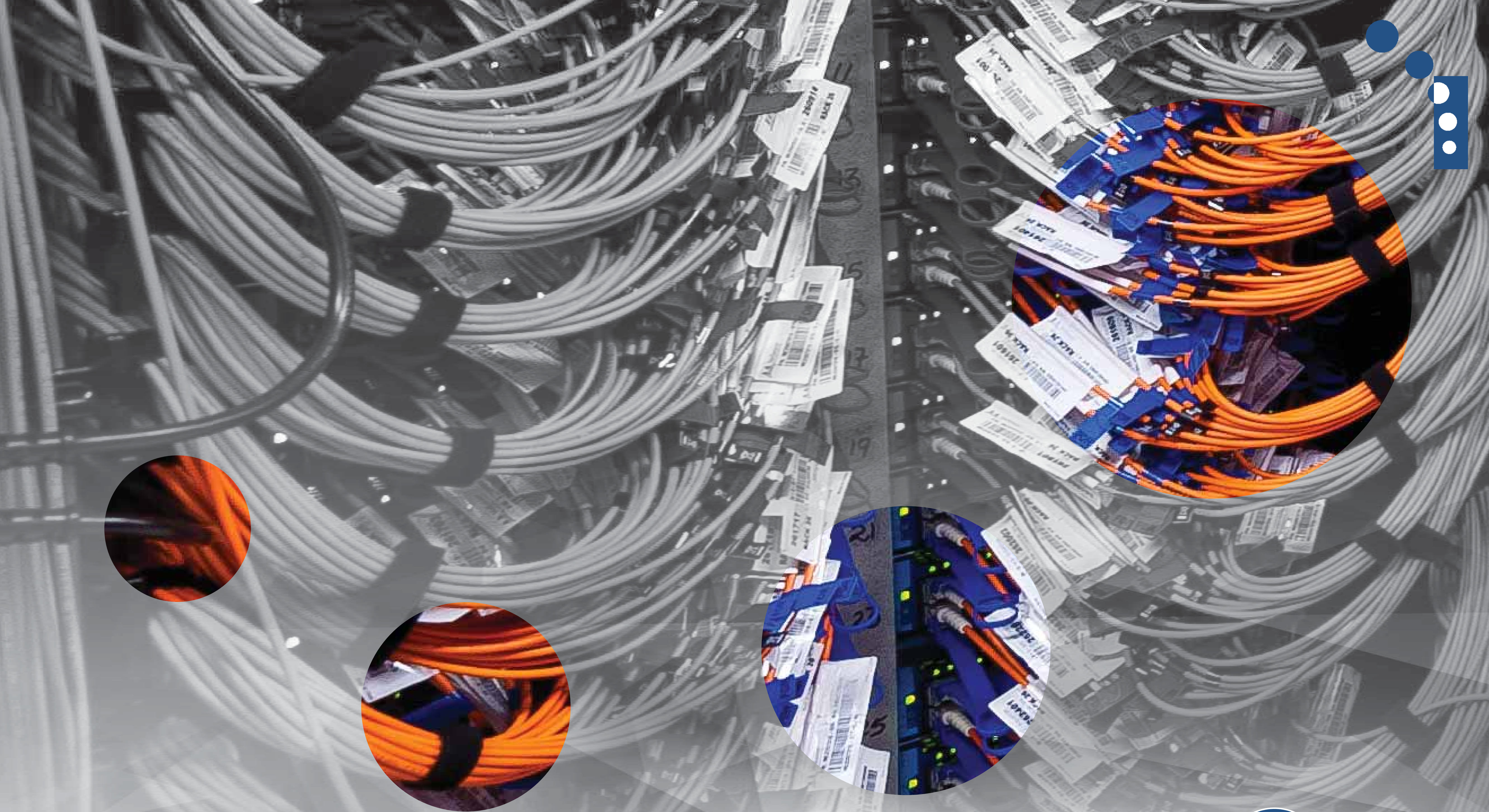
"So it's not quite as simple as making a molecule that will fit to the exact shape of the active site."

The greater the computing power, the more accurately these molecules can be modelled.

"If we had unlimited computing power – and it's probably what will happen in the future as computers advance – we would repeat our experiments 1,000 times to get really robust statistics of how well a certain molecule binds to the protein and therefore how effective it could be as a drug," says Dr Wilson.

"We can do so much more now than even three or five years ago thanks to the way computing keeps advancing."

> *"We can do so much more now than even three or five years ago thanks to the way computing keeps advancing."*



3 Our Infrastructure

Our Vendors

Our Infrastructure

Raijin

- Fujitsu Primergy cluster
- 1.2 PFlops peak performance
- 57,472 Intel Xeon cores (Sandy Bridge, 2.6 GHz)
- Mellanox FDR 56 Gb/sec Infiniband full fat-tree interconnect
- 160 TB main memory
- 10 PB disk storage
- 503M core hours/annum
- 300+ software packages
- Access to 20 PB data repository

Installed for testing in January 2014, Raijin's new Mellanox software accelerators were made available to users in July 2014. Benchmarking using CSIRO's Cubic Conformal Atmospheric Model has shown that the introduction of the accelerators, along with adoption of hyperthreading, has led to a 2.5-fold efficiency in the model's run-time.

This year the HPC Systems Team has also enhanced Raijin's custom job-monitoring dashboard, with the addition of SU usage and per stakeholder, per user, and per project job statistics. These improvements help support staff to work with users to optimise their jobs to increase throughput.

Finally, the team have been evaluating the performance of new generation processors in preparation for NCI's next supercomputer deployment.

EXPERT STAFF

In the course of maintaining Raijin, NCI's expert System Teams often find and repair software bugs. In the past year, the team have contributed five Lustre patches that have since been made available to the open source community by Intel. The team also contributed several bug fixes to Raijin's scheduling software, PBSPro, including bonus time calculation and walltime limits, and fixing an ancient memory leak, which has been incorporated into the upcoming release of PBSPro. These contributions led to an invitation from Altair to deliver talks at Supercomputing '14 and PBS User Group '15.

The HPC Systems Team also contributed a patch to Parallel Debugger, increasing its scalability from 112 cores to theoretically unlimited cores – limited only by physical memory – effectively making the software exascale ready.

Cloud

NCI cloud facilities are spread over three installations: the NeCTAR cloud, available to all users; and the ROHS and Tenjin clouds, available to NCI's official partner organisations. The NeCTAR and Tenjin clouds are built to supercomputer specification with the same hardware foundation and interconnect as Raijin, making NCI's the fastest cloud environment in the Southern Hemisphere.

TENJIN

Tenjin, NCI's supercomputer-grade cloud, was made available to our partner organisations in September 2014. Since then, Tenjin has been maintained at greater than 99.5% uptime.

Tenjin is specifically designed for data-intensive research, such as genomics, earth system science, and geophysics. It is an ideal environment for research requiring access to the datasets held in the NCI Environmental Research Data Collection.

In 2014/15, Tenjin's data storage system has been upgraded from 500 TB to 1 PB capacity.

RHOS

The NCI Red Hat OpenStack (RHOS) cloud environment is our first-generation private cloud. It was commissioned in September 2013.

NeCTAR

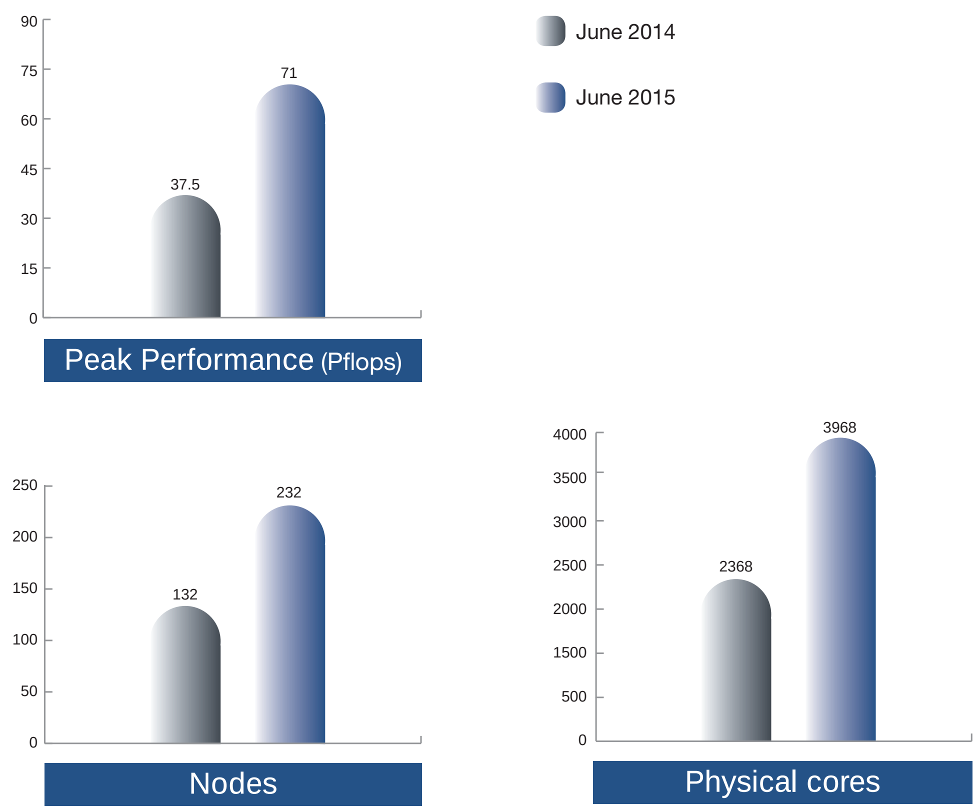
NCI is one of eight nodes of the Australian Government's National eReserach Collaboration Tools and Resources (NeCTAR) federated research cloud initiative. The NCI NeCTAR node, which came online in March 2014, provides 1,600 physical cores to researchers affiliated with Australian universities. Unlike the other NeCTAR nodes, which are based on generic or commodity hardware, the NCI node is of supercomputer specification.

In contrast to Tenjin, which is encompassed within NCI's rich site-wide filesystems, the NeCTAR cloud is managed, like the other nodes of the NeCTAR federation, in a centralised way from the University of Melbourne.

Table 6: NCI's cloud environment

Cloud	Available to	Operating platform	Peak performance (Tflops)	Nodes	Physical cores	Core hardware	Interconnect	Main memory (TB)	Solid State Disk (TB)	Access to NCI's 20 PB site-wide high-speed parallel filesystems
Tenjin	NCI partners	Red Hat OpenStack	33.5	100	1,600	Intel Xeon Sandy Bridge, 2.6GHz	Mellanox FDR 56 Gb/sec Infiniband full fat-tree	25	160	Yes
RHOS	NCI partners	Red Hat OpenStack	4	32	768	Intel Xeon Westmere, 2.6GHz	Dell 10 Gb/sec Ethernet	4.6	12.8	Yes
NeCTAR	Researchers affiliated with Australian universities	Ubuntu OpenStack	33.5	100	1,600	Intel Xeon Sandy Bridge, 2.6GHz	Mellanox FDR 56 Gb/sec Infiniband full fat-tree	25	160	No

Figure 8: Cloud statistics



Globally distributed cloud

In November 2014 NCI teamed up with Singapore's Agency for Science, Technology and Research (A*Star) to improve global data transfer speeds.

Working in collaboration, NCI and A*Star staff used InfiniBand technology to greatly increase the efficiency of the AARNet pipeline that currently links these organisations.

In a demonstration at Supercomputing '14, the team showed that the new system resulted in transfer of a 1.2 TB dataset from Singapore to Australia in just 24 minutes, compared to 9 hours using the standard TCP/IP protocol. The data was then analysed on NCI's Tenjin cloud and the results returned immediately to A*Star.

