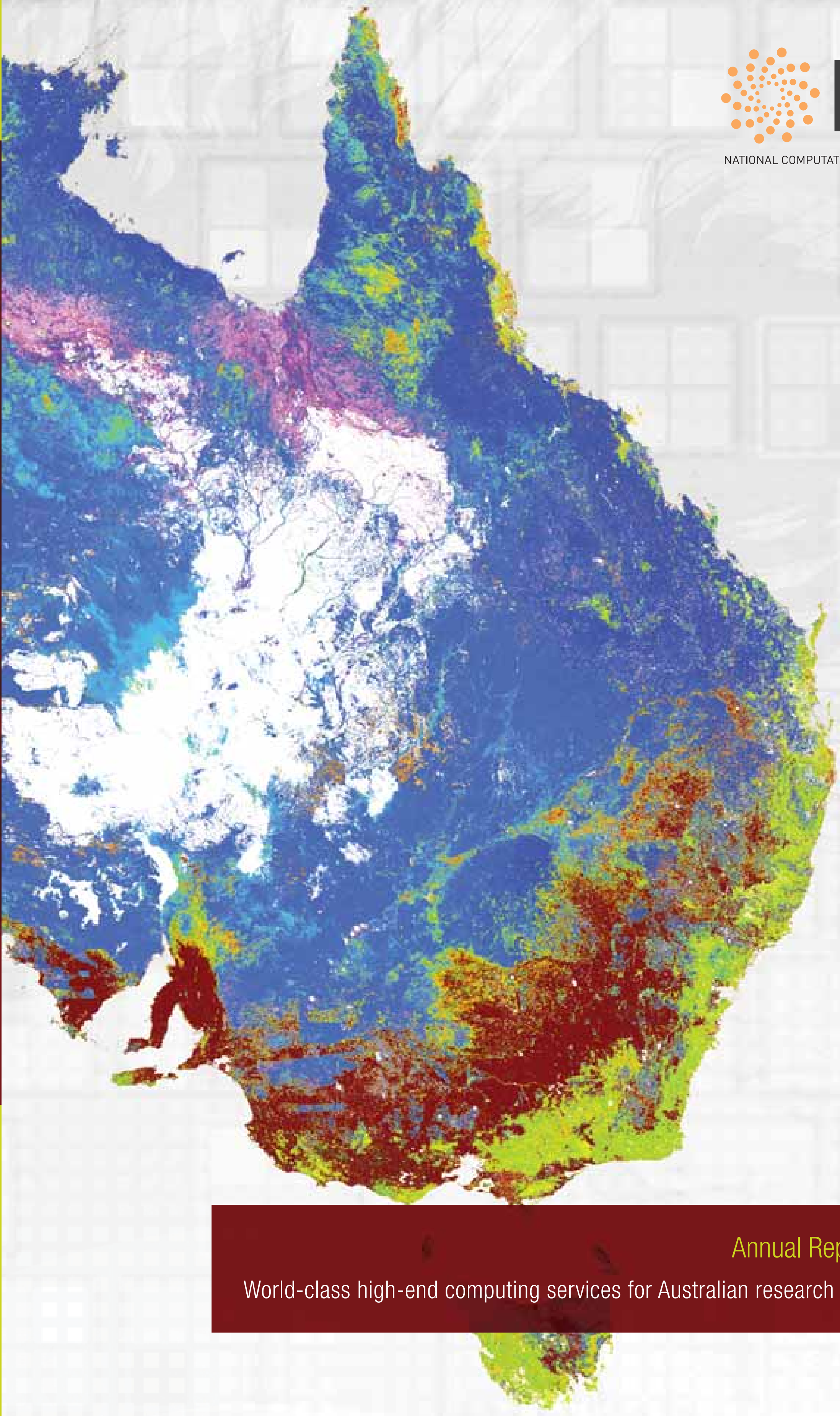
NCI

NATIONAL COMPUTATIONAL INFRASTRUCTURE



Annual Report 2015-16

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

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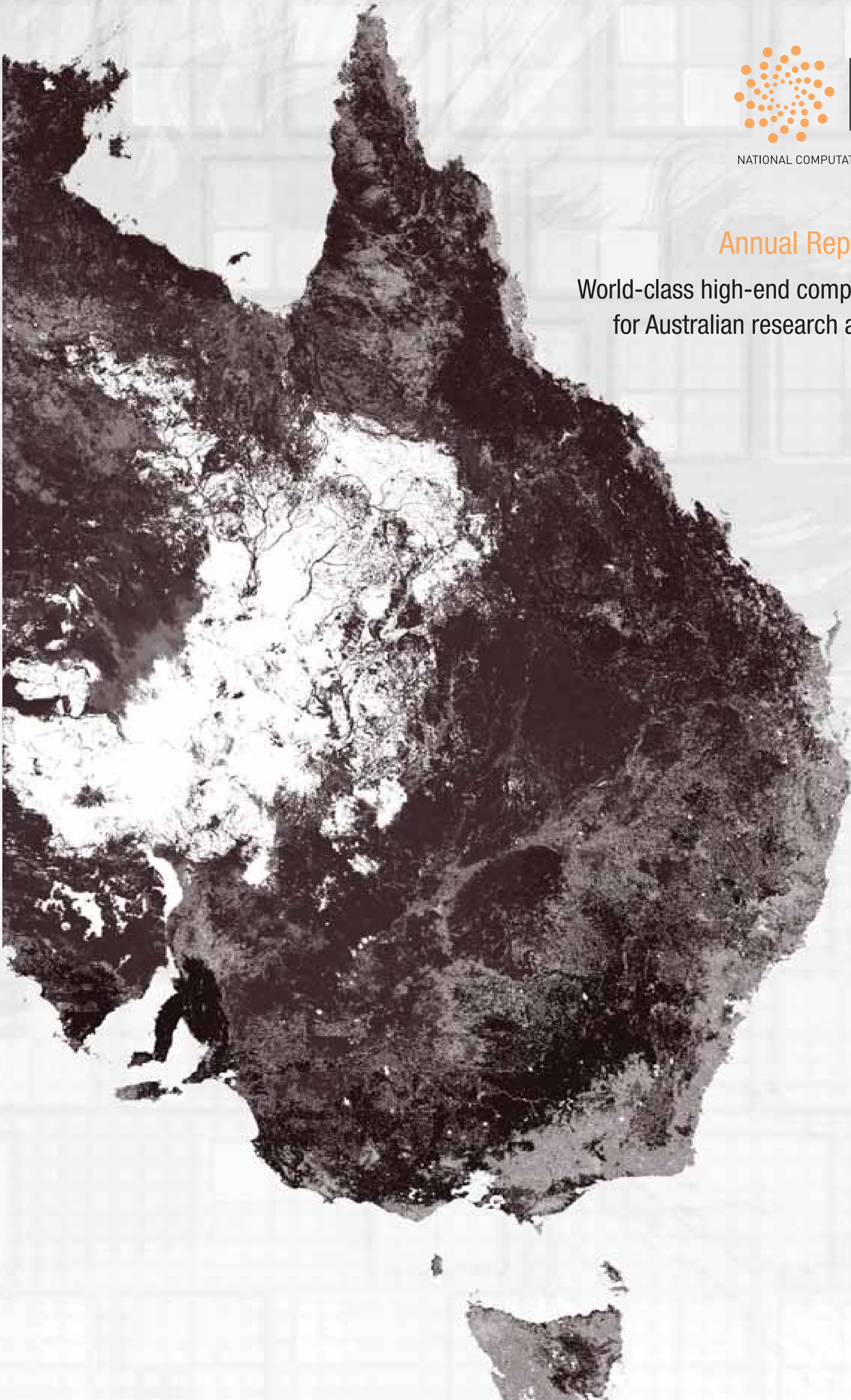

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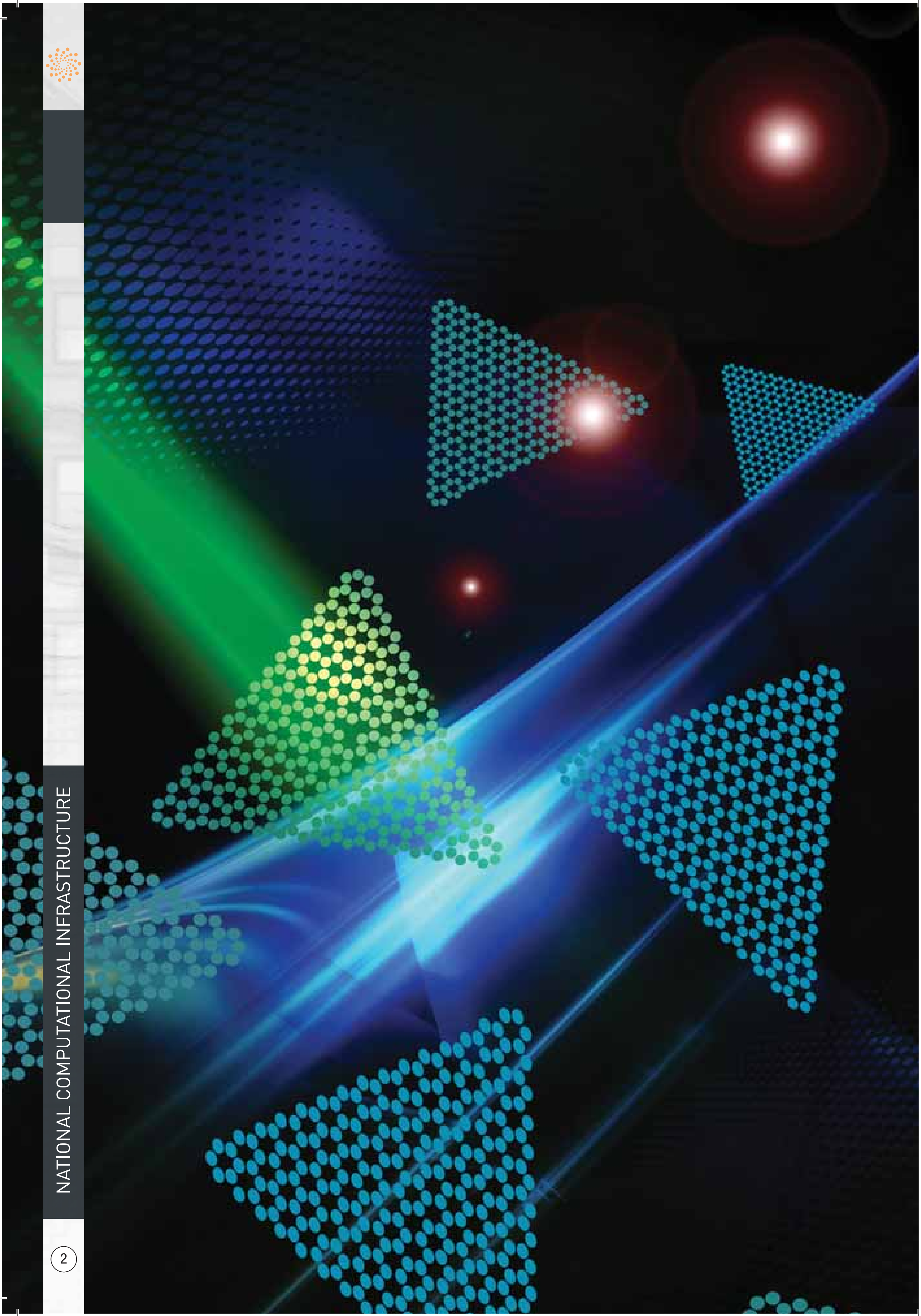

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Introduction

Who we are

NCI Australia is the nation's most highly integrated, high-performance research computing environment. NCI is built to deliver on national priorities and research excellence from across the scientific disciplines. 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, not only in the reach and outcomes of the service that we provide, but also in our funding model, bringing together the shared responsibilities of the Australian Government and the research sector. The Australian Government provides world-class infrastructure to NCI through its National Collaborative Research Infrastructure Strategy (NCRIS), and the research sector, comprising universities, national science agencies, industry and the Australian Research Council (ARC), collectively contribute two-thirds of the annual recurrent costs.

Our values

The realisation of our values through a unique combination of infrastructure, software and skills is pivotal in delivering transformational outcomes that manifest in the advancement of social, commercial, policy and environmental gains for the nation.

- NCI is research and outcomes driven, constantly seeking to develop and evolve its service portfolio to deliver on researchers' requirements, institutional research needs, and national research priorities.
- NCI aims to deliver a national benefit by enhancing the outcomes of individual research projects and longer run research programs undertaken by government, science agencies, universities, and industry from across the country.
- NCI's research-driven agenda is underpinned by deep engagement with a broad range of research organisations, centres and communities across Australia and the world —

which, in turn, drives the relevance, agility and value of its services.

- The quality and depth of NCI's infrastructure, expertise and experience deliver transformational outcomes to researchers that are on par with world's best practice, and, in some cases, are world-leading, maintaining NCI's position as an innovation leader in computationally- and data-intensive methods.

What we do

Based at The Australian National University, we provide integrated high-performance computing and high-performance data services to over 4000 researchers at a number of the national science agencies, including CSIRO, Geoscience Australia and the Australian Bureau of Meteorology, along with 35 Australian universities, five Australian Research Council Centres of Excellence, eight NCRIS capabilities, three medical research institutes, and three industry partners.

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. It also delivers outcomes that inform and benefit public policy, and supports an internationally competitive research environment that attracts and retains world-class researchers for Australia.

About this Report

This NCI Annual Report provides an overview of NCI's activity during the 2015-16 Financial Year.

This includes a description of NCI services, users and infrastructure, as well as research highlights about the work of NCI's partner organisations. The NCI Annual Report also details the financial report for that period.

Chair's Report

It is with pleasure that I write this preface to the NCI Annual Report for 2015–16, and my first since becoming Chair of the Board—a role which I took over from my predecessor, Emeritus Professor Mark Wainwright, who retired as Chair in December 2015. Mark Wainwright was NCI's foundation Chair, commencing his term in November 2007. His legacy, over the following eight years, includes the strong governance for which NCI is known, and the Board's oversight of a uniquely strong national partnership (of universities, government science agencies, research councils, medical research institutes, and industry) that sustains the bulk of NCI's operations, and steers the evolution of its service portfolio.

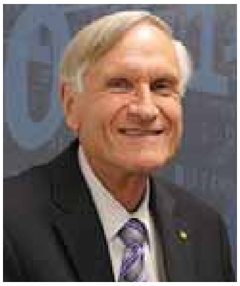
NCI traces its history back nearly 30 years to Australia's first university supercomputer at ANU, the first, national high-performance computing (HPC) services through the Australian Partnership for Advanced Computing (APAC) from 2000, and from 2007 as the NCRIS-funded National Computational Infrastructure. I have enjoyed being a part of this journey in each of these phases, particularly as a member of the APAC Board in the early 2000s, and now again as Chair of NCI. The changes which have occurred during this time are profound, with research competitiveness in, and the social, environmental and economic benefits deriving from, every field of science and technology being now highly dependent, not only on HPC, but also on "big data" methodologies and computational and data science expertise. The world's HPC facilities are responding to this international impetus, and I was most impressed to find that NCI is not only responding, but is amongst the forefront of such developments.

At this time, the Australian Government is developing a new National Research Infrastructure Roadmap and investment plan for the coming decade. The crucial importance of a strong, national advanced computing capability cannot be understated, and I commend the strong and constructive engagement of the Director, and my fellow Board members, in making the case to both government and the Roadmap Expert Group.

Over the past year, the Board has been emphasising to government the urgency of reinvestment in NCI's capital infrastructure, and particularly the replacement of its ageing supercomputer, Raijin. The recent success of NCI's application to the 2015–16 round of the Agility Fund, in which it was awarded $7 million, is a valuable and encouraging signal, and indicative of strong support from government. These funds, together with matching co-investment from the NCI Collaboration, will provide a vital supplement to NCI's computational capability, in advance of Raijin's replacement. The coming year is thus one of challenge but also optimism.

The coming year will also see a change in leadership, with the foundation Director, Professor Lindsay Botten, retiring in May 2017. In reflecting on the substantial achievements of NCI realised during his term as Director, I note the strong and mature base for the ongoing development of national advanced computing services, and the exciting opportunities for the future under a new Director, the recruitment of whom is now underway.

In closing, I thank sincerely the members of the NCI Board for their dedication, commitment and expertise. I particularly acknowledge the insightful support of the Deputy Chair, Professor Robin Stanton, to both me and my predecessor, and also the service of Dr Robert Frater who retired from the Board in June 2016.



Emeritus Professor Michael Barber, FAA, FTSE
Chair, NCI Board

Director's Report

Over many years, investments in high-performance computing (HPC) have delivered astounding benefits in advanced economies, Australia's included—propelling research impact in every field of science and industry application, providing a foundation for the solution of grand challenge problems, and underpinning economic competitiveness. The modern HPC environment has evolved to encompass the imperative of "big data", in addition to its traditional role of computational modelling and simulation. The contemporary HPC environment comprises a highly integrated, high-performance computing and data infrastructure, required for the computationally- and data-intensive workflows of today's research, together with expertise in computational and data science required to leverage value from the infrastructure and enhance the research ambition.

This fusion of big computation, big data, and expertise, today referred to as *advanced computing,* is the pathway along which NCI has evolved in recent years, and a paradigm now widely advocated to national research funding bodies throughout the world. As Australia's most highly integrated and expert e-infrastructure environment, NCI is proud to be in the vanguard of this transformation—shaped through deep engagement with, and by the goals of, the research communities and organisations that we serve—delivering national benefits, heightened impact, and enhanced competitiveness for Australian research and innovation.

The benefits arising from this approach are seen in the exciting research outcomes highlighted in this report, the enhanced capability and performance in data and computational services which have been provided, and the quality and innovation inherent in the NCI portfolio which is driving research to new heights and growth in our business—with four new organisations joining the NCI partnership this year, and with more in prospect in the coming year.