This profound breakthrough in trans-continental data transfer has major implications for internationally collaborative research; high-speed data transfer will enable the possibility of 'globally distributed cloud computing' – the capability to split jobs over multiple intercontinental cloud environments.

NCI has been working with A*Star to grow the 'InfiniCortex' network across the globe; so far the US, UK, Japan, South Korea, France and Poland have all implemented InfiniBand connections via Singapore.

Data Storage

ENHANCED STORAGE CAPACITY

NCI's site-wide parallel Lustre filesystems have been enhanced greatly this financial year, with the addition of 10 PB capacity and an increase in transfer speed from 45 GB/sec to up to 90 GB/sec, and which is expected to increase to 140 GB/sec in the following year.

In January 2015, the upgraded /g/data2 filesystem entered full production service, with an expansion from 4.5 PB to 6.7 PB. Eight major data collections totaling 2,018 TB have been migrated from /g/data1 to /g/data2 to allow for growth and provide improved performance. These infrastructure enhancements have been made possible with funding from the Australian Government's RDSI project.

In April, NCI signed a $2M deal with Fujitsu to work with storage and data management company NetApp to supply and install /g/data3. The new FAS, E-series and EF all-flash storage arrays provide an additional 8 PB of persistent storage capacity, accessible at up to 140 GB/sec on Raijin. /g/data3 will consist of 192 Rack Units of disk array with 2,904 individual drives and more than 520 cables. /g/data3 will hold the RSDI-supported National Environmental Research Data Collection [see page 14].

This year the Data Storage Services Team have also expanded the capacity of NCI's Spectra Logic T950 tape libraries, which hold archival data and provide back up for our site-wide parallel filesystems. The potential raw storage capacity of these libraries has been increased from 25 PB to 49 PB this year, with the installation of more than 1,440 tapes. Together, these libraries currently hold more than 12 PB of data.

Overall, NCI's filesystems have been maintained at greater than 99% uptime this financial year.

Figure 9: Filesystem configuration

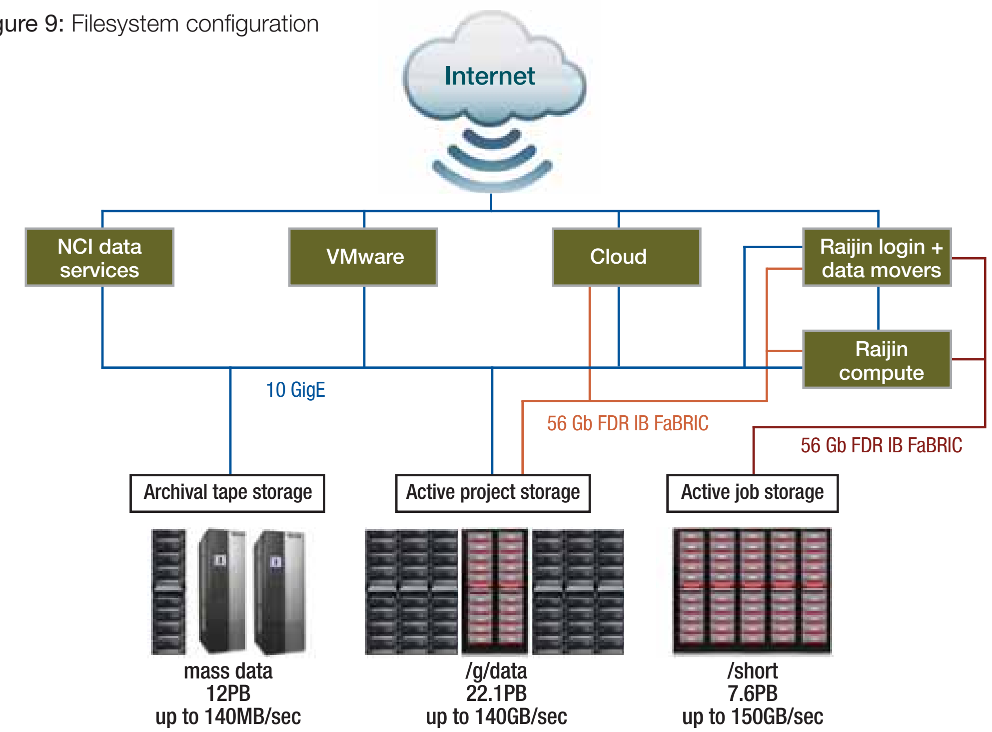
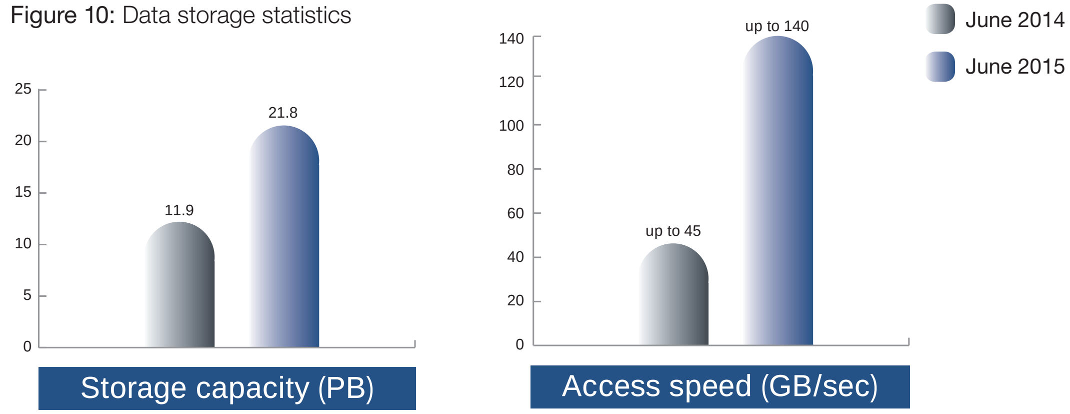


Figure 10: Data storage statistics



ENHANCED TRANSFER SPEEDS

The NCI Data Storage Services and HPC Systems teams have worked together to significantly improve data transfer efficiency within the NCI facility. The result is an increase in data migration rates between filesystems to more than 15 GB/sec with the introduction of an open-source distribution copy tool.

NCI's primary internet connection was also upgraded, in August 2014, to the latest generation AARNET4 link, moving from a capped to a dedicated full bandwidth 10 Gigabit connection. This improved connection has boosted the ingest of nationally and internationally sourced data collections as part of the RDSI project, as well as offering improved transfer speeds to users connecting to Raijin from outside NCI.

Superfast international data transfer

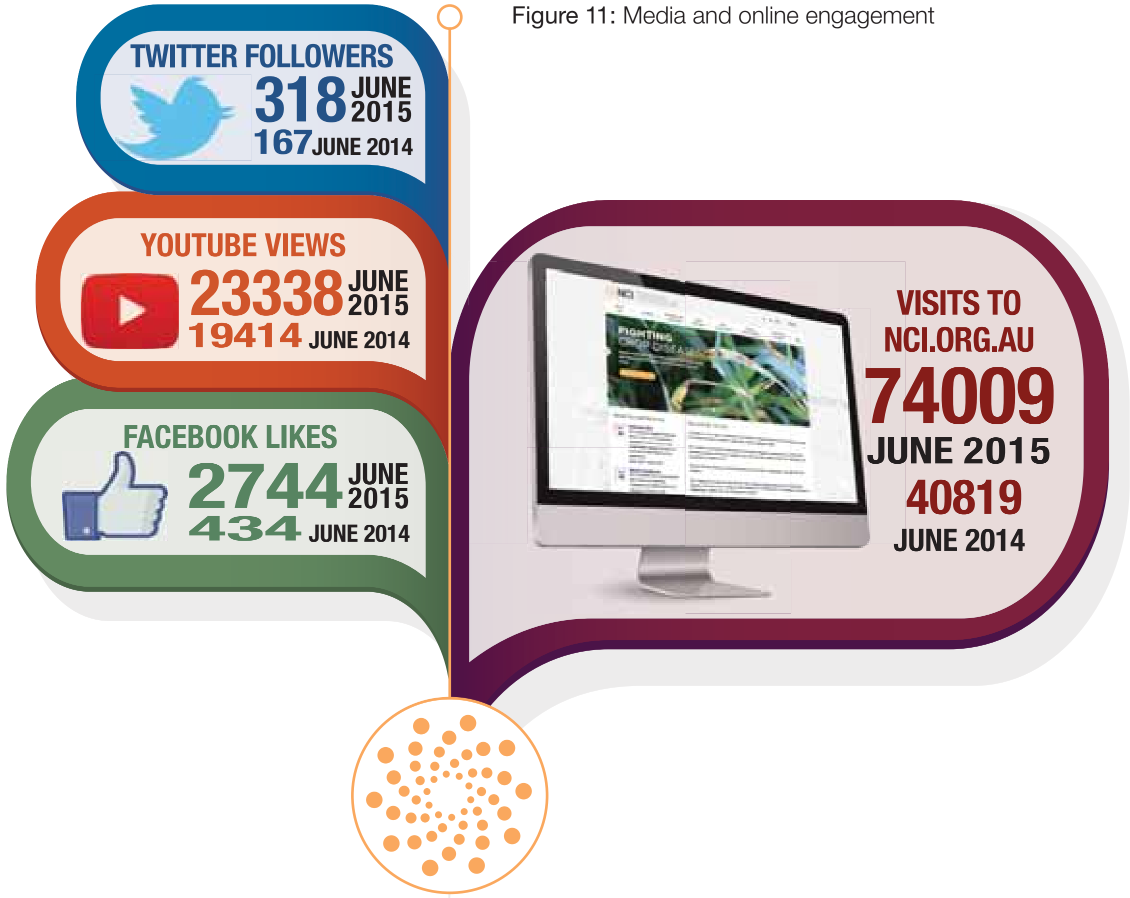
NCI is working with data managers from around the country and the globe to quickly and reliably transfer very large datasets.

So far NCI has ingested 1.5 PB of the Coupled Model Intercomparison Project (CMIP) 5 dataset from the Lawrence Livermore National Laboratory in the USA using high-speed global networks.

This undertaking has only been possible because of the expertise of NCI staff, who have achieved a very high fraction of the theoretical bandwidth of global networks [see page 56].