Today, NCI is truly a national advanced computing service, supporting research in over 500 active projects, involving more than 4000 researchers from 35 universities; eight NCRIS capabilities; five national science agencies (including the Bureau of Meteorology, CSIRO and Geoscience Australia); a growing number of medical research institutes and industry R&D users. NCI's critical role in the national R&D system is seen through its support of more than 200 ARC- and National Health and Medical Research Council (NHMRC)-funded activities (projects, fellowships, industry hubs and six Centres of Excellence) with an annual value approaching $60 million; its acknowledgment in more than 10 research publications per week, i.e., 500 per annum; and its vital role in empowering social, economic and environmental outcomes—through national science agencies, medical research institutes, and industry in areas such as extreme weather and regional climate impacts, environmental and agricultural policy, advanced resource extraction techniques, health and medical research, and new technologies that will underpin future industries. Examples which include 30 per cent improvements in the performance of Australia's weather and climate prediction model; NCI's role (through GA) as the regional Australasian/South-East Asian hub for the EU Copernicus Sentinel satellite data to enable valuable environmental intelligence; and NCI's contribution in enabling high-throughput genomic analysis to understand and solve human diseases such as cancer and auto-immune diseases are sprinkled through this report.

This year marks a crossroad in national research infrastructure strategy, with the development of both a new National Research Infrastructure Roadmap, to set investment priorities and determine implementation, and an e-Research Framework, to shape a future e-infrastructure landscape. Each is critical in shaping the future environment, its implementation and efficiency, the utility of the services for the research and innovation sector, and ultimately Australia's international research competitiveness.

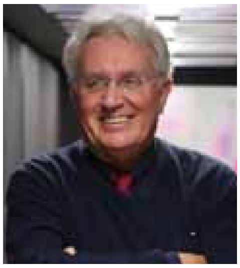
For these reasons, NCI has been active in prosecuting a vision of a research-driven, converged infrastructure and service portfolio, which integrates computational and data capabilities, and which also includes substantially enhanced investment in expertise—a vision that is based on local experience and international directions.

Our vision is grounded in, and validated by, various measures, amongst which is the strong cash co-investment from stakeholders for services, presently $12 million per annum, and a steady growth in the number of organisations and communities wishing to engage. Pleasingly, support from the ARC, through a $1 million p.a. LIEF subscription grant, matched by a number of research-intensive universities, has been renewed for a further three years (2016-18) and highlights our key role in supporting ARC research. Our annual user survey further confirms that the services are highly valued, and also highlights areas in which improvements can be made.

A significant re-investment in NCI by the Australian Government, through a successful allocation to the NCRIS Agility Fund during this year, is particularly welcome and demonstrates confidence in our directions. NCI was granted $7 million (the largest allocation from the $15 million pool), matched equally by co-investment from the NCI Collaboration. This will provide a much-needed, 30-40 per cent boost in the computational capacity of NCI, together with

access to contemporary HPC infrastructure that will rejuvenate international collaborations, as well as the replacement of the oldest of the three persistent filesystems, now at end-of-life. The procurement of the former is well underway and NCI anticipates commissioning the new HPC facility as a supplement to Raijin (until its substantive replacement) early in 2017.

In closing, I note that this is my final contribution to an annual report ahead of my retirement in 2017, having had the privilege of leading NCI since 2008. I offer sincere thanks to the Board Chairs and Deputy Chairs, under whom I have served, for their wise advice and support; to my senior colleagues at NCI for shaping, sharing and prosecuting our vision; to the entire NCI team for its dedication, professionalism and expertise; to the Australian research community whose aspirations have shaped us, and whose successes reflect well on us and build the case for ongoing investment; and to the co-funding partner organisations and the Australian Government through the National Collaborative Research Infrastructure Strategy, the confidence of which is so vital to the continuation and delivery of a world-class, advanced computing service for Australia.



Professor Lindsay Botten,
Director, NCI

Snap shot –
the year at a glance

July 2015
Mancini user self-service portal launched

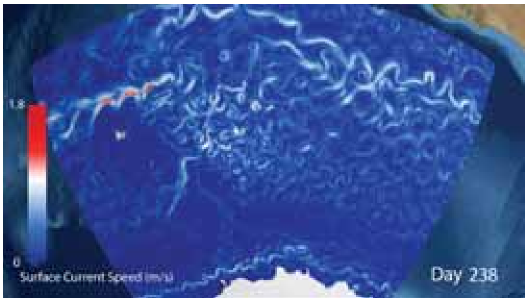
August 2015
NCI's third and newest global filesystem, /g/data3, enters production

September 2015
Ministerial visit: Hon Paul Fletcher MP and Hon Karen Andrews MP

October 2015
Successful renewal of NCI's ARC LIEF grant for three years (2016-18) announced.

Australian Government
Australian Research Council

November 2015
Professor Andy Hogg Antarctica water video released: 29345 views to date



December 2015
Designing solar cells *"Splitting light in the cloud"* with article published in international journal *Optica*.

January 2016
Biosensors for medical diagnosis and research from the ARC Centre of Excellence for Nanoscale BioPhotonics *"Shining new light on the body"*

February 2016
New partner organisations: Garvan, UTS, University of Wollongong

GARVAN INSTITUTE UTS UNIVERSITY OF WOLLONGONG AUSTRALIA

February 2016
RDS data ingest 100 per cent complete

March 2016

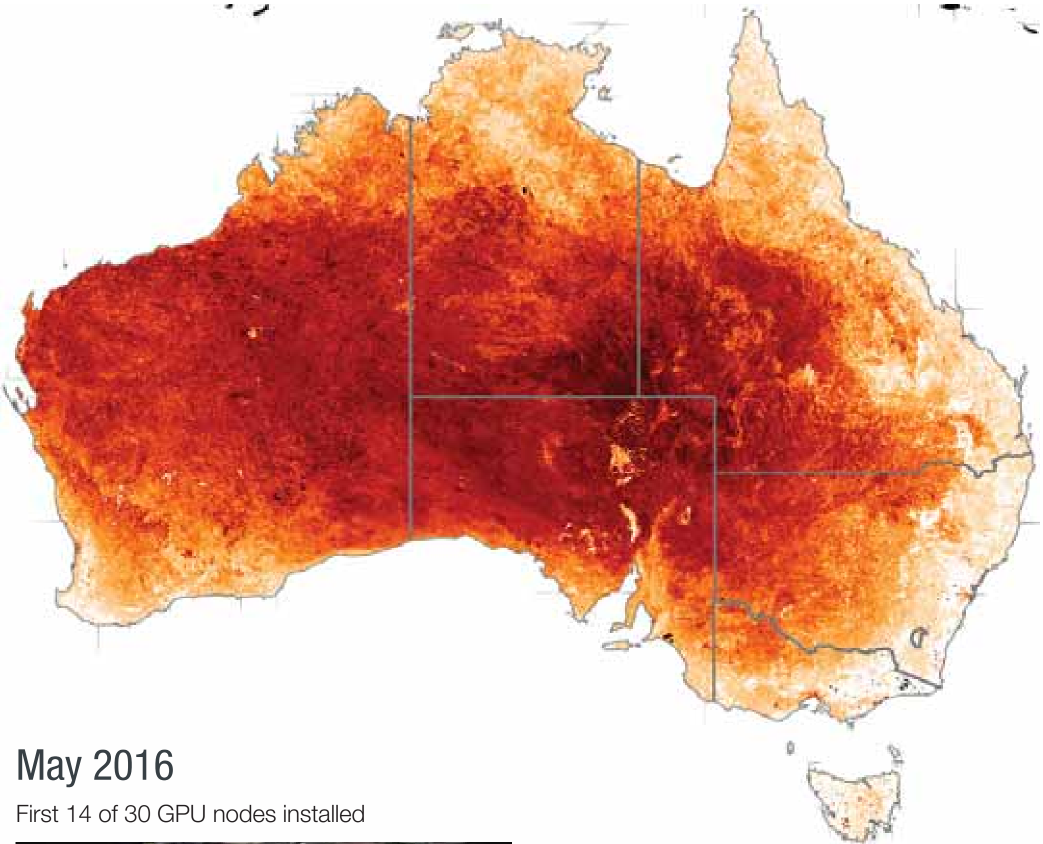
Invited HPC presentation to the National Research Infrastructure Roadmap Expert Group

May 2016

Copernicus service agreement signed with Geoscience Australia; Copernicus data hosting from NCI goes live (see Case Study 4)

April 2016

Australia's Environment website launched: accessible from http://wenfo.org/aus-env/



May 2016

First 14 of 30 GPU nodes installed

May 2016

Invited application for NCRIS Agility Fund—$7 million allocation announced after the election in August

June 2016

NCI designated as the national infrastructure partner in the NHMRC-funded Australian Genomics Health Alliance

June 2016

Latest partner organisation: Macquarie University

System specs at a glance

59 Staff

2 buildings

2 data centres

Over 55 km of cabling

Over 15,000 hard drives

Over 8,500 magnetic tape drives

3 dedicated high-performance computing systems

Raijin:

- Fujitsu Primergy cluster
- 1.37 PFlops peak performance
- 57,864 Intel Xeon cores (Sandy Bridge, 2.6 GHz) in 3609 Fujitsu Primergy nodes
- Mellanox FDR 56 Gb/sec Infiniband full fat-tree interconnect
- 162 TB main memory
- 12.5 PB disk storage
- Over 500 million core hours per year
- 314 software packages
- 29.9 PB of high-performance operational storage capacity

Tenjin:

- Australia's highest performing research cloud
- Dell cluster running OpenStack Cloud operating system
- 33 TFlops peak performance
- 1,600 Intel Xeon cores (Sandy Bridge, 2.6 GHz)
- Mellanox FDR 56 Gb/sec Infiniband full fat-tree interconnect
- 25 TB main memory
- 1 PB Ceph Storage
- Access to 30 PB data repository

Fujin:

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

Fastest filesystems in the Southern Hemisphere (Lustre):

- 7.6 PB scratch storage on Raijin accessed at 150 GB/sec
- 22 PB active project storage accessed at up to 140 GB/sec
- 13 PB archived data accessed at up to 140 MB/sec

Australia's largest research data catalogue:

- Over 10 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

Australian Government
Department of Education

Partner organisations:

Australian National University

CSIRO

Australian Government
Bureau of Meteorology

Australian Government
Geoscience Australia

RMIT UNIVERSITY

INTERSECT

DEAKIN UNIVERSITY AUSTRALIA Worldly

qcif

ACE
ANTARCTIC CLIMATE & ECOSYSTEMS COOPERATIVE RESEARCH CENTRE

UTS
UNIVERSITY OF TECHNOLOGY, SYDNEY

GARVAN INSTITUTE

UNIVERSITY OF WOLLONGONG AUSTRALIA

MACQUARIE University

Australian Government
Australian Research Council

THE UNIVERSITY of ADELAIDE

Australian National University

MONASH University

UNSW AUSTRALIA

THE UNIVERSITY OF QUEENSLAND AUSTRALIA

THE UNIVERSITY OF SYDNEY

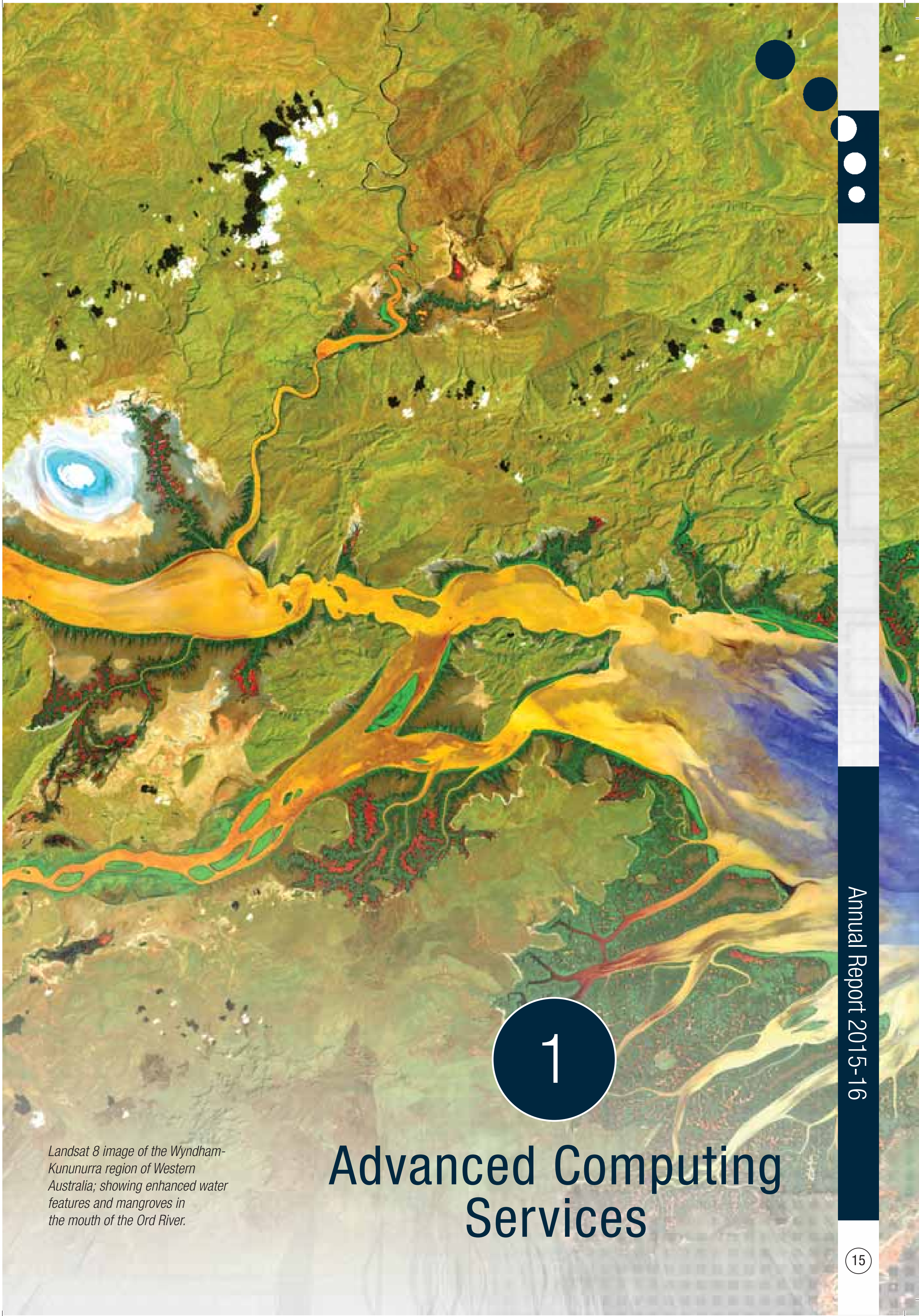
RMIT UNIVERSITY

FUJITSU

A node of

Commercial Partners

Affiliates



Landsat 8 image of the Wyndham-Kununurra region of Western Australia; showing enhanced water features and mangroves in the mouth of the Ord River.

1 Advanced Computing Services

NCI's Integrated e-Research Capabilities

The National Computational Infrastructure is a highly integrated advanced computing facility, dedicated to advancing and making possible research from all areas of science.

By providing high-performance computing, data storage and data services under one roof, NCI brings to the research community an all-in-one resource for compute and data intensive work.

HIGH PERFORMANCE COMPUTING	Ground-breaking Australian computational research is expedited on NCI's high performance cluster, generating experimental results in just days or weeks that would otherwise have taken decades or centuries on a desktop computer.
CLOUD COMPUTING	Enabling collaborative access to specialised computing environments and to more than 10 petabytes of nationally and internationally significant research data.
DATA STORAGE	NCI operates the fastest filesystems in the Southern Hemisphere, linking our high performance computing and high performance data resources, providing an unparalleled service integration for our users.
HIGH-PERFORMANCE COMPUTING INNOVATION	Through maximising research outcomes by developing and optimising codes to run most effectively on a supercomputer, NCI can ensure the most efficient running of high-level models and simulations.
DATA INNOVATION	Meeting the ever-increasing requirements for e-infrastructure investments with 'end-to-end' management of data, including ingestion, curation and delivery.
COLLECTION MANAGEMENT	Simplifying access to petabytes of research data using persistent identifiers and other types of metadata for curation, maintaing a navigable catalogue for users.
VIRTUAL LABORATORIES	Online platforms that make datasets, state-of-the-art analysis and visualisation tools easily accessible in a 'one-stop shop' environment, providing the researcher with everything they need.
VIZLAB	Using cutting-edge visualisations such as image stills, video animations and interactive interfaces to better understand and interpret data across a wide range of scientific disciplines.

Advanced Computing and Data Infrastructure

HPC Systems

The NCI HPC team had an extremely busy and successful year, during which a number of new capabilities were introduced for users of Raijin. This included improved job scheduling, introduction of cgroups to better manage running processes and more than two quarters with 100 per cent uptime.

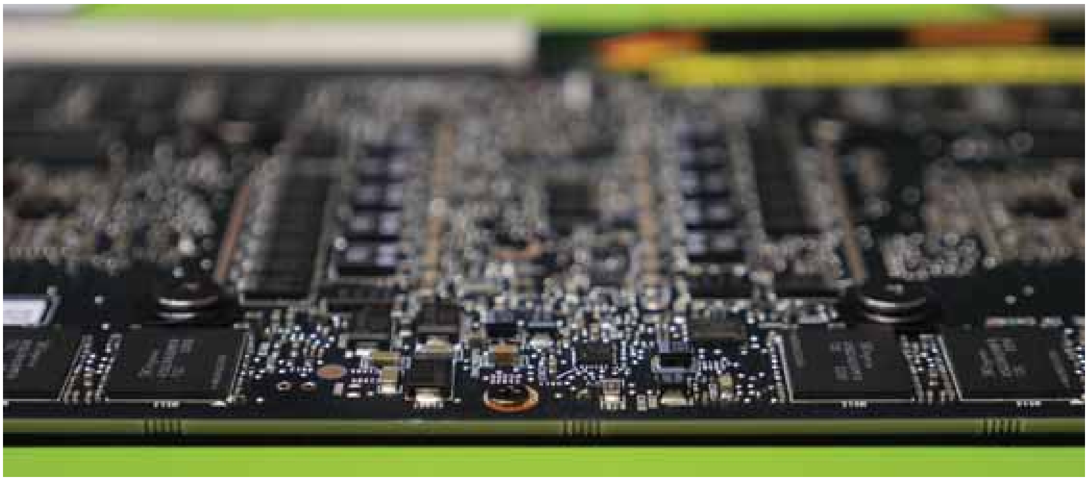
High uptime is a key part of an efficient and reliable supercomputing facility. It makes it possible for researchers to trust that their large compute jobs will run with minimal disturbance. In turn, this means that there is the computer capacity for more jobs to run at once and over the year. In total, Raijin ran at 99.9 per cent uptime during the year, an improvement over its two previous years of operation.