4 Outreach

Figure 11: Media and online engagement



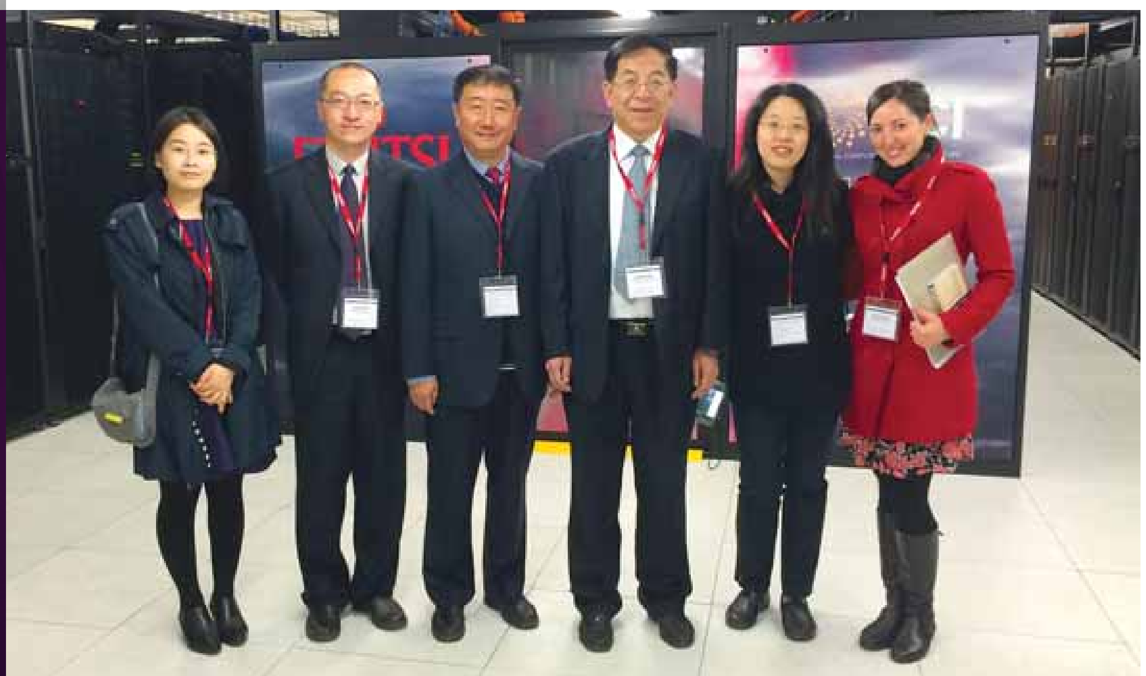
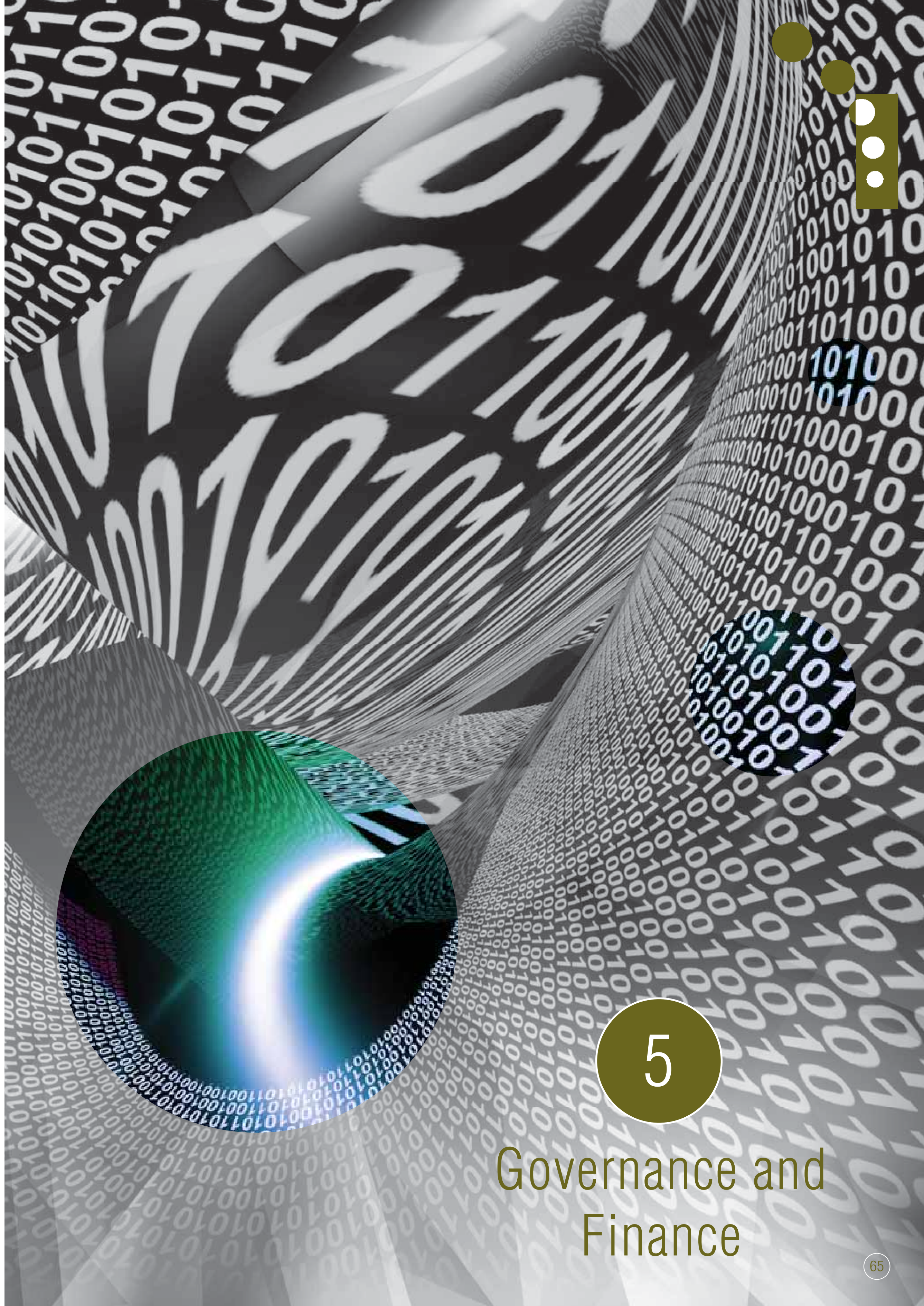


Table 7: Building tours and outreach activities

Group	Date
Group of 8 Communications Directors	10 July 2014
Tuckwell Scholarship candidates	11 July 2014
UNSW eResearch Coordination Group	18 July 2014
Undergraduate students from the ANU Fenner School of Environment & Society	12 August 2014
Public lecture on NCI and supercomputing at the National Science Week Science in ACTion day at ANU	16 August 2014
Delegates from Qatar University	26 August 2014
Building tours for the general public as part of ANU Open Day	30 August 2014
Department of Human Services Data Centre Facilities Management Team	5 September 2014
Australasian Research Management Society Conference	17 September 2014
NCRIS Showcase at Parliament House	30 September 2014
Lake Ginninderra Cub Scouts	15 October 2014
China Scholarship Council	27 October 2014
Council of Australian University Directors of IT delegates	26 November 2014
Yokohama National University	4 December 2014
Pakistani Vice-Chancellors and High Commissioner	10 December 2014
Year 12 students from around the country as part of the National Youth Science Forum	13 & 27 January 2015
ANU Astroinformatics Summer School	13 February 2015
General meeting of the National Science Week Committee	18 February 2015
Tokyo University masters students	26 February 2015
Geochronologists from GA	3 March 2015
Universities Australia Higher Education Conference	10 March 2015
Department of Communications	20 April 2015
Beijing Institute of Technology	21 April 2015
Girls in ICT Day	23 April 2015
ANU Computer Science undergraduates	18 May 2015
Victoria University of Wellington	22 May 2015
LANDSAT Conference	19 June 2015

Table 8: Conference presentations by NCI staff

Conference	Country	Date
Molecular Modeling	Australia	2 August 2014
Drishti Workshop	Australia	4-5 August 2014
American Chemical Society Annual Meeting	USA	10-14 August 2014
Tomography for Scientific Advancement	UK	1-3 September 2014
Drishti Workshop	UK	1-4 September 2014
Oil and Gas Industry Workshop	Australia	15-18 September 2014
Lustre Admin & Developers Conference	France	22-23 September 2014
HPC Advisory Council	Singapore	7 October 2014
OzEWEX Conference	Australia	29 October 2014
Supercomputing	USA	15-20 November 2014
Drishti Workshop	USA	22-24 November 2014
OzViz	Australia	8-9 December 2014
American Geophysical Union Annual Meeting	USA	15-19 December 2014
SGI Data Migration Facility User Group	Australia	18-19 February 2015
Science ICT Network Conference	Australia	26-27 February 2015
Asia Pacific Regional Internet Conference on Operational Technologies	Japan	24 February - 6 March 2015
NeCTAR Virtual Laboratories Workshop	Australia	3-7 March 2015
Oil and Gas Workshop	USA	7 March 2015
Universities Australia Higher Education	Australia	11-13 March 2015
Supercomputing Frontiers	Singapore	17-20 March 2015
Science Meets Parliament	Australia	24-25 March 2015
International Symposium on Environmental Software Systems	Australia	25 March 2015
Parallel Programming and Performance Optimisation Workshop	Australia	25 March, 25 May, 30 June 2015
CECAM Workshop : Charge Transfer Modelling in Chemistry	France	7-10 April 2015
European Geosciences Union Annual Meeting	Austria	12-17 April 2015
Higher Education Technology Agenda	Australia	11-13 May 2015
Model Evaluation Workshop	Australia	19 May 2015
Blue Planet Symposium	Australia	27-29 May 2015
International Workshop on Modelling the Ocean	Australia	5 June 2015
UK Meteorology Office Collaborators Workshop	UK	8-12 June 2015
ICQC Satellite Meeting: Novel Computational Methods	Japan	16-20 June 2015
National Environmental Science Programme Data Workshop	Australia	26 June 2015



5 Governance and Finance

Governance and Finance

The NCI Board

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

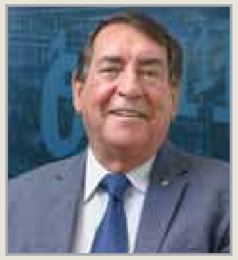
- An independent Chair appointed by the Board
- The Director, NCI
- One member appointed by each of the Major Collaborators (ANU, CSIRO, BoM and GA)
- Additional independent board members appointed for two-year terms by the NCI Board on the basis of their expertise

The Board is advised by:

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

Figure 12: Organisational structure

Board Members

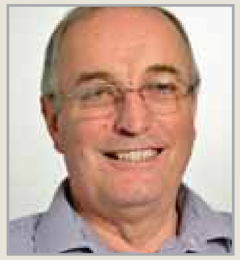


Emeritus Professor Mark Wainwright, AM
Chair

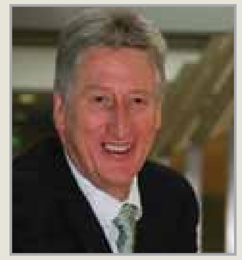
Professor Margaret Harding
Deputy Vice-Chancellor (Research), ANU

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

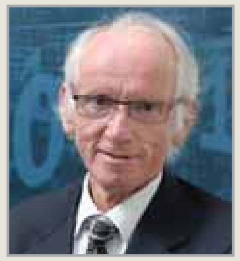
Professor Lindsay Botten
Director, NCI



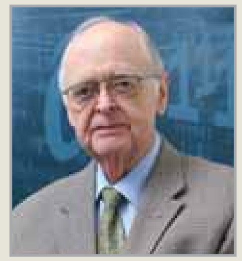
Dr David Williams
Executive Director National Facilities & Collections, CSIRO



Dr Chris Pigram
Chief Executive Officer, Geoscience Australia



Professor Robin Stanton
Independent Member,
Former Pro Vice-Chancellor (eStrategies), ANU



Dr Robert Frater
Independent Member
Vice-President Innovation, ResMed Ltd.

Dr Thomas Barlow
Independent Member
Research Strategist, University of Sydney

Financial report

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.

EXPENSES

NCI, as Australia's national, high-end 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 team of expert staff, high-performance computing infrastructure, and utilities and maintenance to operate this infrastructure. This is reflected in NCI's expenditure profile. Of note is the 'transfers to other' expenditure item; this reflects transfers to other areas of the University for capital works and other internal purchases funded under various contracted projects.

REVIEW/AUDIT

Each funding contract held by 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 the University'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.

Table 9: Financial report

STATEMENT OF INCOME AND EXPENDITURE

For the Period 01 July, 2014 to 30 June, 2015

For the NCI Collaboration and associated project accounts

	Current Period $
Balance as at 1 July 2014	**17,305,665**
Add	
NCI Collaboration Income	8,761,739
Other grant income	8,316,892
Investment Income	201,806
Total Income	**17,280,437**
Total Available Funds Before Expenditure	**34,586,102**
Less	
Salaries & Related Costs	6,287,212
Equipment - Capital	5,476,645
Equipment - Non-Capital	104,072
Utilities & Maintenance	3,461,526
Travel Field & Survey Expenses	402,817
Expendable Research Materials	244
Contributions	150,500
Consultancies	699,118
Consumables	641,852
Other Expenses	149,894
Transfers to other	1,546,064
Total Expenditure	**18,919,945**
Unspent Balance as at 30 June 2015	**15,666,157**

6 Appendix

Compute projects supported by NCI in 2014/15

Project Title	Lead CI, Institution	Total Allocation (kSU)
Properties and Stability of Nanoparticles for Advanced Applications	Amanda Barnard, CSIRO	37820
Seasonal Prediction Systems and Science	Guo Liu, Bureau of Meteorology	24500
BoM ESM research	Michael Naughton, Bureau of Meteorology	23450
The Dynamics of the Southern Ocean	Andrew Hogg, Australian National University	20300
ACCESS	Tony Hirst, CSIRO	20040
Simulation and Phylogenetics to decipher Rubisco structure, function and evolution	Jill Gready, Australian National University	18000
Quantum Modelling of Photo-Electrode Materials	Salvy Russo, Royal Melbourne Institute of Technology	11568
Computational Design of Complex Materials	Ming Liu, Swinburne University of Technology	10521
BLUElink3 Project	Gary Brassington, Bureau of Meteorology	10100
Simulation studies of biological and synthetic channels	Ben Corry, Australian National University	9800
Astrophysical Accretion Disks, Jets and Winds and Interactions with the Surrounding Medium	Geoffrey Bicknell, Australian National University	9364
3D magneto-hydrodynamical stellar modelling and 3D non-equilibrium radiative transfer	Martin Asplund, Australian National University	9000
Joint project on ACCESS-CM2 development	Daohua Bi, CSIRO	8200
Molecular Simulations of Ionic Liquids for Energy Storage Applications	Robert Rees, Royal Melbourne Institute of Technology	7980
Direct Numerical Simulations of Turbulent Combustion	Evatt Hawkes, University of NSW	6324
Electromagnetic Structure of Matter	Derek Leinweber, University of Adelaide	6320
Past, present and future climate variability and change in the Southern Hemisphere	Matthew England, University of NSW	5602
Regional-Scale Seasonal Prediction Over Eastern Australia and the Coral Sea	Anthony Rafter, CSIRO	5344
A Quantum-Chemical Approach to Understanding and Controlling Chemical Processes	Michelle Coote, Australian National University	5300
Mechanisms and attribution of past and future ocean circulation change	Andrew Hogg, Australian National University	5235
Strategic Radar Enhancement Project	Peter Steinle, Bureau of Meteorology	5051
From molecules to cells: Understanding the structural and dynamic properties of cellular components at an atomic level	Alan Mark, University of Queensland	4945
Modelling biophysical connectivity in Australia's territorial waters	Johnathan Kool, Geoscience Australia	4850
CO2 conversion in catalytic MOFs	Aaron Thornton, CSIRO	4299
Computational Earth Imaging	Malcolm Sambridge, Australian National University	4250
Bulk metallic glasses	Michael Ferry, University of NSW	4009

Project Title	Lead CI, Institution	Total Allocation (kSU)
Climate Change Science and Processes	Aurel Moise, Bureau of Meteorology	3900
Performance Enhancement in Access-to-Space Scramjets	Vincent Wheatley, University of Queensland	3853
Performance Enhancement in Access-to-Space Scramjets	Vincent Wheatley, University of Queensland	3853
Towards dynamic tectonic reconstructions	Dietmar Mueller, University of Sydney	3605
Action of Toxins from Venomous Animals on Biological Ion Channels Molecular Dynamics Studies	Shin-Ho Chung, Australian National University	3500
First-Principles Investigations of Processes and Properties in Catalysis, Coatings, and Devices	Catherine Stampfl, University of Sydney	3254
Water Information Services	Adam Smith, Bureau of Meteorology	3250
Atomistic Simulation for Geochemistry and Nanoscience	Julian Gale, Curtin University of Technology	3250
Downscaling future climate change from CMIP5 climate models with an eddy-resolving ocean model	Xuebin Zhang, CSIRO	3017
NCI-Fujitsu Collaboration ACCESS Model Optimisation Project	Mark Cheeseman, NCI	3010
Unified Model porting	Tim Pugh, Bureau of Meteorology	3000
Development and Application of Quantum Chemistry Methods for the prediction of physicochemical properties of ionic materials	Ekaterina Pas, Monash University	3000
High-resolution Downscaled Climate Runs	Jack Katzfey, CSIRO	2898
Geohazard Modelling for the Asia-Pacific Region	Phil Cummins, Geoscience Australia	2750
Computational Nanomaterials Science and Engineering	Sean Smith, University of Queensland	2729
Molecular simulation of carbon fibre composites	Tiffany Walsh, Deakin University	2630
Weather and Environmental Prediction Specialised Forecasting Systems	William Thurston, Bureau of Meteorology	2500
Understanding petrophysical and multiphase flow properties of rock through experiment, 3D imaging and modelling	Adrian Sheppard, Australian National University	2300
Development of volcanic risk models	Adele Bear-Crozier, Geoscience Australia	2257
Structural and Mechanistic Chemistry	Leo Radom, University of Sydney	2256
High-Order Methods for Transitional and Turbulent Flows	Hugh Blackburn, Monash University	2226
Terrestrial modelling within the Centre of Excellence regionalizing land surface processes	Claire Carouge, University of NSW	2150
From Plume Source to Hotspot	Rhodri Davies, Australian National University	2100
Simulation and Modelling of Particulate Systems	Aibing Yu, University of NSW	2057
Molecular Dynamics Simulations of Ion Channels and Transporters	Serdar Kuyucak, University of Sydney	2040
Jet-Driven Turbulence in Star Cluster Formation	Christoph Federrath, Australian National University	2010
Investigations of transitional and turbulent shear flows using direct numerical simulations and large eddy simulations	Julio Soria, Monash University	1974

Project Title	Lead CI, Institution	Total Allocation (kSU)
Direct and Large-Eddy Simulations of Turbulent Reacting Jets Under High Pressure Conditions	John Abraham, University of Adelaide	1930
Instabilities in the convecting mantle and lithosphere	Louis Moresi, University of Melbourne	1805
Atmospheric and oceanic processes and dynamics	Todd Lane, University of Melbourne	1745
The Interplay Between Galaxies and Intergalactic Gas At High Redshift	Edoardo Tescari, University of Melbourne	1700
A search for highly accelerated binary pulsars	Matthew Bailes, Swinburne University of Technology	1700
Geoscience Australia Landsat Data Processing	Wenjun Wu, Geoscience Australia	1700
The Last Minutes of Oxygen Shell Burning in Supernova Progenitors	Bernhard Mueller, Monash University	1697
New materials and fluids for catalysis, battery technologies and sensors	Debra Bernhardt, Griffith University	1584
Mix in high-acceleration implosions driven by multiple shocks	Ben Thornber, University of Sydney	1572
First-principles computational designs for advanced structural and functional materials	Zhe Liu, Monash University	1563
Development and Application of Quantum Monte Carlo methods	Manolo Per, Royal Melbourne Institute of Technology	1530
Development and application of bio/nano interfacial simulations	Tiffany Walsh, Deakin University	1519
Research, development and production computing	Benjamin Galton-Fenzi, University of Tasmania	1340
Computational Studies of the Mn/Ca Cluster in Photosystem II	Robert Stranger, Australian National University	1300
The role of convection in ocean circulation	Ross Griffiths, Australian National University	1300
Computer-Aided Materials Design for Clean Energy	Chenghua Sun, University of Queensland	1292
ACCESS preparation for IPCC AR5	Tony Hirst, CSIRO	1291
Geophysics	James Goodwin, Geoscience Australia	1260
Convective nuclear burning in 3D: Fixing the weak link in stellar models	Simon Campbell, Monash University	1254
Abrupt climate change events in the past, present and future	Katrin Meissner, University of NSW	1216
Regional Climate Modelling in South-east Australia	Jason Evans, University of NSW	1200
Investigating electronic properties of novel oxide materials for spintronic and energy applications	Sean Li, University of NSW	1195
High-magnetic-field liquid-metal flows for fusion power and big-data cooling solutions	Gregory Sheard, Monash University	1178
Advanced Modelling of Biological Fluid Flows	Kerry Hourigan, Monash University	1176
Computational Fluid Dynamics Studies of Bluff Body and Heat Transfer in a Buoyant Channel	Andrew Ooi, University of Melbourne	1050
SSimPL-ACS The Survey Simulation PipeLine: Alternative Cosmologies Study	Pascal Elahi, University of Sydney	1035

Project Title	Lead CI, Institution	Total Allocation (kSU)
Integration of conventional and digital core analysis	Christoph Arns, University of NSW	1020
Transition in Fluid Flows	Mark Thompson, Monash University	1012
Exploring structure-property correlations in advanced materials: Nexus between computational simulation and atomic resolution microscopy	Simon Ringer, University of Sydney	1006
Predicting and understanding Australia's regional rainfall distribution in a changing climate	Michael Reeder, Monash University	1003
Nanomaterials for Energy, Nanoelectronics and Environmental Applications: Contribution from Modelling towards Rational Design	Aijun Du, University of Queensland	1000
Theory and Simulation of Nanomorphology and the Environmental Stability of Nanostructures	Amanda Barnard, CSIRO	1000
Simulation of Enzyme Mechanisms, and Protein Dynamics, Structures and Properties	Jill Gready, Australian National University	1000
South Pacific High-resolution Climate Model Simulations	Kevin Walsh, University of Melbourne	1000
Animal toxins as novel analgesics and pesticides	Rong Chen, Australian National University	1000
Mechanisms of charge-membrane interactions and transport	Toby Allen, Royal Melbourne Institute of Technology	1000
Global scale decadal climate variability in a ACCESS hierarchy of climate models	Dietmar Dommenget, Monash University	995
Theoretical Investigation of novel materials for industrial and biomedical applications	Irene Yarovsky, Royal Melbourne Institute of Technology	987
Computer aided materials design for metal matrix composites reinforcements	Christoph Rohmann, University of Queensland	975
Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanoscale Materials	Nikhil Medhekar, Monash University	971
Bluelink developments	Peter Oke, CSIRO	971
Computational approaches to organic photonic and electronic materials: from strongly electronics to device engineering	Benjamin Powell, University of Queensland	957
Computational Mesoscale Physics, Probing Complex and Hierarchical Material Structure	Adrian Sheppard, Australian National University	950
Hi-res mapping of renewable energy from meteorological records for Australia	Jing Huang, CSIRO	942
Mitigation of Site Specific Errors from Geodetic Time Series	Michael Moore, Geoscience Australia	920
Modelling of the Plasma Production of Nanostructures	Anthony Murphy, CSIRO	911
Precipitation-groundwater interactions over eastern Australia climate change impacts at multiple scales	Jason Evans, University of NSW	910
Modelling and simulation of dynamic bushfire propagation	Jason Sharples, University of NSW	900
Advanced Processing of the GaLactic and Extragalactic All-sky MWA Survey	Randall Wayth, University of Melbourne	900
Towards efficient cosmological tests of modified gravity through numerical simulations	Jason Dossett, University of Queensland	898
Physics of the interactions between high-speed craft and their environment	Russell Boyce, University of Queensland	850