The biggest win in the past year was the testing and deployment of a high-density GPU solution based on state-of-the-art Nvidia K80 General Purpose Graphics Processing Units. NCI has augmented Raijin with 14 high-density GPU nodes, each of which includes four NVIDIA Tesla K80 GPU Accelerators, supplemented by Intel Haswell processors and 256GB of rapid access system memory.

The upgrade gives Raijin a 175 Teraflop increase in performance, a 14 per cent improvement bringing its peak performance to 1.375 Petaflops. The uptake of the new GPU queue by users has been extremely encouraging, demonstrating the high demand for innovative computing solutions in this field. Chemistry and molecular dynamics codes in particular benefit from GPUs, with codes such as NAMD and LAMMPS running respectively 11 and 8 times quicker. Due to the demand for the new GPUs, NCI plans to more than double the number of operational GPU nodes in 2016-17.

In a nod to NCI's position as a leading international facility, the organisation was invited to be part of Intel's early shipment of the latest generation Xeon Phi chips, codenamed 'Knights Landing'. These will be installed and commence operation in the second half of 2016, giving researchers around Australia access to the latest accelerator compute nodes from Intel.

HIGH-PERFORMANCE COMPUTING



Cloud Services

NCI provides high-performance cloud computing services to Australia's research community. This comes in the form of two distinct cloud deployments: a partner cloud, Tenjin; and a participating node of the National e-Research Collaboration Tools and Resources project (NeCTAR).

In 2015-16, the Cloud Services team has continued to contribute extensively to a range of nationally funded activities. These activities show the level of support that NCI provides to national projects on an ongoing basis, helping to maintain and improve services benefiting researchers from institutions around the country.

As part of NCI's commitment to national e-research platforms, NCI forms part of the NeCTAR Core Services team providing technical services, code and process development for the NeCTAR Research Cloud. This year, NCI was the lead participant and provided the core of the consultation, design and code development for a flexible reporting system for the NeCTAR community. This was a very high priority system for the NeCTAR Nodes and Directorate to assist in the management of the National Cloud resources. The quality modular design and development work on the reporting framework has allowed for this solution to also be used for the internal NCI Tenjin cloud, allowing for better reporting to NCI partners.

With the focus on research cyber security, the NCI cloud team under the NeCTAR Work Package program has developed a platform-independent security framework for cloud deployments. This has delivered significant benefits for NCI and NeCTAR Cloud users as it has enabled proactive monitoring of security vulnerabilities on users' virtual machines. The project contributed directly to ongoing NeCTAR security activities, showcasing the contribution NCI makes to nationally significant e-research infrastructure.

NCI's cloud team also continues to innovate with the launch of an open source framework enabling researchers to build and deploy a HPC cluster in the cloud with ease. The cluster provides all the benefits of the NCI cloud environment with a software environment similar to NCI's flagship supercomputer Raijin.

CLOUD COMPUTING

Data Storage Services

During 2015-16, NCI significantly increased its active project data storage capacity. All the data used by active projects running at NCI is kept within four large Lustre filesystems, including three global, persistent data filesystems, made up of thousands of interconnected hard drives delivering 22.1 petabytes of high-performance operational storage capacity. The newest filesystem, /g/data3, entered full production in August 2015, with an initial capacity of 5.7 petabytes. In March, this was expanded to 7.2 petabytes, and is fully integrated into NCI's operations, including access for the supercomputer Raijin.

Over the course of the year, over 48 million files, totalling 3,256 terabytes of data, were migrated between the /g/data filesystems to support the growing need for research project data. Uptime on the /g/data filesystems continues to exceed 99.8 per cent, ensuring reliable access to project data around the clock. A reliable solid file system helps in the efficient running of the data centre, enabling Raijin and other compute and data services to be operated at maximum throughput, maintaining the high productivity that researchers expect of the NCI services.

At the other end of the data storage spectrum, NCI's long-term archival tape storage libraries also received an upgrade with a software update in the second half of 2015, allowing the archival Massdata system to take advantage of the latest generation of tape technology. Each magnetic tape kept within NCI's latest TS1150 library can now store over 20 terabytes of data, at a speed of 360 MB/second.

The NCI tape libraries contain nationally significant research datasets going back to the 1970s. For example, images of Australia taken by scientific flights and early satellites are stored within NCI, and are still being accessed today for land monitoring research projects. Other significant datasets include the data used for the CMIP5 climate modelling exercise and the entire archive of images from the SkyMapper astronomy project. Where needed, a second, identical tape library in a separate building provides a backup for specific data within the NCI collection.

DATA STORAGE

User Support

Mancini

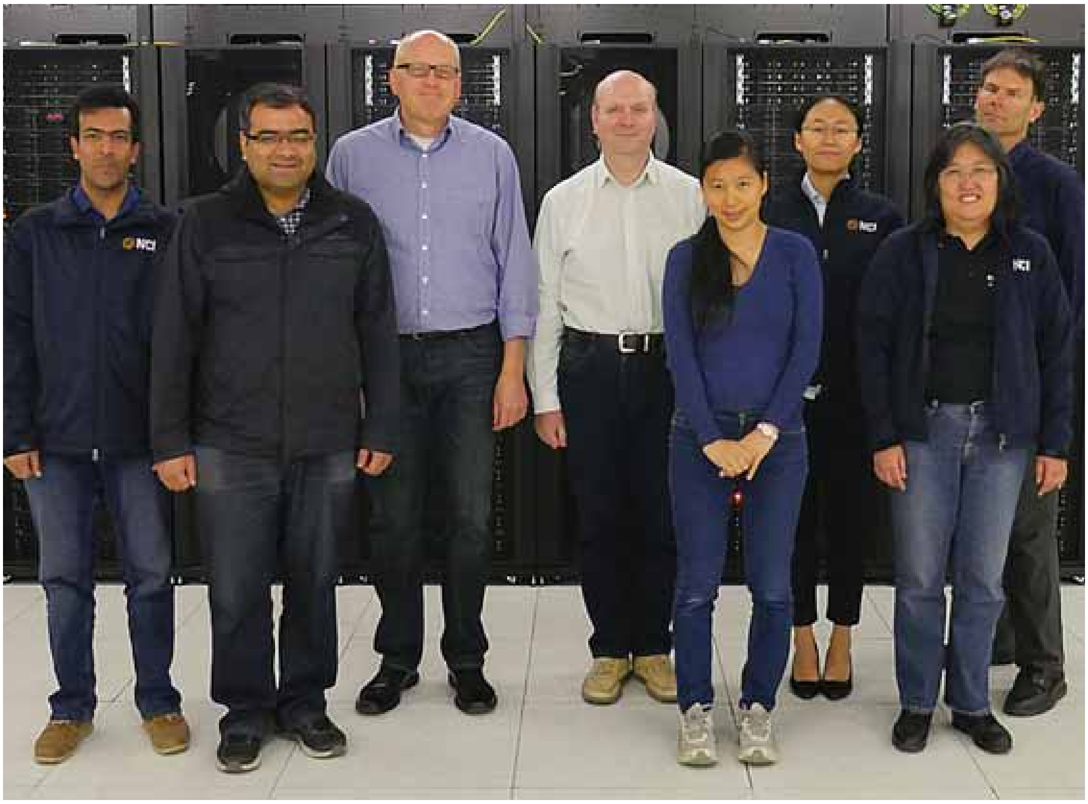
Mancini is NCI's self-service registration system for users. It allows users to register an account at NCI quickly and easily. Once in the system, users are able to submit project proposals directly to NCI and their institution's resource managers in near real-time, without using email. They are also able to see an overview of the projects that they are participating in, and see other projects that they might like to join.

Mancini was released to the user community in Q3 of 2015, a major milestone for NCI User Services. It has been stable and in continuous service since it was released. Mancini provides a major service improvement for NCI's users, streamlining the process of obtaining access to research projects and the NCI systems.

The unified login system at NCI means that this single login can now be used for all the different platforms that users access.

User Services Team

NCI's User Services Team is made up of PhD-qualified staff scientists and specialist programmers, with expertise and experience in various domains of science and the computational methods supporting them. They provide expert science and HPC support to users, as well as offering training and administration of users and projects at NCI.



NCI's User Services Team, from left to right: Mohsin Ali, Gaurav Mitra, Roger Edberg, Andrei Bliznyuk, Ching-Yeh (Leaf) Lin, Yue Sun, Rika Kobayashi and David Houlder.

Training

The User Services group continued to deliver training courses to partner organisations in 2015-2016. An advanced level course “Parallel Programming and Performance on Raijin” was presented at the Bureau of Meteorology and Antarctic Climate and Ecosystems Collaborative Research Centre. Introductory level courses “Introduction to Raijin” and “Introduction to Virtual Desktop Interface Systems” were presented at Geoscience Australia, The Garvan Institute for Medical Research, and RMIT University.

TABLE 1: NCI TRAINING COURSES

Date	Partner/user organisation	Number of attendees	Name of course
30/7/2015	Bureau of Meteorology (Melbourne)	23	Parallel and Performance Programming on Raijin
29/9/2015	ACE-CRC/AGP/AAD (Hobart)	20	Parallel and Performance Programming on Raijin
24/7/2015	Geoscience Australia (Canberra)	15	Introduction to NCI (Raijin)
28/1/2016	Geoscience Australia	18	Introduction to NCI Virtual Desktop Interface Systems
12/2/2016	Garvan Institute	25	Introduction to NCI (Raijin)
23/3/2016 and 24/3/2016	RMIT	20	Introduction to NCI, with special presentation of V3/ Trifid to NCI data migration
3/5/2016	Geoscience Australia	18	Introduction to NCI (Raijin)
20/6/2016	Geoscience Australia	31	Introduction to NCI Virtual desktop Interface Systems (2 sessions)
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

Another aspect of NCI’s collaboration work comes from a specialised project run with Fujitsu aimed at promoting the availability and efficiency of internationally recognised computer programs in quantum chemistry on Fujitsu hardware. NCI staff working on this project have a high level of familiarity with chemistry programs such as ADF, Amber, Gaussian and VASP, which enables them to participate in code development and optimisation along with the Fujitsu scientists.

For example, Gaussian is one of the most widely used chemistry codes in Japan, and testing through its collaboration with NCI is the only way that Fujitsu has to certify that the code runs effectively on their flagship FX100 machines. This testing is done on NCI’s Fujitsu FX10, one of the few available outside Japan. A new release of Gaussian is expected in the coming year, and preparations are already underway to test the code for efficient performance on Fujitsu’s hardware.

NCI’s team is on hand to advise chemistry researchers about ways to improve their codes, assisting both Fujitsu scientists and academic users. This year, they have also frequently attended conferences and presented talks on computational chemistry methods and the use of these codes, in Australia and internationally.

High-Performance Computing and Data Innovation

High-Performance Computing Development Services

Maximising research outcomes, raising the ambition of researchers, and ensuring the most effective use of a very expensive infrastructure like Raijin demands that the software that is run is as efficient as possible in its use of the hardware, and that it scales strongly to make the best possible use of the parallel nature of the supercomputer.

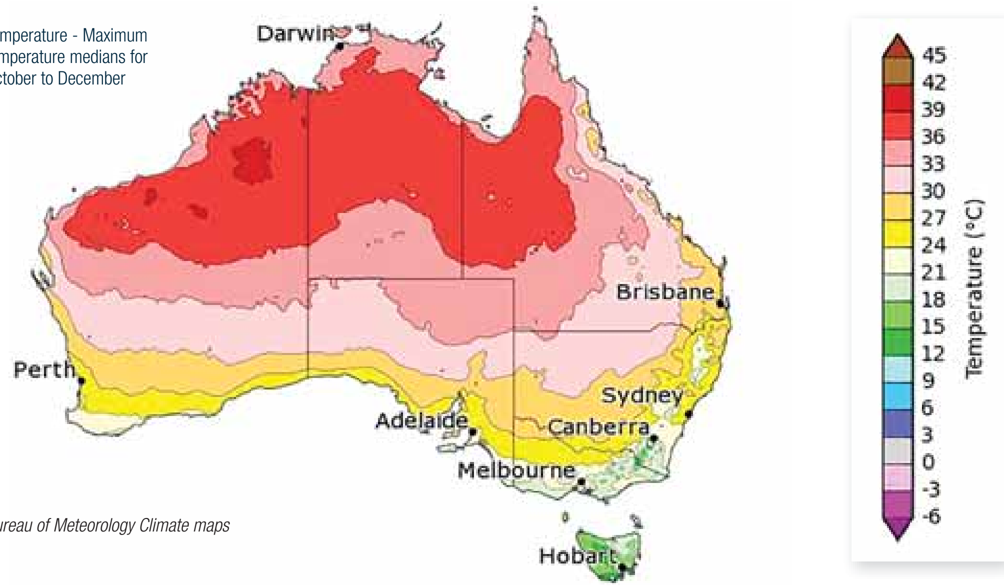
A critical function of the NCI HPC Scaling and Optimisation Team is thus in assisting researchers to identify bottlenecks in the performance of their codes, to rectify these and where possible to optimise them, and where there is the opportunity, to migrate codes onto new and more effective technologies (e.g., accelerators) as they become available. NCI's activities in code optimisation, and performance monitoring, profiling and enhancement, are many and varied, with the expertise available to the NCI community.

There is, however, a particular emphasis on the optimisation of climate and weather codes with staff of the Bureau of Meteorology, supported by a formal collaboration with Fujitsu. The focus of this work is the joint optimisation of ACCESS — the Australian Community Climate Earth System Simulator, which is the mainstay of the BoM weather forecasts and research into the variability and extremes in the world's climate system (see Case Study 5).

The project has made a number of improvements in how to more efficiently use NCI and BoM computational resources, including performance improvements which have been taken up by the UK Meteorological Office; and has scaled the model to much higher resolutions allowing a far better understanding of the physics of the atmosphere and the ocean. Overall, this project has provided impetus for NCI to build an important national capability, whereby complex priority codes, such as ACCESS, can be enhanced to advance both research and the national benefit.

HPC INNOVATION

Temperature - Maximum temperature medians for October to December



Bureau of Meteorology Climate maps

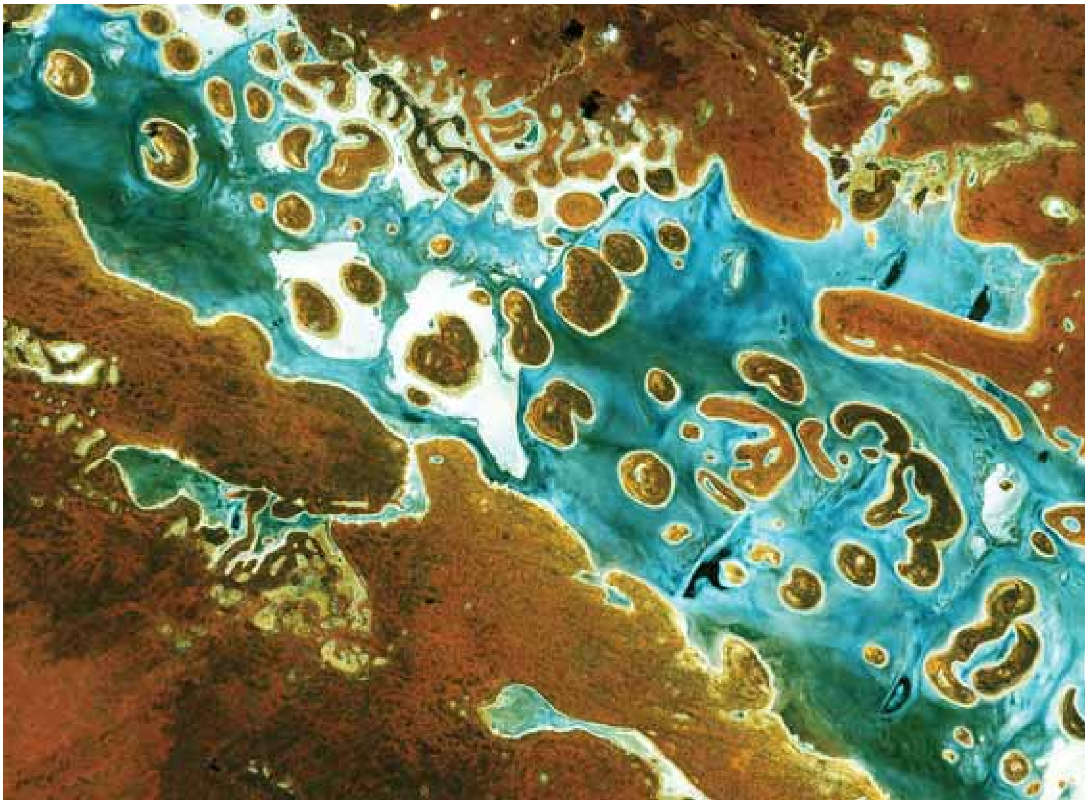
Research Data Services

The Research Data Services team has developed a Data Quality Strategy (DQS) to improve the quality of datasets across different subject domains and, through this, the ease by which the users can discover and access the data. The DQS includes new checks to improve NCI's data quality control and quality assurance methods. These will ensure that new datasets, as well as datasets already in the collections, are as accessible and usable as possible.

The quality control includes compliance with recognised standards and data conventions. These compliance checks improve interoperability, a feature of data archives that makes it possible for different datasets to be used and queried side-by-side. This requires consistent and accurate metadata for each and every file in the collections. With this in place, the content of datasets can be looked at in the context of when and where each was produced, who is its author and what instruments or models were used to generate the data.

In addition to using quality control to make sure that data held at NCI is maintained at a high standard, quality assurance checks are also used to ensure that the data works with a wide range of tools and data services. This enables data consumers to have a high degree of confidence that data they access from NCI will work with their tool of choice such as Python, Matlab or QGIS.