Project Title	Lead CI, Institution	Total Allocation (kSU)
Land Surface Science	Andy Pitman, University of NSW	846
The dynamics of protein-ligand interactions	David Chalmers, Monash University	835
Mechanisms and attribution of changes in Australian climate extremes	David Karoly, University of Melbourne	820
Modelling the formation of sedimentary basins and continental margins	Patrice Rey, University of Sydney	807
Prediction of the Properties of Materials and Nanomaterials	Salvy Russo, Royal Melbourne Institute of Technology	800
Theoretical modelling of protein-inhibitor interactions and chemical reactivity	Elizabeth Krenske, University of Queensland	785
Simulation of hypersonic flows in expansion tubes	David Gildfind, University of Queensland	780
Common envelope interaction and stellar outbursts in the era of time-domain Astrophysics	Orsola De Marco, Macquarie University	741
Turbulence and mixing in the Southern Ocean	Nathan Bindoff, University of Tasmania	725
Metal Nanoclusters as Catalysts for Photoreduction of CO2	Gregory Metha, University of Adelaide	709
Hydrodynamical explosion simulations and radiative transfer for thermonuclear and core-collapse supernovae	Ivo Seitenzahl, Australian National University	700
Modelling of the interaction between Antarctica and the Southern Ocean	Benjamin Galton-Fenzi, University of Tasmania	700
Computational Studies on Voltage-Gated Cationic Membrane Channels	Shin-Ho Chung, Australian National University	700
protein structure calculation using pseudocontact shifts	Thomas Huber, University of Queensland	700
Atomistic simulations of nanoscale liquid flow on solid surface	Luming Shen, University of Sydney	700
Numerical Simulations of Microcombustors	Ananthanarayanan Veeraragavan, University of Queensland	693
ACCSP Dynamical Ocean Downscaling of Climate Change Projections	Matthew Chamberlain, CSIRO	683
Low Reynolds Number Aerodynamics of Flapping Wings	John Young, ADFA	680
Genomic analysis	Gavin Huttley, Australian National University	676
Computational Investigation of Sodium Gated Ion Channels	Serdar Kuyucak, University of Sydney	665
Modelling of Chemical Systems Including Molecular Excited States, Photosynthesis, and Molecular Electronics Applications	Jeffrey Reimers, University of Sydney	659
Mimicking nature: computational design of better antioxidants	Amir Karton, University of Western Australia	650
Coral genomics, transcriptomics and epigenomics	Sylvain Foret, Australian National University	650
Radiative magneto-hyrdrodynamic modelling of interconnected solar interior and atmosphere	Sergiy Shelyag, Monash University	644
Role of subduction zone interface mechanical coupling on subduction dynamics and overriding plate deformation	Wouter Schellart, Monash University	635
Dynamical downscaling hydro-climatic simulations for water resources planning and management in a changing climate	Ashish Sharma, University of NSW	610

Project Title	Lead CI, Institution	Total Allocation (kSU)
Molecular Interactions	Meredith Jordan, University of Sydney	609
Peptronics: Understanding the Relationship between Structures and Properties	Jingxian Yu, University of Adelaide	609
Building a synthetic SAMI galaxy survey	Chris Power, University of Western Australia	600
UWA Modelling and simulating the evolution of spiral galaxies	Dan Taranu, State-based institutions	600
Molecular Simulations of Enzymatic Catalysis	Haibo Yu, University of Wollongong	600
Diagnosing Hydrogen Reionization with metal absorption line ratios	Luz Garcia, Swinburne University of Technology	600
Small Molecule Activation using Transition Metal Complexes	Robert Stranger, Australian National University	600
Large-eddy simulation of atmospheric turbulence	Todd Lane, University of Melbourne	600
Multi-scale modelling of soft condensed matter in functional materials and biology	David Huang, University of Adelaide	599
Impacts of future land-use changes and urbanisation on the local and regional climate of Sydney area	Daniel Argueso, University of NSW	591
Investigation of atypical bushfire spread driven by the interaction of wind, terrain and fire	Jason Sharples, University of NSW	560
Atom-photon interactions in biologically relevant media	Andrew Greentree, Royal Melbourne Institute of Technology	550
Exact Enumerations in Statistical Mechanics and Combinatorics	Iwan Jensen, University of Melbourne	550
Remotely sensed observations for Earth system modelling	Leon Majewski, Bureau of Meteorology	550
First-principles computation study of Zeolite for gas separation: novel molecular sieving mechanism and rational design	Paul Webley, University of Melbourne	550
Interfacial Barriers for the Transport of Nanoconfined Fluids	Suresh Bhatia, University of Queensland	529
Type I Supernovae Modelling Radiative Transfer for Thermonuclear and Core-collapse Explosions	Brian Schmidt, Australian National University	518
Modeling electrocatalytic energy conversion reactions on carbon based materials by DFT for optimal catalyst design	Yan Jiao, University of Adelaide	502
A numerical investigation of turbulent flow over surfaces with spatially varying roughness	Daniel Chung, University of Melbourne	500
Modelling the Australia-Antarctica divorce: quantifying controls on plate motions	Giampiero Iaffaldano, Australian National University	500
Large scale high accuracy computations for studies of Riemann's zeta function, as part of the 8th Hilbert problem	Gleb Beliakov, Deakin University	500
TraitCapture: An Open Source, High Throughput Phenomics pipeline	Justin Borevitz, Australian National University	500
Deciphering the genetic control of diseases	Peter Visscher, University of Queensland	500
Testing Gravity on Cosmic Scales with Weak Gravitational Lensing and Redshift Space Distortions	Shahab Joudaki, Swinburne University of Technology	500
Density Functional Theory Design of Carbon Based Materials for Energy Application	Ting Liao, University of Queensland	500
LES of high Reynolds number turbulent wall bounded flows	Jason Monty, University of Melbourne	484

Project Title	Lead CI, Institution	Total Allocation (kSU)
Developing computational methods to improve the accuracy of structural data obtained from DEER spectroscopy	Evelyne Deplazes, University of Queensland	483
Comparative analysis of gene and protein families in genomes from diverse environments	Mark Ragan, University of Queensland	479
eReefs EnKF Data Assimilation	Emlyn Jones, CSIRO	468
Multiscale modelling of Advanced Engineering Materials and Structures	Chunhui Yang, Deakin University	455
Investigating membrane protein dynamics, substrate recognition and transport	Megan O'Mara, Australian National University	450
Structural characterisation of malarial drug targets	Sheena McGowan, Monash University	448
Bioinformatics, molecular dynamic simulation of biofunctional proteins and mass spectrometric fragmentation mechanisms	John Bowie, University of Adelaide	438
What Regulates Star Formation?	James Wurster, Monash University	418
Chemistry at Semiconductor and Oxide Surfaces	Oliver Warschkow, University of Sydney	405
Free Energy Simulations of Ion Channels and Transporters	Serdar Kuyucak, University of Sydney	405
The spectral details of extragalactic point sources at low frequencies	Andre Rene Offringa, Australian National University	400
The effects of tropical convection on Australia's climate	Nidhi Nidhi, University of NSW	400
Moderate Resolution Imaging Spectroradiometer (MODIS) Thematic Products	Wenjun Wu, Geoscience Australia	380
Theoretical Quantum Chemistry including Quantum Refinement of DNA Structures and Development of new Computational Methods	Lars Goerigk, University of Melbourne	378
Nanoporous membranes for energy applications	Marlies Hankel, University of Queensland	369
First-principles calculations on heterostructures of two-dimensional materials for different applications	Zhimin Ao, University of Technology, Sydney	364
Understanding the Aegean-Anatolia Collisional System	Patrice Rey, University of Sydney	362
Atomic Collision Theory	Igor Bray, Curtin University of Technology	360
Marine Virtual Laboratory	Justin Freeman, Bureau of Meteorology	360
Design and development of new inexpensive materials for efficient hydrogen production and storage	Judy Hart, University of NSW	355
Assimilation of Trace Atmospheric Constituents for Climate	Peter Rayner, University of Melbourne	350
Oceanic Nepheloid Layers and Their Role in Coastal Oceanography	Xiao Hua Wang, ADFA	346
4-D Numerical Models of Plate Tectonics Subduction with an Upper Plate	Fabio Capitanio, Monash University	343
Bias removal in data assimilation systems for flood forecasting	Valentijn Pauwels, Monash University	340
Transients and Variables with the MWA	Martin Bell, University of Sydney	330
Influence of sea surface temperatures and orography on the development of East Coast Lows	Alejandro Di Luca, University of NSW	325
ARC Linkage Wind Generation Project: WRF Wind Climatology	Michael Hewson, University of Queensland	323

Project Title	Lead CI, Institution	Total Allocation (kSU)
Nanostructured optoelectronic devices	Chennupati Jagadish, Australian National University	320
Efficient chemical dynamics in gas phase, solid phase and heterogeneous systems	Terry Frankcombe, Australian National University	320
Novel Atomic Level Investigations of High Temperature Surface Thermodynamics of Molten Steel	Rita Khanna, University of NSW	319
Solar Rain	Alberto Troccoli, CSIRO	318
The dynamics of subtropical anticyclones and the connection to drought, heatwaves and bushfires in southern Australia	Michael Reeder, Monash University	315
The Mechanical Properties of Bio-Macromolecules	Ravi Jagadeeshan, Monash University	314
Harnessing the bioactivity of protein fragments and peptides	Marcela Bilek, University of Sydney	313
Allosteric Control of ATP Hydrolysis in the ABC Transporter Catalytic Cycle	Peter Jones, University of Technology, Sydney	310
Multi-dimensional radiative transfer simulations for Type Ib/c supernovae	Brian Schmidt, Australian National University	300
Coupled Chemistry Climate Modelling of Stratospheric Ozone Depletion and Recovery	David Karoly, University of Melbourne	300
Computation of X-Ray Diffraction Patterns for 3D Model Systems	Thomas Welberry, Australian National University	300
Paramagnetic spin states on diamond: in search of the source of surface noise	Jared Cole, Royal Melbourne Institute of Technology	298
Understanding the Origins of Enhanced Photocatalytic Activity in doped TiO2 Nanostructures Using Density Functional Theory	Dorian Hanaor, University of Sydney	292
A robust, high-throughput system for identifying genetic variation from very large genome sequence datasets	Matthew Field, Australian National University	290
Modelling of high-temperature receivers for concentrating solar thermal energy systems	Graham Hughes, Australian National University	275
Severe Wind and Coastal Inundation Modelling	Craig Arthur, Geoscience Australia	270
Tracking mantle slab dewatering using ASPECT	Craig O'Neill, Macquarie University	255
Investigation of High Entropy Alloys for use in advanced nuclear applications	Daniel King, University of Technology, Sydney	255
Will East coast lows change in frequency or intensity in the future?	Jason Evans, University of NSW	251
Quantum Chemical Modelling of Nanoscale Chemical Processes	Alister Page, University of Newcastle	250
Modelling supernova explosions: Multidimensional simulations for Type Ia explosions	Brian Schmidt, Australian National University	250
Quantitative Goldbach Conjecture	David Harvey, University of NSW	250
Turbulence: Numerical modelling and application to aquatic ecosystem functions	Ivan Marusic, University of Melbourne	250
Modelling Nanoscale Materials for Sensing and Device Applications	Michelle Spencer, Royal Melbourne Institute of Technology	250
Computational investigation of new selective transport materials	Maria Forsyth, Deakin University	243
Disc Brake Squeal	Joseph Lai, ADFA	241