More than two petabytes of the over 10 petabytes of research data collections at NCI are available publicly through the THREDDS data service. This huge repository of geospatial data includes Bureau of Meteorology weather observations, images from the Landsat satellites and videos of the ocean floor from Geoscience Australia. Members of the public are invited to explore the data collection at http://geonetwork.nci.org.au.



Lake Amadeus in the Northern Territory, captured by the European Space Agency's Sentinel 2A satellite on 19 December 2015.

NERDIP: National Environmental Research Data Interoperability Platform

The colocation of large research data collections with high-performance computing and cloud resources at NCI provides a rich environment that enables new types of innovative large-scale interdisciplinary research to take place.

NCI has created NERDIP, the National Environmental Research Data Interoperability Platform, to provide a unifying, standards-based infrastructure and comprehensive set of services for users accessing datasets managed at NCI.

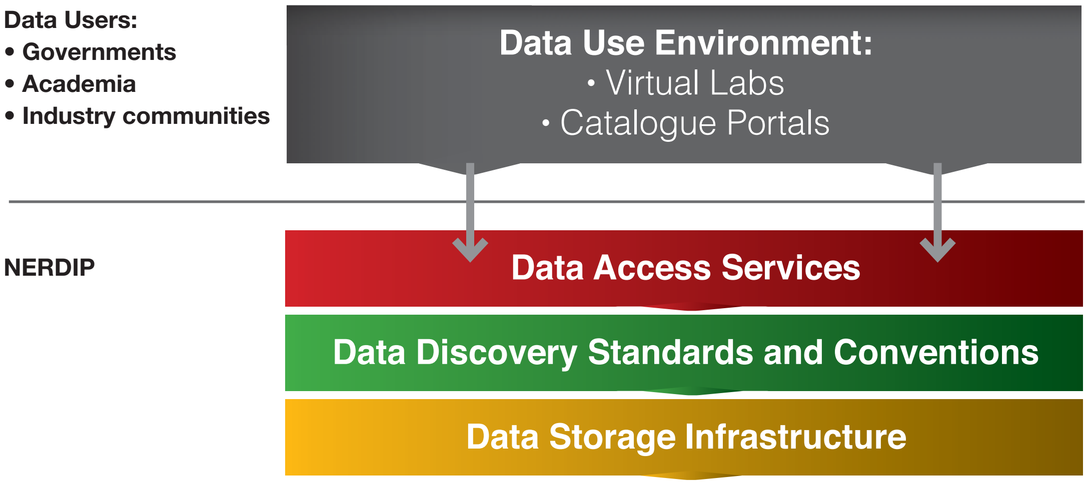
To maximise access by a broad range of users, the data collections are carefully prepared, standardised and harmonised for improved interoperability. This also improves local and remote programmatic access for high-performance analysis across all of NCI's data collections.

Use of common file formats such as NetCDF-CF, along with standard data services and protocols for accessing and analysing datasets, improves the experience for all users, and opens up the data to a new range of users without the need for time-consuming data manipulation. NERDIP provides an integrated data access and analysis environment, enabling interdisciplinary research in many scientific disciplines. Making the datasets interoperable makes it possible for data from different instruments and disciplines to be used together across a range of research domains, despite their diverse origins.

Using international data standards and world-leading data management systems for all of NCI's datasets means researchers now have a platform on which they can search, discover and analyse multiple varied datasets. Accessing the datasets through Raijin, the Virtual Desktop Infrastructure or community Virtual laboratories such as the Climate and Weather Science Lab, users are now able to easily work on a wider range of environmental data than ever before.

Go to http://nci.org.au/systems-services/national-facility/nerdip/ to find out more about NERDIP at NCI.

FIGURE 1: NATIONAL ENVIRONMENTAL RESEARCH DATA INTEROPERABILITY PLATFORM



High-Performance Data

The NCI High-Performance Data team works on the problem of providing simple and reliable access to high-value datasets. This includes providing new ways to view and visualise information, and maintaining up-to-date collections of imagery and observations from many different sources, including satellites and geophysical instruments.

One highlight of the year was NCI's signing of the service agreement with Geoscience Australia for the operations of the Australian Copernicus Hub—following on from the formation of the Australian Copernicus Hub partnership (See Case Study 4) and the agreement between the European Union (EU) and Australia to provide access to the data from the EU Copernicus Sentinel satellites. In a major milestone for NCI as Australia's leading e-research organisation, the organisation will be the Southeast Asian regional hub for all of the satellite observations coming from the European Commission's Copernicus program. The program uses multiple Sentinel satellites from the European Space Agency (ESA) and the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT) to provide imagery and observations about many different variables to do with land, water and the atmosphere. NCI has already commenced the data ingest from the first two of the satellites, with further satellites with different observational specialties to be launched in the coming years.

Through the Australian Copernicus Hub partnership, many different governmental and land management organisations in Australia and throughout the region have expressed interest in the data products to come through the Copernicus Data Hub. The increased coverage, resolution and variety of the Earth observations now available through the Copernicus Data Hub will open up many possibilities for research, policy and industrial uses in the coming years.

NCI will be ideally placed to help the Australian Copernicus Hub partnership in data dissemination for the Southeast Asian region for countries from Myanmar to New Zealand. The value of the satellites and the wide array of data that they capture make them incredibly valuable for all manner of applications in land management and development planning.

Another highlight of the year was a demonstration at the European Geosciences Union conference in Vienna in April 2016 of live data retrieval and manipulation from the NCI data centre. NCI is a partner in the international Earth Server 2 project, along with NASA, the European Centre for Medium-Range Weather Forecasts and others. The team demonstrated the possibility of accessing multidimensional data at NCI, as part of a European Union Horizon 2020 project aiming to support excellence in science, industrial leadership and tackling societal challenges.

Sandstone rock formations Uluru (on the right) and Kata Tjuta (on the left) in the Northern Territory, captured by the European Space Agency's Sentinel 2A satellite.

Data Collections

Taking advantage of the constantly expanding data storage infrastructure at NCI, the Data Collections team reached a major milestone this year. In February 2016, they completed the ingest of over 10 Petabytes of nationally significant data collections, the storage for which was funded by the NCRIS Research Data Services project. Eight nodes around the country are participating in this national data storage and service activity, with NCI having the largest active (on-disk) collection, as well as being the first to complete its data ingest.

Another major development in NCI's collection management over the past year has been the comprehensive infrastructure put in place to support data management in various ways. NCI's Data Collections team now offers robust services such as user-built data catalogues, Digital Object Identifier (DOI) minting, and the introduction of a variety of data provenance and tracking systems. These systems are designed to make accessing and using datasets for research open, transparent and easy. This ensures the owner and original location of the data are always visible and available.

One way that this is happening is with a new data provenance capture infrastructure. This infrastructure, which is currently being tested, links unique identifiers for entities such as datasets in the NCI catalogues with researchers and activities. Once this provenance report is available online, users can follow the footprint of the datasets and reproduce the results to verify and learn more about the research workflow. The datasets that have unique identifiers attached to them provide a much easier way to keep track of their usage in different research projects and publications.

Another improvement in the data collection management system is the Research Data Switchboard. This is a database management tool that helps visualise the relationships between entities such as researchers, datasets, grants and publications. Making use of unique identifiers that each entity in the system is given, this new tool lets users ask questions such as "how many users/publications are related to a particular dataset?" by querying the graph database. The connections between institutions, individuals, and their publications are now displayed by the system, with open access for users to query future relationships.

An RD-Switchboard graph showing connections between a researcher, their publications and the related datasets.

The next benefit to come from the Switchboard is that data owners will be able to track who is accessing their data and whether they have published any papers using it. The Research Data Switchboard opens up new possibilities for tracking and reporting use, but also allows for novel connections between researchers and topics to appear.

Virtual Laboratories

NCI offers virtual laboratory environments for researchers in the areas of climate and weather science, astronomy and geophysics. The three virtual laboratories are online platforms that integrate NCI's high-performance cloud and supercomputing with Australia's largest and highest performance data storage facilities, making it easy to access software, data sets and computing power simultaneously. Having everything researchers need in the one place speeds up the research process and makes collaboration much easier.

During 2015-16, the Virtual Laboratories (VL) team focused on migrating key components of the system to NCI's private cloud, Tenjin. Immediate benefits of this activity include access to Tenjin's world-class performance, plus a much tighter integration with NCI's peak HPC system, Raijin. The common hardware specifications these two systems share enable a close compatibility of software packages between them.

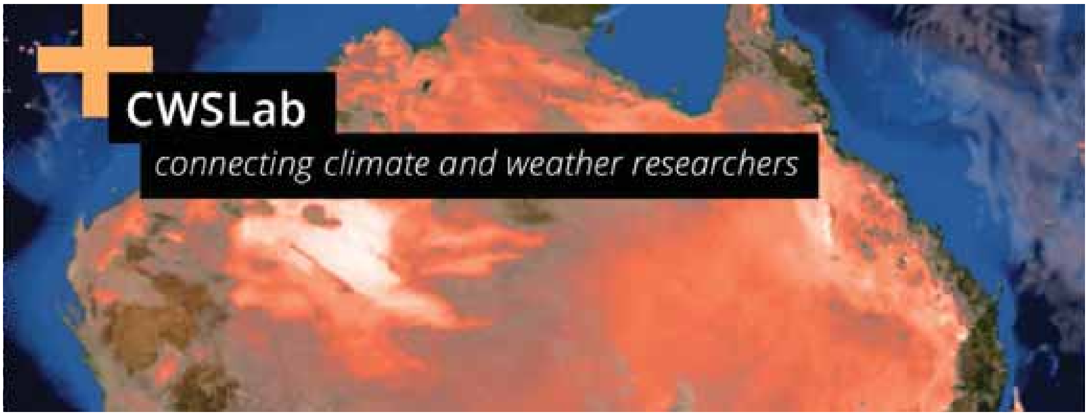
The Virtual Laboratories team develops, deploys and operates a range of systems and services that leverage NCI's major infrastructure (cloud, high-performance computing and storage) to support and enable workflows and virtual analysis environments embedded in NCI's partner organisations.

Services include a range of standards-compliant data services that enable scalable real-time delivery of data from NCI's over 10 Petabytes of scientific data collections. The team also works on systems including the NCI Virtual Desktop Infrastructure (see Case Study 1), which enables seamless interactive access to NCI's full range of infrastructure options, including a comprehensive suite of software packages.

A real-time monitoring system of the services and systems NCI operates, installed as part of the migration, allows for faster and more targeted responses to systems issues, improving both service quality and availability for all users. Detailed monitoring data also enables NCI to identify repeated or problematic issues quickly and accurately. Complementing the monitoring system is a new reporting framework that enables the team to track usage information and capacity issues for each deployed service. They also use it to capture usage information for projects or data collections.

The development and deployment environment developed by the Virtual Laboratories team draws on the best from modern DevOps practices. This provides an added benefit in that it is easily extended to other teams within NCI's Research Engagement and Initiatives section. Thus, the effort invested by the Virtual Laboratories team is able to generate multiplying returns as other teams at NCI incorporate the systems, services and methodologies employed by the VL team within their own activities.

VIRTUAL LABORATORIES



Scientific Visualisation - NCI's VizLab

For more than 25 years, NCI and its predecessors have been working on scientific visualisation as a research tool. The value of the visualisations goes beyond the beauty of the images produced. Rather, the aim is to use them as an investigative tool to gain deeper insights into complex datasets.

Today, NCI's team of specialist visualisation programmers has developed a respected reputation for innovative use of visualisation techniques. They work closely with researchers from NCI's partner organisations to help them gain insights from their data in fields such as meteorology, entomology and materials science.

Innovation in Software Development: Drishti and Drishti Prayog

Drishti is a custom-built software package developed at NCI for visualising volumetric data such as computed tomography (CT) scans. It was developed at VizLab more than a decade ago, and is now available as an open source software package for public use.

Drishti, together with its associated suite of tools, is continuously being enhanced to address the needs of its worldwide user community. In 2015-16, significant additions were made to the widely used presentation tool 'Drishti Prayog', as well as the segmentation tool 'Drishti Paint'.

Drishti Prayog is the interactive Drishti dataset presentation tool. It can be used on touchscreen devices to manipulate volumetric datasets and look inside scanned objects, from fossilised jaws to garden insects. Drishti Prayog encourages users to actively engage rather than passively observe. It has seen significant uptake across the user community in 2015-16, including uses in several science centres in the UK and Australia, such as the Natural History Museum in London.

In particular, VizLab collaborated with Questacon, the National Science and Technology Centre in Canberra, Australia to produce an exhibit called "Spiders", examining spider anatomy. Using data generated from CT scanners at ANU and using touchscreens enabled with Drishti Prayog, visitors at the "Spiders" exhibition in Questacon can explore the bodies of several different spiders in high-resolution detail.

The spider Missulena Bradleyi, endemic to the east coast of Australia, visualised using NCI's Drishti software.

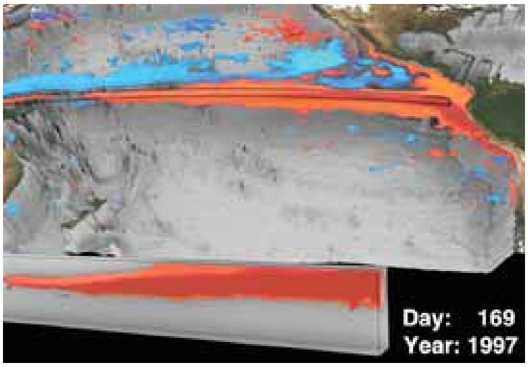
Specialist Services

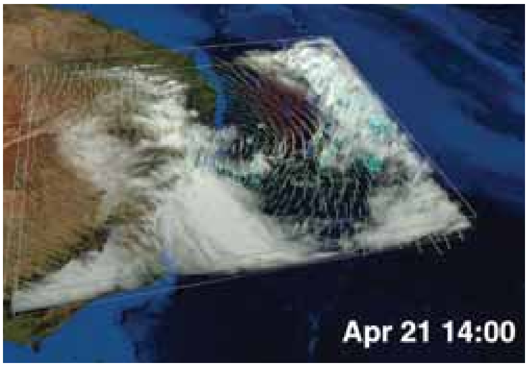
Oceanography

VizLab continues to work closely with ocean modelling researchers from the ARC Centre of Excellence for Climate System Science, including Drs Agus Santos, Alex Sen Gupta and Paul Spence (UNSW), Dr Shayne McGregor (Monash) and Dr Andy Hogg (ANU) to visualise the El Nino/La Nina phenomenon. This visualisation is based on data from a ¼-degree ocean-sea ice model of the global ocean, which is run on Raijin and made possible through NCI's activity in optimising the code for ACCESS, Australia's climate and weather modelling system. This follows on from previous visualisations that have made use of the data outputs produced by high-resolution ocean models.

Meteorology

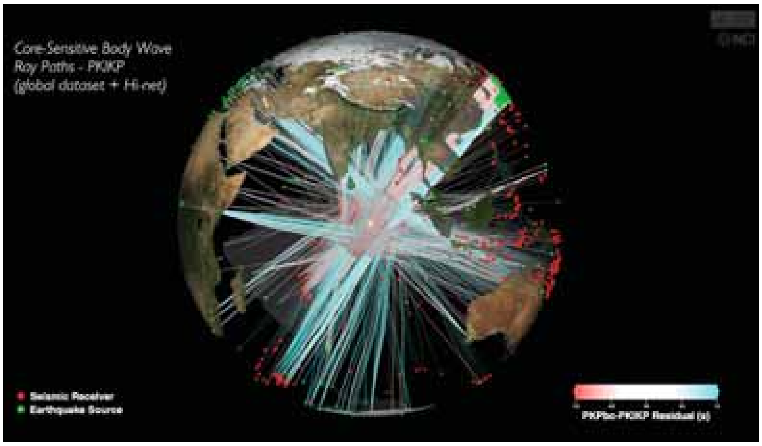
Working with a research version of the ACCESS weather and climate model, VizLab can bring simulations of extreme weather to life. In this case, the simulation shows a severe low pressure system on the east coast of Australia in April 2015, which produced extensive flooding and damage, as well as causing four deaths. White shading indicates clouds, while the vertical blue shafts show rainfall. The coloured-line segments indicate the near-surface wind direction. This visualisation is based on the work of the High Impact Weather Research and Development team at the Bureau of Meteorology, led by Dr Jeff Kepert and Dr Robert Fawcett.





Earth Sciences

Another area of visualisations is the Earth Sciences. This year, VizLab produced animations of seismic waves travelling through the earth, derived from the international IRIS and Hi-net seismic event datasets. The seismic event data is being used by The Australian National University's Dr Hrvoje Tkalčić to tomographically reconstruct the structure and rotational dynamics of the Earth's inner core. Images from the visualisations are destined to be published in a forthcoming book, and have already appeared in significant online coverage.

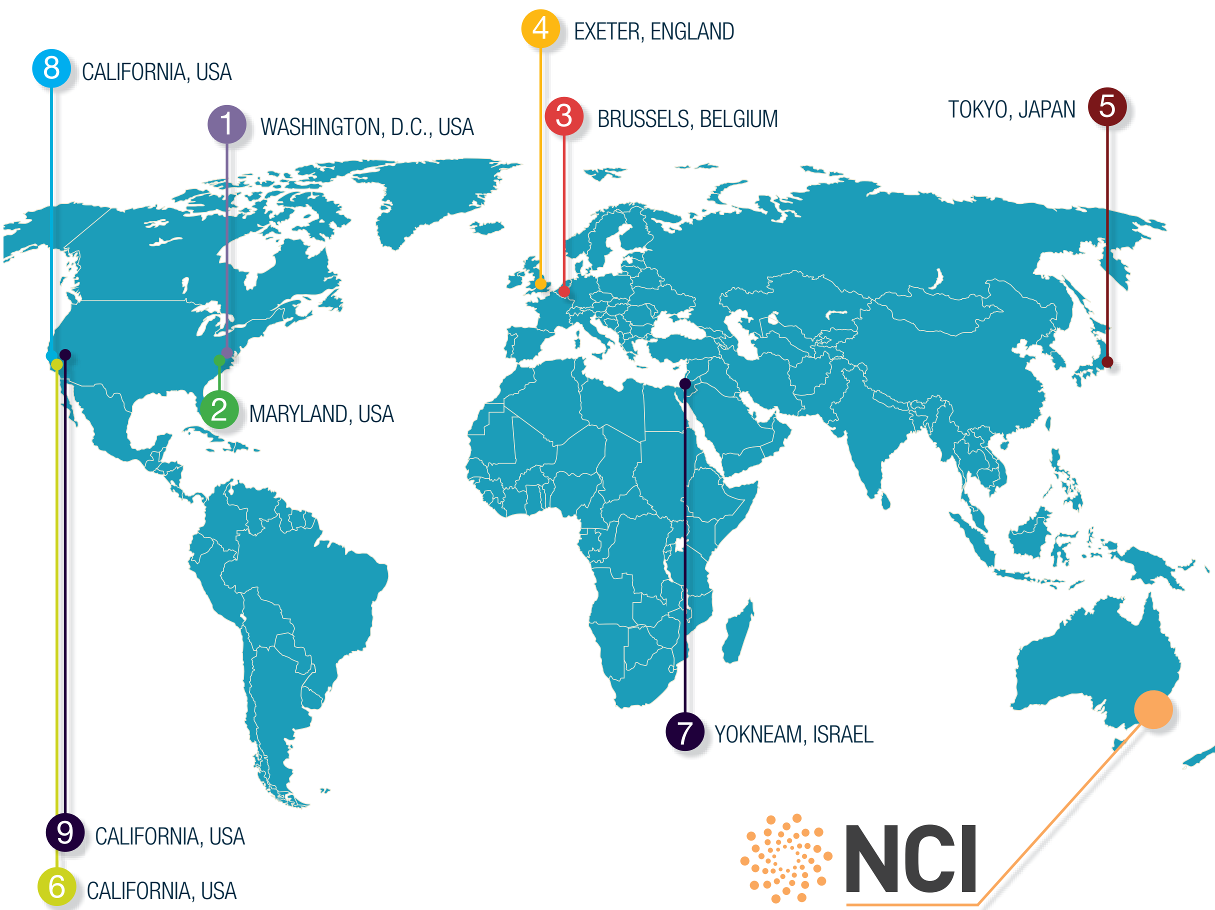


Collaboration

International Collaboration

FIGURE 2: NCI'S INTERNATIONAL COLLABORATORS: MAP OF THE WORLD

1. NASA
2. NOAA
3. European Commission
4. Met Office
5. FUJITSU
6. DataDirect NETWORKS
7. Mellanox TECHNOLOGIES
8. NVIDIA
9. intel



CASE STUDY 1: **VIRTUAL DESKTOP INFRASTRUCTURE**

Speeding up the research process with virtual desktops

A Normalised Difference Vegetation Index time series for mangroves in the Gulf of Carpentaria, from the Australian Geoscience Data Cube.

The Virtual Desktop Infrastructure (VDI) at NCI is simplifying the research process for many data reliant projects across the country. Researchers are able to use these new virtual desktops to access all of the data stored at NCI without having to transfer it to their personal computers. The VDI runs on NCI's private cloud Tenjin, part-funded by the National eResearch Collaboration Tools and Resources project (NeCTAR). By accessing the data remotely instead of needing to transfer it first, researchers are able to manipulate and analyse it in real time.

When Dr Leo Lymburner from the Australian Geoscience Data Cube went to the USA earlier this year to present his data to the United States Geological Survey, he could log in to the VDI and show them the data in the system. "We could do a live demo of our current Landsat satellite data holdings from the other side of the planet, which was pretty cool. They were able to see me log on through NCI and show them a live status of what our Landsat collections look like."

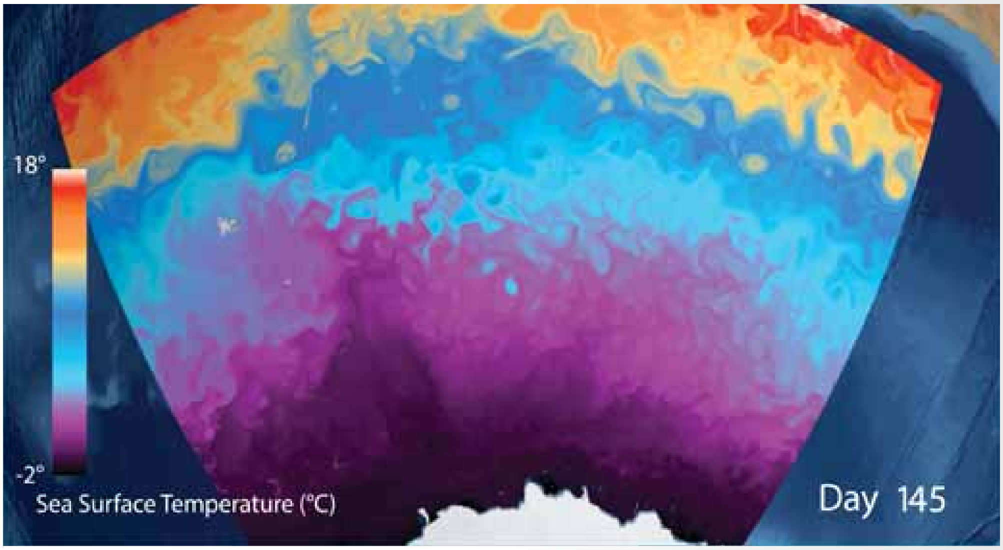
After logging in, researchers can use a standard desktop interface to interact with their data, instead of having to go through a layer of coding first. The interface provides them with many different software tools built in, reducing the need to install software on their local computer. It also provides a number of ways for users to create and share their own virtual environments and specialist packages. This opens up complex computational data analysis to a wide range of researchers, without the need for specialist programming skills.

For Dr Andy Hogg from The Australian National University and the ARC Centre of Excellence for Climate System Science, the big benefit in using a VDI is that he does not need to submit a compute job on NCI's main supercomputer, Raijin. Jobs computed on Raijin sit in a queue before being sent off for processing, which is fine for large jobs taking several hours and many computer cores, but is less ideal for interactive data analysis. "The climate and ocean models we run on Raijin produce huge amounts of data, which we then need to analyse. That's where the VDIs come in. The large memory capacity of the VDI nodes means that I can customise my analysis and try it out on my data in real time," he says.

For users with only a small amount of technical knowledge, the VDI provides a powerful working environment. It looks and feels like a standard computer desktop, but also provides incredibly performant software tools and hugely varied datasets, upgrading its functionality beyond any regular desktop. By eliminating the time and effort required for data transfers and local computation for each user, the VDIs bring the data analysis work of the scientists to the foreground. For this reason, Dr Lymburner says, "I'm absolutely thrilled with it; I use it on a daily basis. It's changed the way I do my work."

CASE STUDY 2: **OCEAN MODEL VISUALISATION**

Understanding the ocean with high resolution models



Eddies in the Southern Ocean, from a visualisation done by Dr Isabella Rosso from ANU and the team at NCI's VizLab.

The NCI's high-performance computing facilities are enabling researchers to model the oceans of the Southern Hemisphere at an unprecedented level of detail.

ARC Laureate Fellow, Professor Matthew England from the University of New South Wales and the ARC Centre of Excellence for Climate Systems Science, is working "to understand the role of ocean circulation in the global climate system." Much of his work focuses on the Southern Ocean, which profoundly affects both the global and Australian climate.

The Southern Ocean, which circles Antarctica, is particularly important to global climate, as the ice sheets and land ice stored on the continent are central to the question of sea-level rise in the coming decades. A slight warming of the Southern Ocean could precipitate melting of the ice shelves and marine grounded ice sheets, potentially leading to dangerous sea level rise.

Professor England has been running ocean circulation models at NCI and its predecessors for more than 25 years, and he says that each computer upgrade gives them new information.

"Every time we get an increase in computational power from NCI, we increase the resolution of our models and that increase in resolution reveals new physics we hadn't previously understood.

"We're actually making discoveries about ocean physics that we never knew about before the higher resolution came along," he says. Since satellites started being used for data-gathering, eddies in the Southern Ocean have become better understood. Now, computational modelling is allowing researchers to get below that scale and see new features affecting the bigger picture. Those features, says Professor England, "are also involved in important things like transferring heat around the ocean and impacting the large-scale circulation."

Professor England says that "computational leaps that are being made are really orders of magnitude advances every decade." When it comes to the benefits of using NCI, "it's an enabling technology, the more computational power we have, the more ocean physics we've discovered in the past and I'm sure that's going to be the same in the future."

CASE STUDY 3: **GENOMIC DATA MANAGEMENT**

The next step in Australian genetic medicine

Australian researchers from the Garvan Institute of Medical Research are developing a ground-breaking database of human genetic information using the unique facilities and expertise of the National Computational Infrastructure.

The Medical Genome Reference Bank (MGRB) being developed by the Garvan Institute and funded by the NSW Office for Health and Medical Research, will comprise more than 4,000 complete human genomes from disease-free seniors. The MGRB participants come from two contributing studies, 45 and Up (Sax Institute, Sydney), and the ASPirin in Reducing Events in the Elderly (ASPREE) clinical trial (Monash University, Melbourne). Participants are 70 years or older and free from cardiovascular disease, degenerative neurological disorders and a history of cancer.

Assembled in a huge genomic database, the fully anonymised information can then be queried by researchers and clinicians. “The power comes from the scale of the population in the study,” says Dr Andrew Stone, Genomics Programs Manager at Garvan. Compared to other genome reference banks, “we have an extensive healthy elderly population, with a well-curated clinical history, and therefore the MGRB will represent the cleanest negative control for any source of genomics-driven clinical experiment.”

As Garvan’s Chief of Informatics Dr Warren Kaplan puts it, a negative control means that if a doctor investigating a particular genetic variation “looked in the MGRB and not a single individual had it, that might be suggesting that that variation is damaging and quite rare.” The negative control indicates that any rare variants that they find in patients that do not occur in the data set are likely to play an important role in causing the disease.

Each completed genome takes up around 100 gigabytes, and reconstructing it from the sequenced data is not easy. “Considering the large amount of data and compute associated with such a massive project, it was immediately obvious to us that we would need to collaborate with NCI,” says Dr Stone.

“None of this would have been feasible”, Dr Kaplan says, “without the expertise that NCI has working with the infrastructure, the security, high-performance computing and cloud. It really is an amazing place and that’s why we’re so enthusiastic about this partnership.”

Once completed, the MGRB will be a major hub for researchers and clinicians from all over Australia. Dr Kaplan says the aim “is to have a single home for all genomic data so all researchers and all clinicians can come and apply their computational method against the data instead of moving the data around the world and to different organisations.”

CASE STUDY 4: **COPERNICUS REGIONAL DATA HUB**

NCI's innovative satellite data imagery hub

The Copernicus Regional Data Hub is a world-leading program to share imagery from the European Sentinel satellites with the Southeast Asian region. An agreement between the Australian Government (through Geoscience Australia) and the European Commission finalised in May 2016 is bringing all of the Sentinel images of our region to a data hub at NCI.

Covering countries from Myanmar to Samoa and much of the Antarctic Territories, the Hub provides up-to-date imagery for scientific, policy and land management uses impacting hundreds of millions of people. To transfer that imagery from its base in Germany to NCI, and then store it and present it to users in a powerful analysis environment brings together many elements of NCI's advanced computing services.

The Copernicus Data Hub Area of Interest, covering Southeast Asia and the Pacific. Image courtesy of Geoscience Australia.

The key elements are international networking to quickly and effectively transfer the data, storage for the data once it is here, high-performance computing to process the data to make it usable and cloud computing to serve the data to Data Hub users.

NCI's High-Performance Data Team Leader overseeing the Copernicus Data Hub Dr Joseph Antony says, "The level of expertise needed to bring the Data Hub to life means that NCI is uniquely placed to do this. No one has tried to transfer such large quantities of data over such a large distance before, so our expertise debugging the international data transfer networks is proving useful in bringing this project to fruition."

All of the data in the Hub is stored in multiple backed-up rapid-access libraries, and it can all be viewed and analysed through NCI's cloud computing platform, the Virtual Desktop Infrastructure (see Case Study 1). This has already led to important uses in Australia, such as recent work monitoring coral bleaching on the Great Barrier Reef and mapping floodwaters using the Sentinel satellites.

"The satellites produce images at such high resolution that coral reefs and individual trees can be seen. The post processing NCI partners and end users do to the data we receive turns it into usable images that many analysis applications can work on. We're excited to facilitate all of the research that will come from this data," says Dr Antony.

Enabling research for a wide variety of users is a key part of NCI's mission. The Copernicus Regional Data Hub is laying the foundations for years of data-intensive science to take place. The data management infrastructure implemented by NCI to support the program continues to demonstrate the quality that NCI users have come to rely on.

CASE STUDY 5: **CODE OPTIMISATION**

Improving weather forecasts through code improvements

Researchers from the Bureau of Meteorology (BoM), CSIRO and the ARC Centre of Excellence in Climate System Science (ARCCSS) are using NCI's high-performance computing facilities and expertise to develop the ACCESS (Australian Community Climate and Earth System Simulator) model used for improved daily weather forecasts all over the country, as well as for understanding the evolution of the world's climate system. While the BoM uses its own supercomputer to run the daily forecasts that go out to the public, advanced work to improve the performance of the model components, and analysis of the performance of future candidate systems are conducted at NCI.

Improvements in computing power make it possible to simulate the atmosphere, water and land much more reliably and accurately than ever before, but to make this a reality, the model's code needs to be improved as well. NCI leads a local team that optimises the next generation of ACCESS code across the different timescales – from numerical weather prediction, seasonal forecasts and climate – that are then used for the Bureau's operational needs. Tim Pugh, Supercomputer Programme Director at the Bureau, says, "The ACCESS optimisation team has a mix of staff from NCI, BoM, and CSIRO, who understand both the models and computational science."

One major improvement by the team reduced the model run time for the Bureau's operational forecast by 30 per cent. This means that the Bureau can now fit more model runs inside their set forecasting schedule, or make additional improvements to the model. That produces better outcomes for the Australian public, and a huge time and cost benefit to the Bureau. "Our weather applications share common code with the climate applications, so benefits in weather modelling translate into benefits in climate modelling. If CSIRO researchers are doing a 200-year simulation, saving 30 per cent of the elapsed time is enormous," says Mr Pugh.

Any performance and scalability improvements to the ACCESS model code are also regularly incorporated into the Unified Model (UM) of the UK Meteorological Office, on which ACCESS is based. Other weather and climate centres and research teams using the UM are then able to apply the improvements to their own modelling. For the operational ACCESS model that runs at the Bureau, the improvements are due to appear in the newest modelling systems to be released next year.

The UK Met Office UM collaboration partners are currently working to improve the convection scale modelling in ACCESS in higher resolution grids. Convection models, which describe the movements of air in the atmosphere, work best when the resolution gets to the order of hundreds of metres. Going from the 1.5-kilometre resolution that is currently in the next operational model down to hundreds of metres in key forecast areas of interest, such as populated areas, will involve a huge increase in computing power and more effective computing solutions built into the code.

Mr Pugh explains, "Whenever we have more computational power available, we can always improve the modelling through improved data assimilation, physics and dynamics. The NCI computational specialists have been doing a great job. We've seen a lot of very significant computational advancements in the software from their work, and each of those has resulted in a more efficient modelling system in our operations."

2

Our Users

Our Users

NCI aims to enable groundbreaking research by providing our users and partner organisations with all the tools and expertise they need to move science forward. The research goals of our users drive our developmental work.

We cater for the full research spectrum, from fundamental investigation to applied, strategic and industry-driven research—in every field of science and technology. This includes providing integrated computation and data services to three of the national science agencies – CSIRO, Geoscience Australia and the Bureau of Meteorology – as well as researchers from 35 of Australia's universities, six Australian Research Council Centres of Excellence, an Australian Research Council Transformation Hub and three industry partners.

Altogether, NCI provided support for over 4,000 users in 2015-16, with over 900 new users and 260 new projects coming on board during the year. One of the major new institutions to join the NCI collaboration this year was the Garvan Institute of Medical Research, the Southern Hemisphere's largest genome sequencing centre. The collaboration will mean that large-scale genomic data generated at Garvan can be archived in a cost-effective and secure manner, and then analysed by research partners using NCI's high-performance computing infrastructure.

Professor Carola Vinuesa from The Australian National University, profiled on page 45, is also involved in research into clinical uses of genetics. Her work adds to the diversity of disciplines that NCI supports, from astrophysics to materials science, molecular design, climate modelling and genomic analysis.

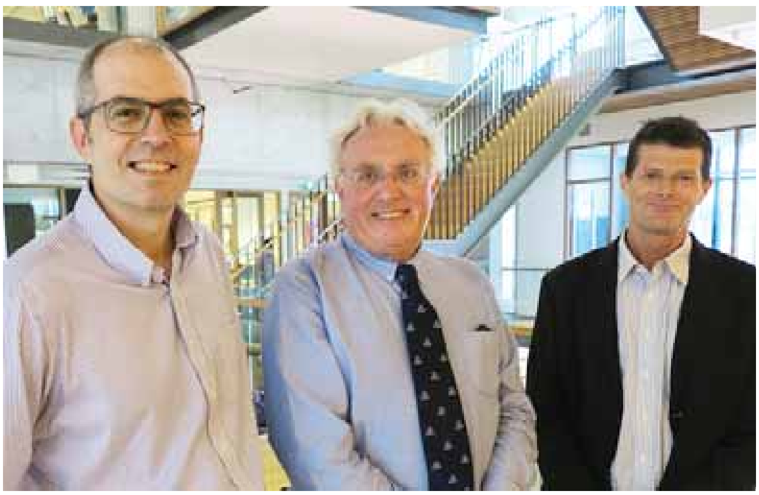
FIGURE 3: OUR USERS

New Partnerships in 2016

Five new institutions joined the NCI Collaboration in 2015-16, including three universities and one medical research institute. This brings the total number of universities making use of NCI's computational capabilities to 35. The University of Wollongong, the University of Technology Sydney, Macquarie University, and the Garvan Institute of Medical Research have all joined the collaboration to provide their researchers with access to Raijin and NCI's associated data storage and collection management infrastructure.