Project Title	Lead CI, Institution	Total Allocation (kSU)
Improving cosmic expansion and neutrino mass measurements with new simulations	Christopher Blake, Swinburne University of Technology	240
Swinburne Testing the cosmological model at low redshift: Mock catalogues for the 6dF and Taipan surveys	Christopher Blake, Swinburne University of Technology	240
Atomic scale modelling of reaction between complex carbon-bearing materials and metallic phase towards a novel approach for recycling waste polymers for sustainable environment	Narjes Gorjizadeh, University of NSW	240
Computational Bio-inorganic and Supramolecular Chemistry	Ian Dance, University of NSW	233
Shear induced platelet aggregation characterising shear forces in in-vitro geometries	Kris Ryan, Monash University	228
Designing Better Catalysts	Brian Yates, University of Tasmania	225
Functionalized graphene for next generation nanoelectronics	Jiri Cervenka, University of Melbourne	225
Developing a materials understanding of the silicide accident tolerant fuels: an atomic scale study	Simon Middleburgh, Australian Nuclear Science and Technology Organisation	225
Gravitational Lensing in Coupled Dark Matter: Dark Energy Cosmologies	Hareth Mahdi, University of Sydney	224
Using numerical simulations to enhance cosmological tests of f(R) gravity	David Parkinson, University of Queensland	221
Numerical Study of Tropical Cyclone Formation, Structure, Landfall Processes and Climate Variability associated with Land-surface Changes	Kei-Wai Kevin Cheung, Macquarie University	220
Magnetotelluric and Electrical data inversion	Jingming Duan, Geoscience Australia	210
DFT and TD-DFT Studies of Organometallic and Metal Cluster Systems	Robert Stranger, Australian National University	210
Simulations of wintertime storms across Southeast Australia, Tasmania and the Southern Ocean	Steven Siems, Monash University	208
Purging and destratifying of thermal and saline pools in Australia's inland rivers	Nicholas Williamson, University of Sydney	206
Interactions and self-assembly of colloidal nanorods: Establishing design rules for creating new nano-structured materials	Asaph Widmer-Cooper, University of Sydney	203
A combined experimental and computational approach to understanding and developing solid-state ionic conductors	Chris Ling, University of Sydney	203
Dynamics of DNA Clamps and Clamp Loaders	Aaron Oakley, University of Wollongong	200
ANU Mathematical Sciences Institute	Andrew Chew, Australian National University	200
Novel methods for phylogenetic inference using genome-scale data	Jason Bragg, Australian National University	200
Geodetric research to measure surface deformation of the Australian continent	Matthew Garthwaite, Geoscience Australia	200
Simulation of expected sky signal for the BigHorns project	Marcin Sokolowski, University of Western Australia	194
Fundamental Understanding of the Role of Singlet Molecular Oxygen in Spontaneous fires	Mohammednoor Altarawneh, University of Newcastle	185
Analysis of complex genomes	David Edwards, University of Queensland	184

Project Title	Lead CI, Institution	Total Allocation (kSU)
Multiscale mechanics of metal/semi-conductor/bulk metallic glass (BMG) systems, mixed lubrication and graphene-polymer composites	LiangChi Zhang, University of NSW	181
Vibrational Frequency changes in carboxylate ligands coordinated to manganese as a function of the metal oxidation state	Elmars Krausz, Australian National University	180
Locating defects in doped semiconductor lattices	Scott Medling, Australian National University	175
Computer Simulation of Glassy Materials out of Equilibrium	Stephen Williams, Australian National University	175
Understanding patterns of evolutionary and ecological diversification	Marcel Cardillo, Australian National University	170
Theoretical understanding and computational design of perovskite solar cells	Yun Wang, Griffith University	170
Theory of multiple atomic ionization	Anatoli Kheifets, Australian National University	165
The Anatomy of Social Media Popularity	Lexing Xie, Australian National University	165
Impacts of environmental change on coastal ecosystem health: application of the eReefs coupled hydrodynamic-biogeochemical model	Katherine O'Brien, University of Queensland	162
Searching for highly conductive molecules for future molecular circuits and sensors	Xiaolin Wang, University of Wollongong	161
The evolution and stability of vortex rings and synthetic jets moving parallel to a flat plate	Kris Ryan, Monash University	161
Numerical investigation of the impact of low-level jets on fire behaviour	Colin Simpson, ADFA	160
Design, analysis and application of Monte Carlo methods in statistical mechanics	Timothy Garoni, Monash University	158
Mesoscale modelling of urban landscapes for assessing heat adaptation and mitigation strategies with climate change	Ailie Gallant, Monash University	157
Biology needs rheology	Prabhakar Ranganathan, Monash University	155
Numerical modelling of MHD effects and sunspot interior structure and dynamics	Paul Cally, Monash University	152
Fluid-thermal-structural interactions for high-speed flight and propulsion	Andrew Neely, ADFA	150
Theoretical study of 2D and 3D topological materials	Anh Pham, University of NSW	150
Reconstructing the Antarctic Ice Sheet through high resolution numerical modelling	Matthew King, University of Tasmania	150
Molecular Dynamics Investigation of Epitopes and Biosurfactant Structural Stability	Natalie Connors, University of Queensland	150
Analysis and interpretation of mass redistribution on Earth derived from space gravity observations	Paul Tregoning, Australian National University	150
DFT and Ab Initio Studies of Inorganic and Organometallic Complexes and Drug DNA complexes	Graham Ball, University of NSW	146
Assessing geothermal energy potential for the Australian Continent	David Lescinsky, Geoscience Australia	145
How does insulin work?	Naomi Haworth, Australian National University	145

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Small molecules for organic photovoltaics and light emitting diodes	Ante Bilic, Curtin University of Technology	142
eReefs Marine Modelling GBR1	Mark Baird, CSIRO	138
Structural and functional simulations of protein drug targets	William Church, University of Sydney	136
Particle-based simulations of fluctuating hydrodynamics for fluid-structure interactions at micro/nano scales	Sergio De Luca, University of NSW	131
Separation of ions and small molecules using Molecular Dynamics simulations	Stefano Bernardi, University of Queensland	130
Modelling surface electrochemistry-transport coupling in AlGaN/GaN-based sensors	Dino Spagnoli, University of Western Australia	125
Mechanism of ferromagnetism and spin manipulation in oxide diluted magnetic semiconductors	Jiabao Yi, University of NSW	125
Analysis and interpretation of space gravity observations	Paul Tregoning, Australian National University	125
(East) Antarctic sea-ice kinematics derived from high-resolution satellite imagery	Petra Heil, University of Tasmania	125
Liquidity Traps and Forward Guidance Monetary Policies: a new computational dynamic game perspective	Timothy Kam, Australian National University	123
Molecular and Dissipative Particle Dynamics Simulations of Polymeric Systems	Ahmad Jabbarzadeh, University of Sydney	121
Extended Hydrological Prediction modelling	David Kent, Bureau of Meteorology	120
Catalysts for Clean Energy from experimental data to reaction mechanisms	Rosalie Hocking, James Cook University	120
Hybrid 2D Materials	Mike Ford, University of Technology, Sydney	118
Australian Water Resource Assessments Calibration Test	Dave Penton, CSIRO	118
Modelling of multi-layered and adaptive structural systems	Gianluca Ranzi, University of Sydney	117
Mesoscale Modelling of Rainfall for Sea	Marie Ekstrom, CSIRO	111
Non-equilibrium plasma conversion of toxic halogenated compounds and waste halogenated refrigerants to value added polymers	Eric Kennedy, University of Newcastle	110
Catalytic Reactions on Metal-oxide and Metal-chloride Surfaces, and Hybrid Molecular Electronics on Semiconductor Surfaces	Marian Radny, University of Newcastle	106
Electronic structure of boron nitride and other novel coating systems	Dougal McCulloch, Royal Melbourne Institute of Technology	105
Catalytic Reactions in the Gas Phase and on Metal-oxide and Metal-chloride Surfaces	Juita Juita, University of Newcastle	102
Resistive Random Access Memory	Robert Elliman, Australian National University	101
Direct simulation of transition for natural convection flow in inclined differentially heated cavities	Steven Armfield, University of Sydney	101
Quantum Simulator	Willy Susilo, University of Wollongong	101
Large scale online learning with a mixed regularization model	Alistair Rendell Account, Australian National University	100
Realistic Modelling of the Effects of Solvent and Additives on Crystallisation	Andrew Rohl, Curtin University of Technology	100

Project Title	Lead CI, Institution	Total Allocation (kSU)
Large scale high accuracy computations for studies of Riemann's zeta function	Gleb Beliakov, Deakin University	100
Atomistic investigation of high temperature polymer chemistry for novel recycling solutions and sustainable environment	Mohammad Al Assadi, University of NSW	100
Computer Aided Design of Ebola Vaccines and Therapeutics	Nikolai Petrovsky, Flinders University	100
Investigation of structural transitions in the insulin receptor	Tristan Croll, Queensland University of Technology	100
Whole genome analysis of Eucalyptus: Australia's foundation tree	William Foley, Australian National University	95
Scale Resolving Turbulence Simulations of Multi-layer Orthogonal-offset Plate Arrays	Zbigniew Stachurski, Australian National University	95
Modelling Dehydroxylation of Clay Structures for CO2 carbonation applications	Alejandro Montoya, University of Sydney	93
SRTM DEM processing	Nerida Wilson, Geoscience Australia	93
The evolution of the mitochondrial genome	Madeleine Beekman, University of Sydney	92
Flow and Heat Transfer Behavior in Fluid Bed Reactors	Zongyan Zhou, University of NSW	92
Brain structure, cognition, and ageing a magnetic resonance imaging investigation	Nicolas Cherbuin, Australian National University	90
Piezoelectric bone remodeling analysis by finite element method	Qing-Hua Qin, Australian National University	90
Diamond-based quantum devices	Snjezana Tomljenovic-Hanic, University of Melbourne	88
National Remote Sensing Processing Facility	Edward King, CSIRO	85
Australian Solar Energy Forecasting System	Merlinde Kay, University of NSW	84
An investigation on the interaction of heavy metal ions (As and Hg) with Surface Enhanced Raman Spectroscopy materials	Suresh Bhargava, Royal Melbourne Institute of Technology	84
Conformational regulation of enzyme function	Ashley Buckle, Monash University	83
Design using genetic algorithms	Mark Hoffman, University of NSW	83
EODS Web Services Delivery	Aaron Sedgmen, Geoscience Australia	80
Primary production in space and time	Bradley Evans, Macquarie University	80
Multiphase fluid flow and heat transport modelling with Tough2-MP	David Lescinsky, Geoscience Australia	80
Production of Linear Alpha Olefins Mechanistic and Applied Investigations	David McGuinness, University of Tasmania	80
Quantum Chemical Molecular Properties	David Wilson, La Trobe	80
Computational investigation of oxygen activation in metalloenzymes	Gemma Christian, Avondale College	80
Supercritical CO2 Turbomachinery	Ingo Jahn, University of Queensland	80
Future Air Quality Projection	Martin Cope, CSIRO	80
Computational Quantum Chemical Studies of Stereoselectivity of Organic Reactions	Michael Paddon-Row, University of NSW	80

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Computational Electronic Structure of Animal Pigment Molecules of Strategic National Importance	Seth Olsen, University of Queensland	79
Molecular Dynamics Study of Gas Storage and Transport in Coals	Junfang Zhang, CSIRO	76
Urban areas in regional and meso-scale models the role of urban parameterizations, climate change and adaptation/mitigations strategies	Jason Beringer, Monash University	75
Computer simulations of biomolecular systems	Haibo Yu, University of Wollongong	73
A powerful mixed effect model approach for novel genetic discoveries using joint analysis of multiple complex traits	Riyan Cheng, Australian National University	70
Computational Quantum Chemistry	Alan Chaffee, Monash University	70
Nanoscale materials and Nanoscale Interactions: From Catalysts through to Hydrophobic Soils	David Henry, Murdoch University	70
Climate Change Impact on Southeast Queensland Water Supply	Wenju Cai, CSIRO	69
Application of quantum electronic-structure methods to protein crystallography and photosynthetic function	Jeffrey Reimers, University of Sydney	68
Understanding the deep driving forces of Earth's large-scale topography through time	Nicolas Flament, University of Sydney	67
Solid Oxide Fuel Cells	Eric Kennedy, University of Newcastle	65
Development and application of new quantum chemistry algorithms	Peter Gill, Australian National University	65
Electrochemical Conversion of CO2 and N2	Luis Miguel Azofra, Monash University	63
Machine Learning for Computer Vision	Stephen Gould, Australian National University	63
First-Principles Modeling of Functional Titanium Dioxides and Hybrid Metalorganic Perovskites	Varghese Swamy, Monash University	62
Optimization and structural analysis for additive manufacturing and maintenance	Wenyi Yan, Monash University	61
SkyMapper and the Southern Sky Survey	Brian Schmidt, Australian National University	60
Deformation and failure of constrained fragmented structures	Elena Pasternak, University of Western Australia	60
Epeirogeny and basin dynamics of Australia	Karol Czarnota, Geoscience Australia	60
Landsat Dynamic Land Cover	Leo Lymburner, Geoscience Australia	60
Performance Analysis and Optimization of Large-scale Scientific Simulations	Peter COMP3320, Australian National University	60
A Computational Study of Dual Orbital Interactions in Radical Cyclization and Addition Reactions	Uta Wille, University of Melbourne	60
Theoretical Study of Perovskite Solar Cells	Yecheng Zhou, University of Melbourne	60
Modulating the function and structures of bio-macromolecules by small molecules	Johannes Zuegg, Australian National University	60
Information flow in Vicsek Models	Terry Bossomaier, Charles Sturt University	59
Learning from big data with generative and discriminative strategies	Geoffrey Webb, Monash University	56