The addition of these four institutions to the NCI Collaboration demonstrates the continuing demand for the advanced computing services available at NCI. For example, the Garvan Institute of Medical Research is using NCI to analyse and securely store whole human genomes for their Medical Genome Reference Bank, a collection of genomes from disease-free Australian seniors, to be used for understanding the impact of specific genes on human health (see page 34). The field of genomics is a new and growing space in which NCI can contribute, and one that heralds profound results such as improved health and medical outcomes in the coming years (see below) and better management of the national health budget.

The increasing demand from all sections of the Australian research community for access to advanced computing services at NCI is a testament to the high-quality and reliability of the NCI systems and the breadth and depth of the expertise of its staff. NCI is constantly working to improve its services for users, facilitating the research work now being done in more places and covering more disciplines than ever before.



Dr Warren Kaplan (Garvan), Prof Lindsay Botten and Prof Chris Goodnow (Garvan)

Australian Genomic Health Alliance

To support the introduction of genomic medicine to healthcare in Australia, a new research organisation, the Australian Genomic Health Alliance (AGHA), has brought together 47 research bodies from around the country. NCI will play a key role within the AGHA as its data repository and hub for data access. In 2015, the AGHA was awarded a $25 million grant from the National Health and Medical Research Council's Targeted Call for Research into Preparing Australia for the Genomics Revolution in Healthcare. Over the course of the five-year grant, the AGHA will support genomics in both clinical and research environments, helping to realise the full potential of genomic medicine in routine healthcare. The Alliance will focus its work on rare diseases and cancer, using genomic medicine to improve diagnosis, treatment and clinical care.

Australian Genomics Health Alliance

New AAS Fellows

Two users of NCI have been announced as new Fellows of the Australian Academy of Science. Professors Susan Scott and Simon Foote, both from The Australian National University, have been recognised for groundbreaking scientific work during their careers.

Professor Susan Scott focuses on gravitational waves and general relativity, and is a member of the LIGO Scientific Collaboration that recently announced the first direct measurement of a gravitational wave.

This work has involved understanding background noise at a variety of detectors, including the Gravitational Wave Facility at ANU. Professor Scott was also part of the first Australian-led search for gravitational waves, looking at the neutron star Cassiopeia A in our galaxy.

She says "Both of these programs were important stepping stones in the final years leading to the first direct detection of gravitational waves on 14 September 2015."

Professor Simon Foote is the Director of the John Curtin School of Medical Research. He was involved in the first attempts to map the human genome and more recently has been looking at the genetics of diseases that affect isolated and less affluent populations, such as malaria.

He has found a new function for platelet cells in the blood, being part of the innate immune response to malaria. This work is now helping him and his team to design drugs that work inside the human host of the disease, meaning that the mosquito carriers cannot develop resistance to the treatment as easily.

His group has also used NCI to analyse whole genome sequences from Indigenous Australians, looking for the molecular basis of the kidney disease that is so common in their communities.

Since 2010, 37 NCI users have been named Fellows of the Australian Academy of Science. This equates to a quarter of all the new Fellows announced in that time, showing the significance of NCI to the Australian research community. The Fellows' research covers all fields of science, from human genetics to nanotechnology, astrophysics and climate modelling. NCI is proud to support their work, and congratulates them on their ongoing scientific achievements.

Australian Academy of Science

Access

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) access 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 NHMRC, and determining allocations through an independent, expert panel.

For 2016, NCI provided almost half of the total NCMAS resource allocation, nominally 75 million hours (15 per cent of the facility). Only one-third of the requested compute allocations for NCI were able to be granted, with 149 projects from institutions all over the country sharing the resources. 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 provides substantial resources for projects identified by the NCI Board as being of high impact or national strategic importance. The scheme currently supports a number of ARC Centres of Excellence (in climate 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 under the provisions of the NCI Collaboration Agreement or NCI's Commercial Service Contract.

If you represent a university, or research institution that would like to work with NCI, please contact **enquiries@nci.org.au**

TABLE 2: COMPUTE ALLOCATIONS BY RESEARCH INSTITUTION

		Stakeholder	Total allocation (kSU*)
MERIT ALLOCATION		National Computational Merit Allocation Scheme	97,112
	Flagship	ARC Centre of Excellence for Climate System Science	12,000
		ARC Centre of Excellence for All-sky Astrophysics	7,950
		Astronomy Australia (NCRIS)	2,000
		ARC Centre for Nanoscale BioPhotonics	800
		ARC Research Hub for Basin Geodynamics and Evolution of Sedimentary Systems	400
		Terrestrial Ecosystem Research Network (NCRIS)	80
PARTNER SHARE	Collaborators	CSIRO	117,230
		Australian Bureau of Meteorology	97,741
		The Australian National University	96,942
		Intersect Australia**	18,411
		Geoscience Australia	14,748
		Deakin University	696
		QCIF	2,778
		Antarctic Climate & Ecosystems Cooperative Research Centre / Australian Antarctic Division	7,494
		University of Technology Sydney	699
		Garvan Institute of Medical Research	3,154
		University of Wollongong	3,184
		RMIT University	13,233
	Universities supported by an ARC LIEF Grant	The Australian National University	see above
		University of New South Wales	8,384
		Monash University	8,059
		University of Adelaide	8,063
		University of Queensland	8,059
		University of Sydney	7,578
		Developmental Share (incl. commercial projects)	20,838
		Total	**560,052**

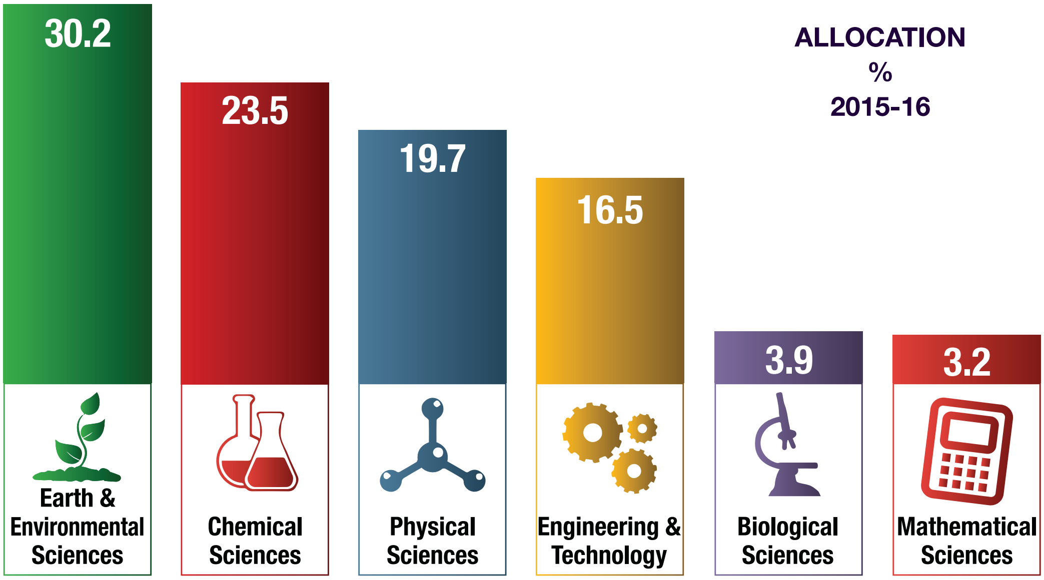
*kSU stands for kilo Service Unit, or a thousand Service Units. A Service Unit is equivalent to the work done by one compute core in one hour.

**Supported by an ARC LIEF Subscription Grant

TABLE 3: 2015 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
Antarctic Gateway Project	250	0%	0%	0%	0%	$-	$-	$-	$-
Australian National University	20,690	89%	12%	28%	94%	$8,875,026	$857,849	$921,282	$10,654,157
CSIRO	1,500	67%	0%	13%	80%	$-	$-	$691,358	$691,358
Curtin University of Technology	1,200	100%	0%	92%	100%	$820,133	$-	$690,613	$1,510,746
Deakin University	1,400	71%	0%	57%	71%	$344,000	$-	$400,000	$744,000
Flinders University	0	-	-	-	-	$-	$-	$1,428,571	$1,428,571
Griffith University	500	0%	0%	0%	0%	$-	$-	$-	$-
La Trobe University	250	100%	0%	100%	100%	$-	$-	$-	$-
Macquarie University	0	-	-	-	-	$-	$-	$-	$-
Monash University	13,420	97%	7%	42%	98%	$6,975,743	$730,861	$5,305,990	$13,012,594
Murdoch University	120	100%	0%	100%	100%	$-	$206,495	$1,200,000	$1,406,495
Queensland University of Technology	1,700	100%	0%	100%	100%	$-	$-	$-	$-
Royal Melbourne Institute of Technology	2,500	76%	0%	36%	92%	$4,527,714	$-	$1,424,806	$5,952,520
Swinburne University of Technology	600	100%	0%	0%	100%	$200,070	$-	$-	$200,070
University of Adelaide	1,490	67%	0%	16%	83%	$3,922,416	$-	$311,000	$4,233,416
University of Melbourne	7,720	92%	0%	64%	100%	$2,246,193	$77,707	$11,166,024	$13,489,924
University of Newcastle	850	100%	0%	0%	100%	$250,000	$-	$-	$250,000
University of NSW	19,000	89%	1%	86%	99%	$2,138,104	$2,556,468	$6,847,351	$11,541,923
University of Queensland	6,850	97%	45%	46%	100%	$1,415,581	$1,269,658	$11,989,616	$14,674,855
University of Sydney	8,300	99%	0%	75%	99%	$5,287,611	$-	$965,206	$6,252,817
University of Tasmania	3,800	87%	0%	33%	93%	$679,261	$-	$2,648,646	$3,327,907
University of Technology, Sydney	360	44%	0%	56%	100%	$242,600	$-	$107,250	$349,850
University of the Sunshine Coast	100	100%	0%	100%	100%	$-	$-	$50,000	$50,000
University of Western Australia	1,000	100%	0%	0%	100%	$131,740	$108,770	$415,891	$656,401
University of Western Sydney	100	100%	0%	0%	100%	$111,500	$-	$1,818,949	$1,930,449
University of Wollongong	1,560	62%	0%	84%	100%	$250,887	$-	$1,938,416	$2,189,303
UNSW Canberra	1,585	100%	0%	90%	100%	$235,500	$-	$5,147,760	$5,383,260
Total	**96,945**	**90%**	**7%**	**53%**	**96%**	**$38,654,078**	**$5,807,808**	**$55,468,729**	**$99,930,615**

FIGURE 4: MERIT ALLOCATION SCHEME COMPUTE ALLOCATION BY RESEARCH FIELD



"A lot of what we do would be impossible without resources like NCI" - **Dr Jenny Fisher, Atmospheric Chemistry researcher at the University of Wollongong**

"Working on dark matter is not only a large data problem, but also a complex physics problem, and you do need supercomputing to do this." - **Associate Professor Csaba Balasz, Theoretical Physicist at Monash University and the ARC Centre of Excellence for Particle Physics at the Terascale.**

"Working with NCI has allowed us to model longer and wider than we ever have before. Overall, we've been extremely pleased with the collaboration. It's had an absolutely amazing impact on the problems we've been able to solve." - **Simon Mortensen**, Group Executive for Port and Navigation for the DHI Group.

RESEARCH HIGHLIGHT

Treating autoimmune diseases using genome sequencing

Patients with autoimmune diseases will be receiving more personalised treatments, thanks to the work of scientists sequencing the human genome to look for uncommon variations.

"Autoimmune diseases are diseases like lupus, type 1 diabetes and rheumatoid arthritis, and we are more and more convinced that rare gene variants are going to be very informative in understanding these diseases," says Professor Carola Vinuesa from The Australian National University—an NHMRC Fellow and Director of the ANU Centre for Personalised Immunology, an NHMRC Centre of Research Excellence.

Autoimmune diseases are often quite rare and hard to diagnose, and the genetic causes have previously been almost impossible to discover. Thanks to recent improvements in genomic sequencing and analysis combined with the computational power of Raijin, Professor Vinuesa and her team are pinning down several distinct variations in the genome that could be at fault.

Bridging the gap between applied medicine and groundbreaking research, they are helping to identify better treatments for individual people living with chronic illness while learning about the genetic basis of certain diseases. This will make it possible to help similar cases more effectively in the future.

Professor Vinuesa says "even if a particular protein mutation might only be identified in one patient, there could be patients with the same disease or even related types of diseases that might have mutations in the same protein but at a different location. The discovery of a protein that's relevant for a disease will then illuminate the disease of many other patients."

Without NCI, says Professor Vinuesa, "it would be impossible to deal with whole genomes. NCI has been extremely helpful as we needed to increase our usage of their computing capacity and storage. I admire the way they are thinking big in terms of dealing with large datasets and doing things that could have a nationwide application."

For now, this team is one of the few around the world using whole genome sequencing to look into the genetic causes of complex immune diseases. "We now have an amazing database that can incorporate all of the variants of every individual we have sequenced into a single place, so we can interrogate it for variants that we have found in all of our patients."

They have already made significant progress, but Professor Vinuesa and her team are just getting started. "If we are interested in a variant we can immediately ask, 'Has this been found in any other patient?' In the end that's what we want, to try and find tailored treatments for patients with immune diseases."

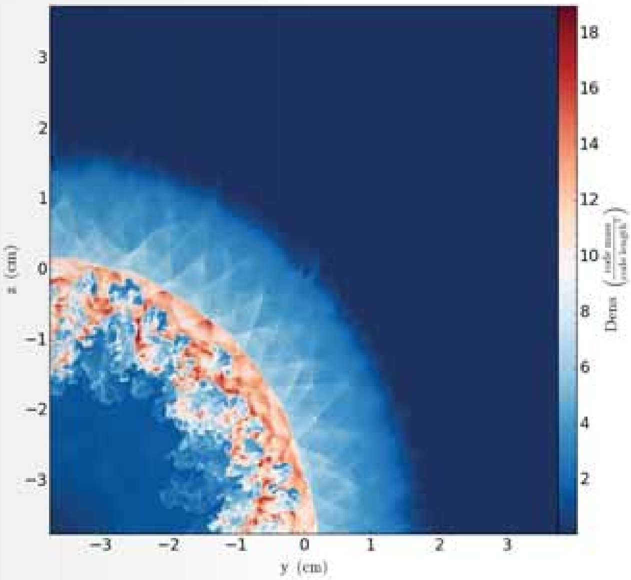
Australian National University

RESEARCH HIGHLIGHT

Modelling nuclear fusion

Researchers from the University of Sydney are modelling a form of nuclear fusion to understand how it can one day be used as a source of energy.

"Inertial Confinement Fusion provides a potential pathway towards utilisation of fusion power as an energy source," says Dr Ben Thornber. This method of producing fusion involves using lasers to heat a small capsule of the Hydrogen isotopes Deuterium and Tritium to the required pressure and temperature for it to implode and fuse the atoms into Helium.



A still from an animation showing one stage of the nuclear fusion modelling, from Dr Thornber and Dr Flaig.

Fusing two lighter atoms into a heavier one releases huge amounts of energy, but the pressure and temperature required to get there are similar to those found in the centre of the sun. Working with such extreme conditions makes physical experiments very difficult, so simulations on supercomputers are used to assist the experimental research being performed around the world.

Dr Ben Thornber, along with Dr Markus Flaig, is using Raijin to model the interaction between the various layers of the capsule as they get compressed in the experiment. "The NCI facility is critical to our research. We use up to 16,000 cores on Raijin to generate our results," says Dr Thornber.

Often, mixing between the capsule's layers stops the core from getting hot enough to fuse. "Our research aims to understand how the instabilities develop and transition to turbulence, and thus inform the future design of the fuel capsules."

"We run computations with up to 16 billion points in total," says Dr Flaig. "This enables us to develop simplified models which substantially improves our understanding of mixing and the subsequent impact on the fusion process."

Even with so many points, it is not always easy to include all the physical details. The challenge, says Dr Thornber, "is to define a case which includes all of the key physics involved in the real problem, but that we can solve on today's supercomputers. This involves a judicious simplification of the problem to its core essence."

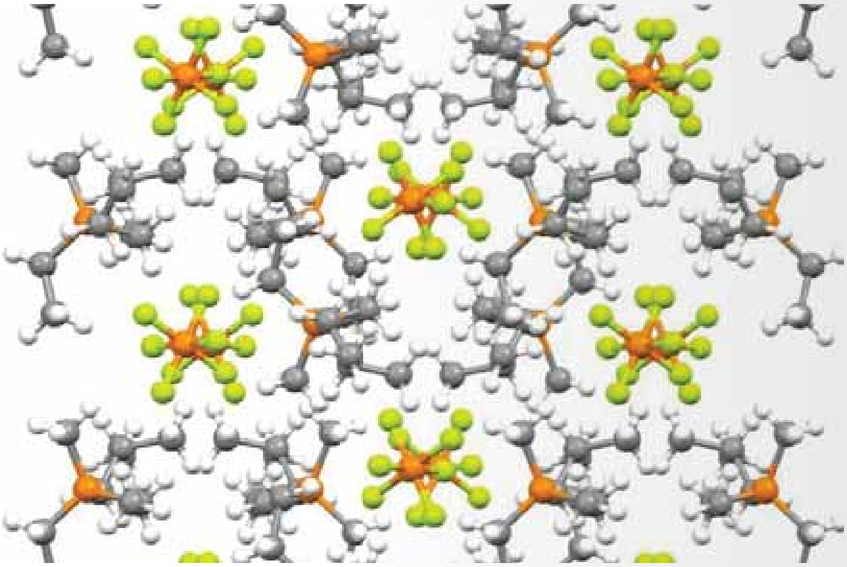
Powering our homes with nuclear fusion power plants is still decades away, but work like this helps us understand the steps to take while learning about nuclear physics and fluid dynamics in the process.

INTERSECT

THE UNIVERSITY OF SYDNEY

RESEARCH HIGHLIGHT

New materials for energy storage



One of the organic ionic plastic crystals that Professor Forsyth and her team are looking into for their energy storage potential.

Energy storage and energy generation technology are improving, thanks to the work of Laureate Fellow Professor Maria Forsyth from Deakin University and her group from the ARC Centre of Excellence for Electromaterials Science.