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CFDMECH	Tracie Barber, University of NSW	55
Dark Matter Discovery	Balazs Csaba, Monash University	52
Comparative genomics pap056	Alexie Papanicolaou, CSIRO	51
HPC for fluid dynamics and molecular dynamics	Weimin Gao, Deakin University	51
The heavy element composition of post-AGB stars and planetary nebulae	Amanda Karakas, Australian National University	50
BEC manipulation through pulse sequences and quantum feedback control	Joe Hope, Australian National University	50
Improving capacity and stability of hydrogen storage materials	Judy Hart, University of NSW	50
Multiscale mechanics of metal/semi-conductor/bulk metallic glass (BMG) systems, mixed lubrication and graphene-polymer composite	LiangChi Zhang, University of NSW	50
Electron beam induced etching and deposition	Mike Ford, University of Technology, Sydney	50
Testing the drivers of Southern Annular Mode changes over the last millennium	Nerilie Abram, Australian National University	50
Atomistic Modelling of Carbon Nanostructures	Nigel Marks, Curtin University of Technology	50
Scintillation and the structure of turbulent gas in the Milky Way	Paul Hancock, University of Sydney	50
Structure-function analysis of PfL-M17 for the discovery of anti-malarial drugs/ MD Analysis of DNA Repair Enzyme MutS	Peter Jones, University of Technology, Sydney	50
Self-assembly of Polyphiles via Espresso Simulations	Stephen Hyde, Australian National University	50
Understanding the drivers of Australian climate variability and change	Steven Phipps, University of NSW	50
DFT study of Diamond/AlN heterojunctions for UV emitting devices	Francois Ladouceur, University of NSW	50
Molecular Potential Energy Surfaces by Interpolation	Michael Collins, Australian National University	48
Theoretical calculations on reactive molecules, intermediates and prebiotic chemistry pathways	Curt Wentrup, University of Queensland	47
Accurate activation energies for aqueous CO2/amine reactions	Jim Smitham, CSIRO	47
Multiscale Simulations of Polymeric Systems	Ahmad Jabbarzadeh, University of Sydney	46
Simulation of Nanoparticle Films Self-Assembly for Breath Analysis and Non-Invasive Medical Diagnosis	Antonio Tricoli, Australian National University	45
Investigation of nanoporous materials for carbon dioxide capture and catalysis	Brad Wells, CSIRO	45
Modelling the interactions and influences of organic compounds in zinc-bromine redox flow battery systems	Tony Vassallo, University of Sydney	44
Nonlinear Dynamics of Ocean Currents	Andrew Kiss, ADFA	43
Insulin-IR complex	Anastasios Papaioannou, University of Sydney	43
Fluid-structure Interactions and Complex Flows in Biological and Biomedical Systems	Fangbao Tian, University of NSW	41

Project Title	Lead CI, Institution	Total Allocation (kSU)
Numerical study of transport, separation, and chemical reaction of particles in multiphase flow systems	Shibo Kuang, University of NSW	41
Studying the Dynamics of Multiple Planetary Systems	Robert Wittenmyer, University of NSW	41
The catalytic oxidation of ammonia	Alejandro Montoya, University of Sydney	40
Computational approaches to sustainable chemistry Towards the prediction of electrochemistry and reaction kinetics in ionic media	Douglas MacFarlane, Monash University	40
Active Control of Light in Photonic Nanostructures	Andrey Sukhorukov, Australian National University	40
Extremal graph theory	Brendan McKay, Australian National University	40
Mechanisms for hydrogenation and dehydrogenation of complex aluminium hydrides and borohydrides	Debra Bernhardt, Griffith University	40
Massively Parallel Computing for Coupled Fluid Flow Dynamics using LBM	Huilin Xing, University of Queensland	40
Measuring the laws of Nature across the Universe	John Webb, University of NSW	40
Lyman Alpha and stellar emission from high redshift galaxies	Luke Barnes, University of Sydney	40
EQRM	Mark Leonard, Geoscience Australia	40
Computational Applications in Equilibrium and Instabilities of Advanced Plasma Confinement Geometries	Matthew Hole, Australian National University	40
Potential Field Modelling in Spherical Coordinates	Ross Brodie, Geoscience Australia	40
Tackling the unconventional resources challenge with multiphysics simulations	Thomas Poulet, CSIRO	40
Large-scale Holistic Scene Understanding in Video	Xuming He, Other Australian Research Institute	40
Inversion AEM data	Alan Ley, CSIRO	37
Electronic Structure of High Oxidation State Complexes	Mark Riley, University of Queensland	32
Space weather modelling	Michael Terkildsen, Bureau of Meteorology	31
The structure of the MACPF/CDC giant pores	Michelle Dunstone, Monash University	31
A project on voxelwise, heritability and genome-wide association study (vGWAS) of human brain structure and function	Wei Wen, University of NSW	31
Computational Studies for Intelligent Organic Reaction Design	Christopher Thompson, Monash University	30
Catalysis and Organometallic Chemistry	Allan Canty, University of Tasmania	30
Microscopic and Macroscopic Studies for Nuclear Reactions	Cedric Simenel, Australian National University	30
Subtle quantum mechanical forces of ions in solution	Drew Parsons, Australian National University	30
Nanophotonic devices based on semiconductor and plasmonic materials	Kenneth Crozier, University of Melbourne	30
Computational Investigation of the Chemistry of Reactive Intermediates	Stephen Blanksby, University of Wollongong	30
Simulation of Photonic Nanostructures	DukYong Choi, Australian National University	30

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Optimization of plasmonic nanoantennas and metamaterials	Matthew Arnold, University of Technology, Sydney	28
Electronic Structure of Organic/Inorganic Dyes for Photovoltaic Applications	Gregory Wilson, CSIRO	26
High resolution studies of cosmogenic beryllium isotopes (10Be and 7Be) in Law Dome ice cores, Antarctica	Greg Doherty, Australian Nuclear Science and Technology Organisation	25
Least cost energy pathways for the Australian Grid	Roger Dargaville, University of Melbourne	25
Efficient Algorithms for Finding Influential Communities in Large-Scale Networks	Weifa Liang, Australian National University	25
Integration of wave-ice interactions into the CICE/ACCESS model	Luke Bennetts, University of Adelaide	24
Materials Design for Self-toughening Bulk Metallic Glasses	Chunguang Tang, University of Sydney	24
The Structural Behaviour of Hollow Fabricated Columns with High Strength Steel Tubes and Double Skin Concrete-Filled Columns with Corrugated Steel Skins	Amin Heidarpour, Monash University	23
Quantum Turbulence	Tapio Simula, Monash University	22
Nanostructures for Advanced Photovoltaic Applications	Ross McPhedran, University of Sydney	22
Nacre inspired structures based on ceramic/polymer composites	Andrey Molotnikov, Monash University	21
Transportation Modelling and Automation Group	Hussein Abbass, ADFA	21
Kinematic study of Galactic bulge planetary nebulae	Quentin Parker, Macquarie University	21
Molecular dynamics simulation of polymers	Saeed Masoumi, University of NSW	21
Developing an Australian Landsat-MODIS Blending Infrastructure	Tim McVicar, CSIRO	21
Evolution, Selection and Estimation of Polygenic Epistatic Networks in Quantitative Traits	Cedric Gondro, University of New England	20
Investigating the structures and energetics of molecular ions	Evan Bieske, University of Melbourne	20
DFT studies of structure-function relationships in materials containing hydrogen	Evan Gray, Griffith University	20
Automatic Corpus Callosum Shape Analysis for Brain MRI images	Girija Chetty, University of Canberra	20
Effect of Na and K on solar cell absorber materials Cu(In1-x,Gax)Se2: A first-principles study	Gujie Qian, University of South Australia	20
Data mining and geostatistical modelling for geoscience applications	John Wilford, Geoscience Australia	20
Modelling of micro-flows in micro-devices	Jong-Leng Liow, ADFA	20
An investigation of ageing brain structure in health and disease	Nicolas Cherbuin, Australian National University	20
Spherical geometry in chemistry and physics	Pierre Loos, Australian National University	20
Quantum Chemical Modelling of Biomolecular Systems	Thilagam Lohe, University of South Australia	20
Regional Data Assimilation	Chaojiao Sun, CSIRO	18
ACCSP and PACCSP	Michael Grose, University of Tasmania	18

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Finite-element and discrete study of pipe belt conveyors	Qijun Zheng, Monash University	18
From Saturn's hexagon to Earth's polar vortex elucidating shear-layer instability in rotating flows	Tony Vo, Monash University	18
Water property rights in regulated rivers	Rupert Grafton, Australian National University	17
The use of state-of-the-art 3-D chemical transport modelling to unravel the effects of atmospheric chemistry on climate	Nicholas Jones, University of Wollongong	16
Earth Observation and Informatics	Robert Woodcock, CSIRO	16
General Share for User Code Development and Testing	Robert Bell, CSIRO	16
New Generation High Strength Insulating Vacuum Glazing	Marcela Bilek, University of Sydney	15
On the Performance of Integrated Hydrologic Models for Simulating Land Surface Fluxes Under Scenarios of Climate and Land Cover Change	Hoori Ajami, University of NSW	15
The next generation of environmental model-data assimilation and forecasting systems	Albert Van Dijk, Australian National University	15
Finite Element Modelling of Engineering Systems	Shankar Kalyanasundaram, Australian National University	15
WRF simulations of Tropical Cyclones	Thomas Loridan, Macquarie University	15
Spectroscopy of gas-phase ions	Stephen Blanksby, University of Wollongong	15
Nanoplasmonic Solar Cells	Kylie Catchpole, Australian National University	14
Advanced Applications of Optimal Tax Theory to Tax Design	Patricia Apps, University of Sydney	14
ESG CMIP5 data processing pipeline	Tim Erwin, CSIRO	13
Modelling Porous Breakwaters using SPH method	Alireza Valizadeh, Monash University	12
The transcriptome of the Eastern mosquitofish, Gambusia holbrooki	Bob Wong, Monash University	12
Plasmonic based components for Nanotechnology	Malin Premaratne, Monash University	12
Data Cube Rangelands and Crop Mapping Applications	Matt Paget, CSIRO	12
Small molecules for OLEDS (organic light emitting diodes)	Melissa Skidmore, CSIRO	12
4D Numerical Models of Lithospheric and Mantle Interaction	Rebecca Farrington, Monash University	12
CFD Study of Wind Engineering Effects of Parabolic Trough Solar Collectors	Abbas El-zein, University of Sydney	11
Climate Adaptation Strategies for Rural Livelihoods in Nusa Tenggara Barat Province, Indonesia	Dewi Kirono, CSIRO	11
Multiscale Simulation of Unsaturated Soil Response to Impact Loading	Luming Shen, University of Sydney	11
Bayesian risk forecasting with flexible volatility models	Richard Gerlach, University of Sydney	11
A novel, weight saving alternative for aircraft flaps and slats utilizing no moving components	Sammy Diasinos, Macquarie University	11
Multiscale simulation of particle flows	Haiping Zhu, University of Western Sydney	10
Computer Simulation of Nanofluidic Systems	Billy Todd, Swinburne University of Technology	10