"What we do in my group is look at electric conductivity in ionic materials. This ionic conductivity is important for optimising how well a battery will work or how well a fuel cell will work in different devices," she says.

The ionic materials that the group is looking at include solids called organic ionic plastic crystals. "The reason we call them that is, despite being crystalline, they still have a high degree of dynamics, both in terms of rotation or reorientation of the ions in the lattice sites but more importantly in terms of diffusion of ions within the lattice."

The fact that the ions are able to diffuse through the lattice means that they are able to carry an electrical current. This makes the plastic crystals ideal for use in batteries, but more research needs to be done to understand exactly how they work and which materials are most effective.

"What we've been doing is using simulation to understand how the dynamics occur and how the structure can affect those dynamics," says Professor Forsyth, who accessed compute time on Raijin through the National Computational Merit Allocation Scheme.

"What the molecular dynamics modelling really helped us understand is that in the crystal itself there may be areas of high order and areas of low order. The ions in that low order region are more dynamic, they contribute more to the conductivity."

The team is focused on increasing their understanding of ionic crystals and liquids to achieve their goal of designing better battery materials. Gradually, they are starting to look at being able to predict new ionic materials that would suit their purposes.

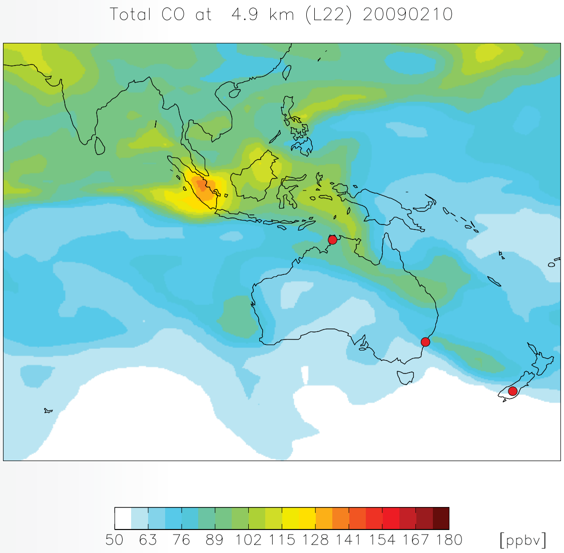
Professor Forsyth says, "That's where I want to see us go, what ion or what material should we be trying to synthesise? More rational design of electrolyte materials and electrolyte-electrode interfaces is the next big challenge."

ARC Centre of Excellence for Electromaterials Science

DEAKIN Worldly

RESEARCH HIGHLIGHT

Tracking chemical processes in the atmosphere



Carbon monoxide simulated by the GEOS-Chem model, from Dr Fisher's research.

Dr Jenny Fisher and colleagues from the University of Wollongong Centre for Atmospheric Chemistry are using computer modelling to understand the chemical processes happening in the atmosphere. These processes drive the dispersion of air pollution, greenhouse gases and airborne particles from cities in Australia and around the world.

Dr Fisher uses meteorological models as the basis of her work. She says that "we take the wind and the temperature and all the stuff that comes out of weather models and use that as inputs to look at what's going on with the chemistry in the atmosphere."

The NCI supercomputer is used in Dr Fisher's work because it speeds up the modelling stages of the research. "Chemistry is very computationally expensive to do in the atmosphere," she says, "I work with chemistry-only models, but integrated chemistry climate models where you actually take into account climate impacts from something like ozone, while also accounting for the effect of the climate on how much ozone is formed, are much more computationally intensive than the climate on its own."

Dr Fisher says that "by using these separate detailed atmospheric chemistry models, we can work out which parts of the chemistry have the biggest impacts and are important to include within broader climate models."

This modelling work can help improve the way researchers understand air pollution in and around cities, and feeds in to the atmospheric branch of climate change studies. Comparing the model output to the readings from different kinds of instruments also allows a better understanding of how all the measurements work together.

The idea "that the choices made in one place can have an impact very far away, that the pollution can be transported really big distances and have pretty big ecological impacts somewhere else" is what originally attracted Dr Fisher to the field of air pollution and atmospheric chemistry. Now she is using supercomputers and satellites to advance her research.

"A lot of what we do would be impossible without resources like NCI," says Dr Jenny Fisher.

Ongoing projects are now aiming to combine long-term measurements with the modelling, making full use of the data, the satellite instruments and the supercomputer facility.

UNIVERSITY OF WOLLONGONG AUSTRALIA

RESEARCH HIGHLIGHT

Studying biomolecules with atomic precision

Researchers from the University of Queensland are using NCI to study the behaviour of biomolecules such as proteins and cell membranes with atomic precision.

Of particular interest is the way these biomolecules interact. Understanding the way that proteins and other molecules bind to cell membranes is challenging because of the variety and complexity of the processes involved.

ARC DORA Fellow Professor Alan Mark explains that "Experimentally you can't observe these systems in atomic detail. The only way to really understand how these molecules move and interact is by calculation." The team uses molecular dynamics simulations to model up to half a million atoms interacting together.

The erythropoietin hormone in red, bound between two receptor molecules in grey, themselves embedded in an organic membrane. Alan Mark's team is trying to understand the coupling taking place in the region shown as small spheres.

Using what they know from experimental data, the team can design and test the simulations to be as accurate as possible. Once the simulations succeed in predicting experimental results, they can be used to investigate novel problems. "If we can predict the properties of systems we know well, we can not only trust that the simulations are behaving correctly but we can then look at other things that aren't observable experimentally," says Professor Mark.

The movement of molecules as they interact, such as the rotation of a hormone receptor following the binding of a hormone to turn on a cell, is impossible to visualise directly. These computational methods allow the researchers to discover exactly what is going on in those systems.

The long-term goal of the research is to model cell self-assembly. When cells form, all of the proteins and lipids inside them assemble spontaneously. "The membrane that forms the outside of the cell, together with its many components, self-assembles into a vast array of structures and functional complexes purely based on the underlying thermodynamics and the interactions between the atoms," says Professor Mark.

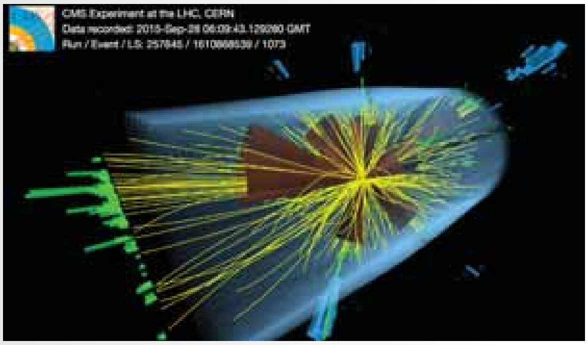
"We've been trying for a long time to understand the true complexity of the biological membranes," he says. Modelling individual components of these complex systems is already providing new information on key elements controlling cell behaviour.

> "The more accurately we can simulate these systems, the better we will be able to understand life at an atomic level"
> - **Professor Mark,** University of Queensland.

THE UNIVERSITY OF QUEENSLAND AUSTRALIA

RESEARCH HIGHLIGHT

Advancing our knowledge of dark matter particles



The products of a nuclear collision captured by the Large Hadron Collider, where research into dark matter is being conducted.

Associate Professor Csaba Balazs from the ARC Centre of Excellence for Particle Physics at the Terascale (CoEPP) and Monash University is using the NCI supercomputer to advance our knowledge of dark matter particles.

Dark matter is a previously unknown kind of fundamental matter that makes up around 25 per cent of the universe but is impossible to see. It helps explain the unexpectedly high gravitational cohesion measured within galaxies but, despite knowing that it exists, we still do not know much about its microscopic properties.

Computer simulations are used to understand how dark matter interacts with ordinary matter by modelling the microscopic theories of dark matter. By bringing experimental data from satellites and underground detectors to these dark matter models, Professor Balazs and his team can learn about dark matter in new ways.

"We take the experimental results and impose them as constraints on the theoretical models. What happens is that in the theoretical models we find correlations between experiments. Underground detectors exclude some theoretical parameter regions. Same with satellites, for different regions. And so we can go back to the experimentalists and guide them towards areas that are not excluded yet."

Because there are hundreds of models that aim to describe dark matter, and the correct model is unknown, researchers are not sure if there are multiple dark matter particles or just one. By gradually excluding different parameter regions of various models, such as very heavy or very light particle masses based on the combined experimental data, the groups can hone in on the physical properties of dark matter particles.

Professor Balazs suggests that many models based on the supersymmetry theory of particle physics naturally predict a single dark matter particle. "Most supersymmetric models predict a non-decaying massive particle. This particle has no electric charge, it doesn't interact strongly, only gravitationally and weakly with the rest of the world. It's a perfect dark matter candidate."

Dealing with the complex theories that describe dark matter involves many parameters spanning dozens of dimensions. When it comes to running the more than one million lines of code more than one million times, the calculation is impossible for any standard computer to deal with, which is where the NCI comes in.

"Without computers like NCI we couldn't do anything. NCI is very important, it's fuelling the whole work that we are doing," says Professor Balazs.

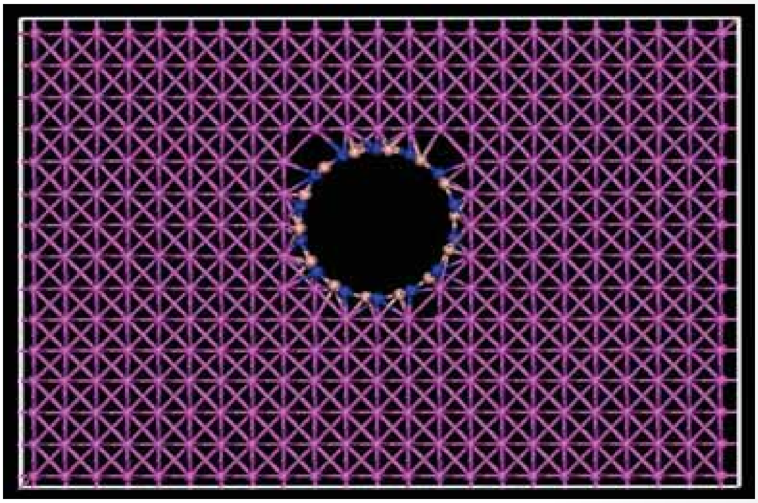
"Working on dark matter is not only a large data problem, but also a complex physics problem, and you do need supercomputing to do this."

CoEPP
ARC Centre of Excellence for Particle Physics at the Terascale

MONASH University

RESEARCH HIGHLIGHT

Nanomaterials designed for space travel



A boron nitride nanotube in an aluminium matrix, modelled by Dr Rohmann at the University of Queensland.

Researchers are using NCI's supercomputing facility to investigate the interaction of nanomaterials with metals that could be used in future space travel. Postdoctoral Research Fellow Dr Christoph Rohmann from the Australian Institute for Bioengineering and Nanotechnology at the University of Queensland is researching new composite materials: metals that are reinforced with boron nitride nanotubes (BNNTs).

Dr Rohmann says that BNNTs have remarkable properties. These include "a heat and oxidation resistance exceeding 700 ^{0}C, a molecular structure 100 times stronger than common steel at a fraction of the weight, and a radiation shielding 1,000 times that of lead."

He is working with scientists from NASA to produce these new materials and test them for use in future space travel. "A composite that offers a reduction in weight, increased strength and protection from radiation will further push the boundaries of space exploration and manned missions," he says.

NCI plays a crucial role in the research process by providing the resources necessary to model these large systems. Supported by the Queensland Cyber Infrastructure Foundation, Dr Rohmann says that his research uses NCI to "model the integration of metal and BNNTs, which represent extremely large systems that need a significant amount of computing time and memory. Therefore we are grateful for the computing resources NCI provides."

Working with scientists at NASA provides Dr Rohmann with the experimental data and insight required to accurately model the composites. He can compare his computational results with the experiments conducted at NASA and make predictions of experimental outcomes. For example, the strength of the binding between BNNTs and metal in the structure obtained from the calculations allows for a good approximation of what to expect in the experiments.

A strong binding will likely result in the disintegration of the BNNTs, causing the formation of unwanted by-products which are often brittle and therefore would weaken the new material. The results from the calculations help NASA scientists in their choice of metal, showing the value of modelling to the experimental work they do. As Dr Rohmann says, "the NCI supercomputer is of significant importance to this project."

qcif THE UNIVERSITY OF QUEENSLAND AUSTRALIA

RESEARCH HIGHLIGHT

Developing the latest climate model

The National Computational Infrastructure is a key part of Australia's climate modelling efforts. The CSIRO is using the supercomputing capability available at NCI to lead the development of the ACCESS climate model, in conjunction with the BoM and the ARC Centre of Excellence for Climate System Science (ARCCSS).

ACCESS, the Australian Community Climate and Earth-System Simulator, couples together models of the atmosphere, oceans, land and sea ice to understand the behaviour of the Earth system as a whole. Recently, the team at CSIRO has added a carbon cycle model to ACCESS, producing an even more realistic representation of the interactions taking place within the climate system worldwide.

Running these models is a hugely data intensive process that cannot happen anywhere other than at NCI. By providing highly parallel computing infrastructure to the researchers, NCI makes this kind of large scale modelling possible. Lead Chief Investigator Dr Tony Hirst* says that "All the ACCESS climate modelling is done on NCI."

The ACCESS model gives Australia an important role in international climate change planning.

CSIRO and the ARCCSS produced simulations for the Intergovernmental Panel on Climate Change's Fifth Assessment Report in 2013, all of which were done on NCI. "We did 3700 years of simulation in total. It's important to do several simulations for each of the CO_2 emissions scenarios in order to separate the underlying trend from the variability."

The data from the simulations has now been connected to a global network of Earth data, the Earth System Grid Federation, through a dedicated NCI node. Researchers around the world can easily get access to the data and download the model output. This data has now been used in around 250 scientific papers in the last two years alone.

The partnership between NCI and CSIRO remains vital to Australia's climate modelling capability. As Dr Hirst says, "We see ourselves as doing all our work on NCI going forward. Without exception, there is no other facility in Australia that allows us to work in the climate space in this way."

*Dr Tony Hirst has been working at the Bureau of Meteorology since July.

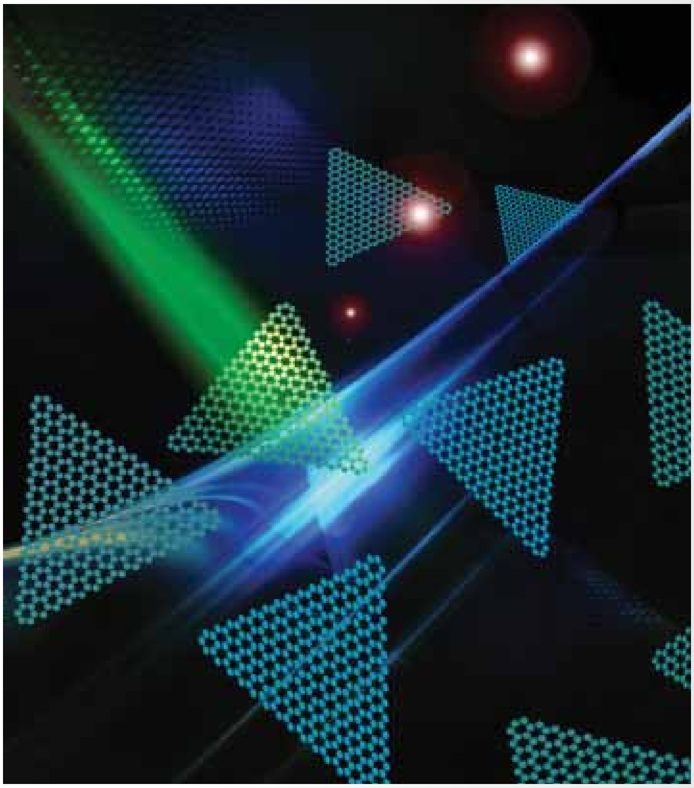
RESEARCH HIGHLIGHT

Exploring the physics of two-dimensional materials

Researchers from the University of Technology Sydney (UTS) are investigating the properties of a wide variety of two-dimensional materials. These materials, made of one atom thick sheets, have radically different properties to their more common bulk counterparts.

Professor Mike Ford is trying to understand the electronic properties of some of these materials using computer simulations on NCI's supercomputer.

> "These are very large compute intensive calculations that would not be possible without access to the NCI high-performance computing facilities."
> - **Professor Ford,** University of Technology Sydney



Artist's impression of quantum emission from 2D hexagonal boron-nitride, from the journal Nature Nanotechnology.

Producing and researching two-dimensional materials experimentally is very difficult, so Professor Ford uses NCI to simulate the materials first, allowing him to find the most useful ones for further study. "You want to do the calculations to identify where the interesting materials are. And then you can try and make them.

"Because they're so thin, they're a good building block for new devices, such as all-optical chips," says Professor Ford. The potential for the use of two-dimensional materials in industry and manufacturing is huge, but most researchers are still exploring the fundamental characteristics that all of the many different materials display.

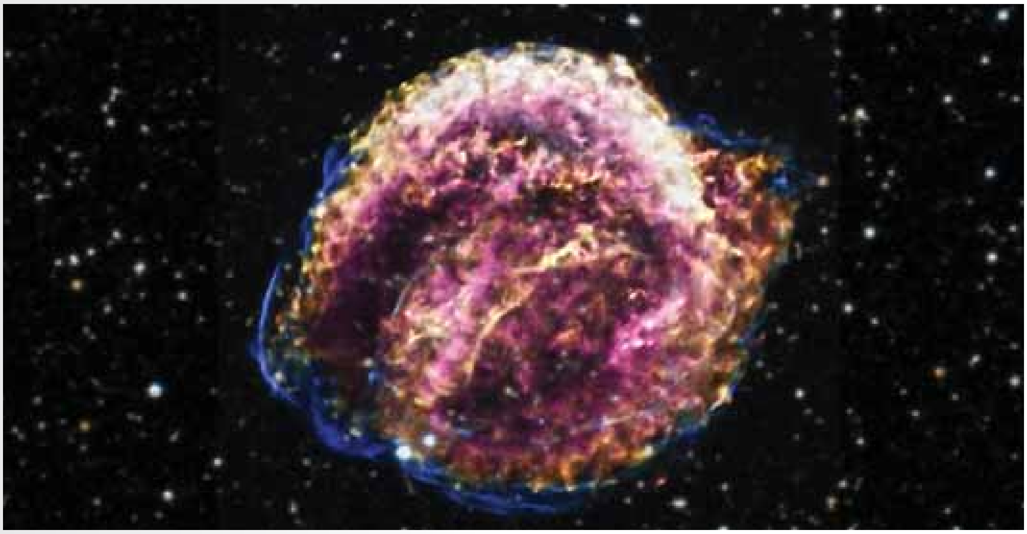
Professor Ford and co-workers are currently interested in the physics underlying quantum emission from defects in two-dimensional materials and their application in optical devices.