Project Title	Lead CI, Institution	Total Allocation (kSU)
Catalytic Reactions in the Gas Phase and on Metal-oxide and Metal-chloride Surfaces	Bogdan Dlugogorski, Murdoch University	10
eMast Model-Data Assimilation	Damian Barrett, CSIRO	10
Applications of Electronic Structure Computations to the Solution of Molecular-Scale Problems	Damian Moran, Macquarie University	10
Bioinformatic analysis of agriculturally important plants, pathogen and pests	James Hane, Curtin University of Technology	10
Structure of the nucleosome remodeling and deacetylase complex	Joel Mackay, University of Sydney	10
Interaction of wood extractives with model surfaces	Karen Stack, University of Tasmania	10
Investigation of High Entropy Alloys for advanced nuclear applications	Michael Cortie, University of Technology, Sydney	10
Monitoring Landscape Scale Vegetation State and Trend from Landsat and ALOS archives	Peter Scarth, University of Queensland	10
Quantifying the Role of Aerosols in Australian Rainfall Trends and Rainfall Variability	Robert Bell, CSIRO	10
A Flood Mapping Framework for the ACT	Rudy VanDrie, Australian National University	10
X10 programming language: High performance runtime and scientific applications	Steve Blackburn, Australian National University	10
Investigating Carbon Cycling in the Australian and Southern Ocean Region	Tilo Ziehn, CSIRO	10
Optimising the Damage Resistance of Advanced Composite Aerostructures Subjected to Impact Loading	Wenyi Yan, Monash University	10
Integration Site Analysis	Shoba Ranganathan, Macquarie University	10
Defects in Germanium and Silicon	Heiko Timmers, ADFA	8
Development of earthquake fragility model using OpenSees	Hyeuk Ryu, Geoscience Australia	8
The Australian Continental Carbon Budget	Vanessa Haverd, CSIRO	8
The role of mantle convection for present day lithosphere dynamics	Sascha Brune, University of Sydney	8
Quantum Lattice Models in Condensed Matter and Particle Physics	Chris Hamer, University of NSW	7
Computational design of dehalogenase enzymes	Tom Peat, CSIRO	7
Modeling of sea level change and variability in the Pacific	Xuebin Zhang, CSIRO	7
An Experimentally-Validated Thermo-Hydro-Mechanical Theory for Geosynthetic Composite Lining Systems under Low Pressure and High Temperature	Abbas El-zein, University of Sydney	6
X-Ray Bursts	Alexander Heger, Monash University	6
Investigation of the electronic structure of highly correlated electronic systems especially of novel multiferroics by density functional methods	Annemieke Mulders, ADFA	6
Simulation of Underground Coal Mines and Mineral Grinding	Chandana Jayasundara, CSIRO	6
Static and dynamic analysis of Z-machine reinforced non-pneumatic tires with high energy efficiency	Ehsan Bafekrpour, Monash University	6
Development of Antioxidant Agents from Natural Products	Joachim Mai, Intersect	6

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Machine Learning and Natural Language Understanding	Mark Johnson, Macquarie University	6
Reconstruction and modelling of cell-material interactions based on high resolution electron imaging	Jing Fou, Monash University	6
Computational modeling of allosteric binding sites in nicotinic acetylcholine receptors	Thomas Balle, University of Sydney	6
The Evolution of stripe rust virulence	Benjamin Schwessinger, Australian National University	5
What makes states good war fighters? Evidence from two centuries of military engagements	Charles Miller, Australian National University	5
Natural Resource Information	Chris Inskeep, Geoscience Australia	5
Bluelink III	Graham Symonds, CSIRO	5
Interrogation of novel Metal-boron bonding situations through computational chemistry	Manab Sharma, Australian National University	5
Decadal Changes in Southern Ocean Ventilation	Mark Holzer, University of NSW	5
Syntax-aware Language Modelling	Matthew Honnibal, Macquarie University	5
Monash Partner Share Management Project	Paul Bonnington, Monash University	5
The AUStralian community ocean model ReAnalysis project (AURA)	Terry OKane, CSIRO	5
Spectral Wind-Wave Development	Russel Morison, University of NSW	4
From molecules to minerals: Network-free stochastic kinetic modelling of iron oxide formation in aquatic environments	Andrew Rose, Southern Cross University	4
Large geospatial national wide data processing with HPC	Chen Hoofa, CSIRO	4
Simulation of Wind and Solar Energy Sources	Christopher Russell, CSIRO	4
Modelling oxidative degradation of natural products	Dave Winkler, CSIRO	4
ICTIS science support project	Duncan Gray, Geoscience Australia	4
WIRADA 2.2 Gridded Foundation Data Sets	Edward King, CSIRO	4
Remote Sensing of Inland Water Quality	Erin Hestir, CSIRO	4
Improving hydrological processes in CABLE land surface scheme	Francis Chiew, CSIRO	4
Modelling sea level extremes in response to global warming	Frank Colberg, University of Tasmania	4
Constructing a Coupled Economic-Climate System Model	Ian Harman, CSIRO	4
Climate projections and SST drivers	Ian Watterson, CSIRO	4
Dynamical Subgrid-scale Parameterisations for Atmospheric and Oceanic Models	Jorgen Frederiksen, CSIRO	4
TAPPAS - HYSPLIT Integration	Kerryne Graham, CSIRO	4
Computational study of 3D breaking deep water, shallow water and shoaling water waves	Michael Banner, University of NSW	4
Numerical simulation of multi-material flows	Petar Liovic, CSIRO	4
Statistical Image Processing of Remotely Sensed Data	Peter Caccetta, CSIRO	4

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CSIRO Mk3.6 GCM output for IPCC	Robert Bell, CSIRO	4
Lattice Models of Condensed Matter and Lattice Gauge Theory	Robert Bursill, University of NSW	4
ASTER satellite imagery	Robert Woodcock, CSIRO	4
A high-resolution 60-year wave hindcast dataset for southeastern Australia	Ronald Cox, University of NSW	4
Parallel Implementation of Shallow Water Bathymetry Retrieval from Earth Observation Imagery	Stephen Sagar, Australian National University	4
Climate and Weather Science Laboratory	Tim Pugh, Bureau of Meteorology	4
Assembly of next-generation sequencing data for microbial metagenomes	Torsten Thomas, University of NSW	4
Tests of Unification Theories in Atomic Phenomena	Victor Flambaum, University of NSW	4
Conformational Stability in Neurodegenerative Diseases	Vidana Epa, CSIRO	4
Spectroscopic and Thermochemical Properties of Small Molecules	George Bacskay, University of Sydney	4
Analysis and Modelling of National Scale Landscape and Surface Climate Data	Michael Hutchinson, Australian National University	3
Simulation fluid flow through NFR	Abdul Shaik, University of NSW	3
Rational design of novel multiferroic materials for energy harvesting and energy efficiency	Claudio Cazorla, University of NSW	3
Protocol for the Analysis of Land Surface models	Gab Abramowitz, University of NSW	3
Fluid-Structure Interaction for Aeronautical Applications	Gareth Vio, University of Sydney	2
CSIRO ICT Social Media Analysis	David Milne, CSIRO	2
q-Hypergeometric function Transformation	Gary Bosnjak, Australian National University	2
Attribution and Projection of Climate Variability and Changing Weather Systems	Jorgen Frederiksen, CSIRO	2
Elucidating molecular origin of energy dissipation in nanosensors via high-fidelity, large-scale molecular dynamics simulations	Naida Lacevic, University of Melbourne	2
Woodland Eucalyptus Genomics	Rose Andrew, University of New England	2
Wide Field Spectrograph	William Roberts, Australian National University	2
Numerical simulations of the coupled plates/mantle dynamics	Giampiero Iaffaldano, Australian National University	2
Photocatalysis of transition metal doped substrates	Nicholas Lambropoulos, CSIRO	1
Advancing dynamical understanding in the East Australian Current Optimising the ocean observation and prediction effort	Moninya Roughan, University of NSW	1
MD simulation for DEJ Lab	Rima Chaudhuri, University of Sydney	1
Quantum mechanical modelling of molecular structures of inulin	Andrea Gerson, University of South Australia	1
Sparse Sieve Density Estimation	Artem Prokhorov, University of Sydney	1
Space Weather in Planetary Systems	Bradley Carter, University of Southern Queensland	1
Estate Tax and Annuities in Entrepreneurship Model	Cagri Kumru, Australian National University	1

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Gait generator for humanoid robots	Chao Chen, Monash University	1
Koala genome project, genome annotation	Denis O'Meally, University of Sydney	1
Direct geothermal systems ground heat exchangers modelling	Guillermo Narsilio, University of Melbourne	1
Engineering Materials simulation	Hamid Valipour, University of NSW	1
Delivering real-time water management information and regional crop water use productivity benchmarking across the cotton industry using IrriSAT	Jamie Vleeshouwer, CSIRO	1
Aboriginal Child Language Acquisition	Jane Simpson, Australian National University	1
Population genomics of psyllid-induced eucalypt dieback	Markus Riegler, University of Western Sydney	1
Electronic & Thermodynamic Properties of Hybrid Organic-Inorganic Nanostructures	Nicholas Lambropoulos, CSIRO	1
Fire activity modelling for use in smoke predictions	Sean Walsh, University of Melbourne	1
Molecular dynamics simulation of interphase precipitation in metal alloys	Weimin Gao, Deakin University	1
Quark Gluon Plasma in Lattice QCD: From Big Bang to Small Bang	Mushtaq Loan, Australian National University	0.8
Control Strategies of Surface Quality of Stainless Steels	Zhengyi Jiang, University of Wollongong	0.8
Understanding the nature of abrupt regional shifts in a changing climate	Roger Jones, Victoria University	0.7
The Nonlinear Dynamics of gait Analysis	David Miron, University of New England	0.6
Calculation of social network centrality measures using R	Jenny Jiang, University of NSW	0.6
The hunt for Ribonucleic Acid riboswitches and genetic sensors of metabolic flux in plants	Christopher Cazzonelli, University of Western Sydney	0.5
Computer-intensive statistical methods	Hanlin Shang, Australian National University	0.5
De novo genome assembly using pacbio long reads	James Hane, Curtin University of Technology	0.5
NeuRA bipolar test project	Janice Fullerton, University of NSW	0.5
Effective implementation of payments for environmental services in Lao PDR	Jeff Bennett, Australian National University	0.5
Determination of potential satellite calibration sites by analysis of the Australian Landsat data archive (or alternatively GA Datacube)	Michael Caccetta, CSIRO	0.5
Implementation of IDL Virtual Machines for satellite-image processing	Petra Heil, University of Tasmania	0.5
Structure and Reactivity of Coinage Metal Nanoclusters	Richard O'Hair, University of Melbourne	0.5
ACCESS UM Modelling	Martin Dix, CSIRO	0.4
Theoretical Study on Chlorophyll Modification and Its Spectral Extension in Oxygenic Photosynthesis	Min Chen, University of Sydney	0.3
Uncertainty quantification algorithms for acoustic and electromagnetic models	Stuart Hawkins, Macquarie University	0.3
WildCountry Science Project	Brendan Mackey, Australian National University	0.1