In the coming years, as UTS increases its share of NCI compute time, Professor Ford is looking to start simulating "hybrid materials, they have really interesting properties." Hybrid materials, where sheets of different two-dimensional materials are layered on top of one another, can have a wide range of properties with many uses. The challenge lies in calculating how the different sheets interact with each other to produce the final desired material properties.

UTS
UNIVERSITY OF TECHNOLOGY, SYDNEY

RESEARCH HIGHLIGHT

A simulation of supernova formation



The Kepler supernova, a type Ia supernova, captured by NASA's Chandra X-Ray Observatory.

Working as part of the ARC Centre of Excellence for All-Sky Astrophysics (CAASTRO), scientists from The Australian National University (ANU) are learning about the formation of a certain type of supernova by modelling its explosions on Raijin.

Type Ia supernovae remain a mystery to astrophysics researchers, Dr Ivo Seitenzahl says. "The details of what kind of stellar systems give rise to these supernovae are still unknown." Researchers do know that white dwarf stars are involved, but the details of how they come together to form Type Ia supernovae remain a mystery.

The research team, made up of scientists from ANU as well as Queen's University Belfast, are using theory to simulate what this supernova formation might be like. "We take a theoretically proposed model and follow the dynamics of the thermonuclear explosion. In three dimensions we need a supercomputer," says Dr Seitenzahl. "NCI supplies us with the computational resources, storage, and a very reliable architecture to let us perform the calculations needed for our research."

Based on the models, they can predict the quantities and locations of hundreds of chemical elements produced in the supernova explosion, as well as other observables such as light curves and gravitational waves. "We then aim to compare the predictions of our model with observations of real supernovae. In doing so we make progress in our quest to find the elusive progenitors of Type Ia supernovae," explains Dr Seitenzahl

The models looking at the light coming from supernovae explosions are the hardest to run on regular computers. "The three-dimensional calculations that compute the light escaping from our explosion models are even more computationally demanding, as we need to follow 200 million particles to adequately sample all relevant interactions and obtain sufficient signal for all directions," says Dr Seitenzahl.

The findings of this modelling are challenging some previous ideas about how these supernovae are formed. They are also suggesting new ways that supernovae in neighbouring galaxies could be measured in the future, for example by using gravitational wave observatories in space.

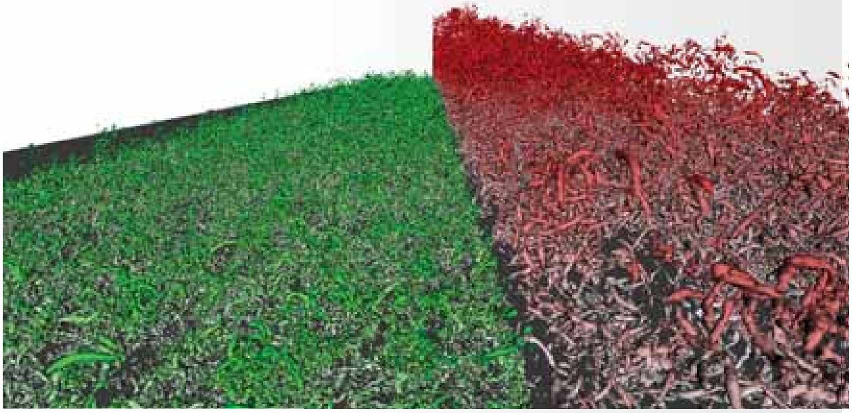
CAASTRO ALL-SKY ASTROPHYSICS

Australian National University

RESEARCH HIGHLIGHT

Simulations of fluid flow turbulence over surfaces

Researchers from Monash University are simulating turbulent fluid flows, which affect airplane aerodynamics and design. The research uses direct numerical simulations (DNS) of turbulent flows to understand more about what is happening in the thin layer of air or water close to a solid surface, known as the turbulent boundary layer, which is responsible for drag on airplanes, cars, trains and ships.



Instantaneous vortex structures of contiguous boundary layers, from one of Professor Soria's simulations.

ARC DORA Fellow Professor Julio Soria explains that "We're simulating every aspect of the turbulent flow, from the large scales right down to the smallest scales where the energy is being dissipated into internal energy. Every detail is being computed." The simulation process allows them to measure variables that are very hard to measure experimentally.

Things like pressure and vorticity are almost impossible to measure at the required precision with current instruments on a physical model, but "in a direct numerical simulation, we can measure all these and more at all the relevant scales, we actually get all of that information."

This is because DNS provides a perfect representation of fluid physics, one where the data at every point is measurable. Every physical feature can be accurately reproduced digitally, right down to things like the fine scale structure of turbulence, and where energy is dissipated. In this way, mechanisms to reduce drag can be investigated.

The NCI supercomputer has enabled the team to run the largest DNS in the world for an adverse pressure gradient turbulent boundary layer. Using 25 million CPU hours at NCI and the Pawsey Supercomputing Centre in Western Australia to run these simulations and collect data fields for statistical and structural analysis, the computer needs to keep track of over 30 billion individual points throughout the calculation. As Professor Soria says, "We are simulating every aspect of a turbulent flow, because we have to know every detail in order to understand the mystery of turbulence."

Professor Soria runs DNS at NCI and physical experiments in wind and water tunnels, each one helping to inform the limitations of the other. Understanding the boundary conditions to impose on the equations, for example, is one of those limitations. "We've got to cut the simulation off somewhere in space, where you cut it off is quite important, and the experiment guides us in this aspect."

The team at Monash is looking forward to continuing this work into the future. "As the computers get more powerful, this allows us to push the resolution even higher, it also allows us to bring in real geometric complexity." For now, they are focusing on fully understanding the details of the physics involved in turbulent flows, because "this gives us a lot more insight into the dials that we need to turn in order to manipulate the flow to our desire and control it."

MONASH University

RESEARCH HIGHLIGHT

The ice sheets and ice shelves of the Antarctic Ocean

Scientists from the Antarctic Climate & Ecosystems Cooperative Research Centre (ACE CRC) are modelling the evolution of ice sheets and ice shelves in Antarctic waters. In partnership with the University of Tasmania, the Antarctic Gateway Partnership and the Australian Antarctic Division, they are looking to better understand the processes taking place in the Southern Ocean.

A snapshot from a particle model of the Totten Glacier ice shelf (from below), showing basal crevasse formation. Image by Sue Cook (ACE CRC, UTAS).

Dr Ben Galton-Fenzi says that "a large part of the uncertainty in future projections of climate change is around exactly how Antarctica will interact with the Earth system. Our efforts are designed to understand how Antarctica will respond to change."

His group are working on models of ice loss through calving and melting of ice sheets, trying to understand the different factors involved on land and under the surface. By using experimental data to guide the design of their modelling, they can run more realistic models and achieve more accurate results than in the past.

Accurate results also come from running various models throughout the research process. Idealised models are used in the development and testing stage, before realistic models are used for things such as sea level rise predictions and for comparison against observations. For dealing with this variety of models, Dr Galton-Fenzi says, "NCI is a fantastic resource." Covering the entire Antarctic continent and surrounding ocean, one model with over 35 million elements produces more than 100 terabytes of data every time it is run.

This data lets the researchers understand the ice-ocean interactions of the region, while also providing information about which areas would be best to target for future field placement of instruments. In this way, the modelling and the experimental data work together to complement each other's strengths.

While the models they use are similar to others from around the world, the researchers have had to adjust them to suit their purposes. "We've spent a significant amount of time adapting the models to be applicable to the specific problem that we have. These models haven't been designed to be applied to high latitude regions," says Dr Galton-Fenzi.

He says that in the coming years, "we are moving towards wanting to do more coupled modelling. We realise that what we really need to answer our questions is a coupled model with atmosphere, ocean, sea ice, ice sheets and solid earth all together."

RESEARCH HIGHLIGHT

Investigating the properties of quantum particles

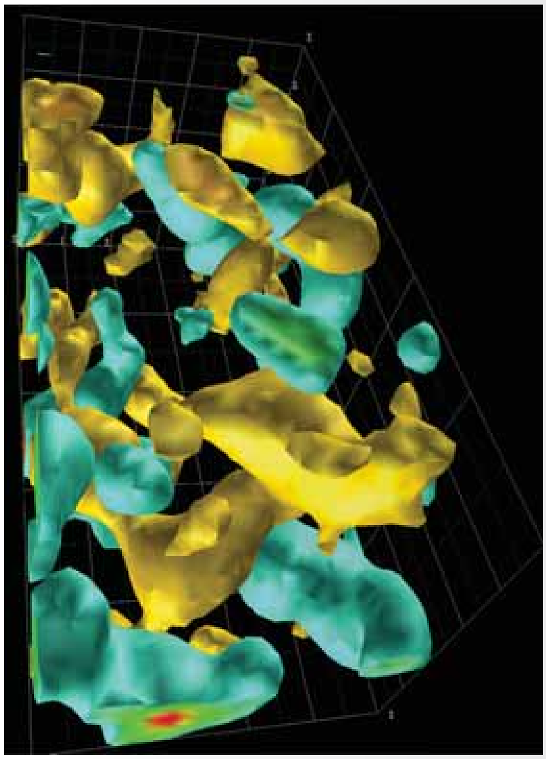
Scientists from the University of Adelaide have been modelling the behaviour of quantum particles using Raijin's advanced computing capabilities.

ARC Future Fellow Dr James Zanotti says, "Our group has been a heavy user of the NCI facilities, and without them our group in Adelaide would have really struggled to exist. The fact that we have access to NCI means that our measurements are able to have an impact internationally. "

He has been trying to understand protons and their quantum properties for more than 15 years using the theory of Quantum Chromodynamics (QCD). One of the problems he is trying to understand is the theoretical basis for why neutrons are heavier than protons, even though they share almost all of the same properties.

To look into this question, Dr Zanotti and his team use a computer lattice that is designed to have the exact quantum properties they are interested in, including contributions from not only QCD, but also QED (or Quantum Electrodynamics). Their current lattice is a cube-shaped grid, 32 units high, long and wide, and covers a period of about 20 yoctoseconds in 64 time steps. One yoctosecond is a trillionth of a trillionth of a second, a 1 preceded by 23 zeros after the decimal point.

To understand more about the proton, they need to mathematically add various quantum background variables and the proton itself into the lattice. After this, they end up with a system of about 200 million distinct numbers that represent the entire lattice and everything inside it. Finally, they need to solve around two million simultaneous equations in order to calculate the behaviour of the proton over the 20 yoctoseconds of the lattice simulation.



Gluon and photon field fluctuations in the lattice designed by Dr James Zanotti, Mr Joshua Charvetto and Professor Derek Leinweber at the University of Adelaide.

"Because this is a quantum field you can't just take a single snapshot of it, you need to look at the order of a thousand snapshots. So we need to generate the 200 million numbers a couple of thousand times," explains Dr Zanotti.

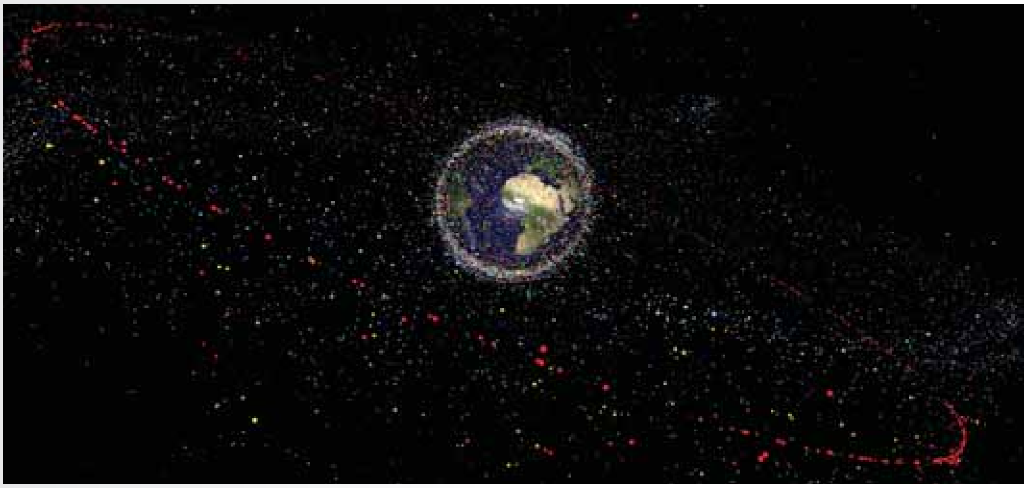
That much data to compute at once makes these calculations impossible to do without sophisticated technology.

> "QCD is a very complicated theory, you're not able to solve it analytically on a piece of paper, and you can only get close to achieving this feat by performing large-scale calculations on a supercomputer." **- Dr Zanotti,** University of Adelaide.

THE UNIVERSITY of ADELAIDE

RESEARCH HIGHLIGHT

Space junk tracking backed by supercomputer power



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

The NCI supercomputer is being used by RMIT researchers in a major space, atmosphere and satellite navigation research centre. The Satellite Positioning for Atmosphere, Climate and Environment (SPACE) Research Centre uses high-performance computing to work through large quantities of data from satellites and ground observation stations.

The centre focuses on a variety of atmosphere-based projects, including using radio waves from satellites to accurately describe the structure of the atmosphere. These real-time findings have already provided a 10-hour improvement in predictability and reliability for Bureau of Meteorology weather forecasts.

Another project that the SPACE Research Centre is working on is about monitoring space junk. Professor Kefei Zhang, Director of the SPACE Research Centre, says "Everything nowadays relies on space technologies. The impact of space junk is that it can disable all that functionality such as the Internet, weather forecasting and disaster monitoring.

"There's too much space junk, over 100 million pieces bigger than 1 millimetre endangering the operation of satellites. If we don't do anything, satellites in space will not be usable in the next 30 to 40 years," says Professor Zhang.

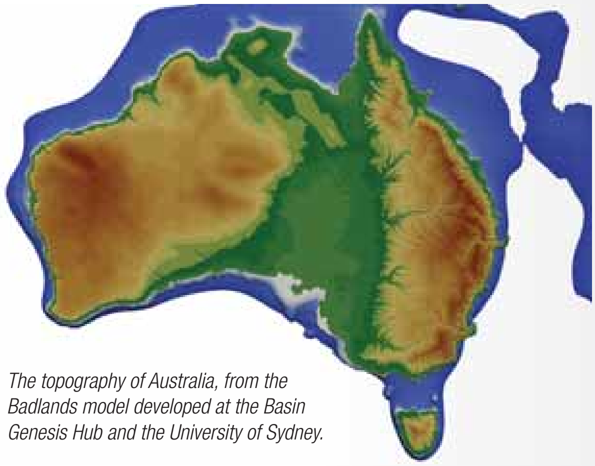
Keeping track of historical weather and satellite records and combining them with current data requires the SPACE Research Centre to use the NCI to store and process the data. Following methods testing and development on smaller local computers, the researchers move their projects to NCI to compute. "We really need, firstly the parallel system to speed the research up, secondly the capacity for storage, and thirdly the memory to run the software," explains Professor Zhang.

"A huge amount of data is generated by modelling, and if we want to do things such as collision avoidance, monitoring extreme weather events, cyclones and flooding, we have to do real-time data streaming. Everybody relies on these technologies and this research is what makes other things possible."

RMIT UNIVERSITY

RESEARCH HIGHLIGHT

Understanding geological formations with precision modelling



The topography of Australia, from the Badlands model developed at the Basin Genesis Hub and the University of Sydney.

Researchers from the ARC's Basin GENESIS Hub (BGH) are running models on Raijin that were previously impossible to compute, to gain an understanding of how continents and sedimentary basins are formed.

Associate Professor Patrice Rey from the University of Sydney says the Hub's purpose is "to understand the formation of continental margins and sedimentary basins in the context of the global Earth, in which we account for the mantle flow, tectonic processes and surface processes."

The team is working with four different computer codes, each looking at a different element of the sedimentary basin process, including mantle flow, plate tectonics and surface effects. Researchers at BGH are progressively working to couple the individual codes, so that all the important factors of the Earth's geodynamics are being taken into account in one all-encompassing model.

Such a model is still a couple of years away, but in the meantime, they are making world-leading findings. Researchers have been able to model the evolution of the Australian landscape over the past 150 million years, using the Badlands computer code that they developed to look at erosion and sediment transportation.

"The capacity of Badlands to simulate the evolution of a landscape, that's really mindboggling," says Professor Rey. "That has definitely attracted a lot of attention from our colleagues and industry partners here. I don't think there is any place in the world where this has been done before. So it's definitively a first."

To run all of these models, the group was awarded one of the top four allocations across the country for 2016, 11 million computing hours on Raijin and other supercomputers, through the National Computational Merit Allocation Scheme. Professor Rey says, "We are really excited about the future and we are really grateful to have access to such a numerical infrastructure here in Australia."

"This is a very exciting time in science. The equations we solve are the Navier-Stokes equations. Those equations have been with us for 150 years, but it is only right now that we can really use those mathematical concepts developed a century and a half ago, combine it with computer science from the mid-twentieth century and now we have the infrastructure, the computational power to make use of all these developments, and that's really exciting."

The work of the Basin GENESIS Hub team relies on the high performance computing that NCI and other HPC facilities around the country provide.

"We are not aware of any other infrastructure that can accommodate our numerical modelling. That kind of computational power is out of reach of most universities so we rely on national infrastructure for our research" **- Professor Rey,** University of Sydney.

BGH

THE UNIVERSITY OF SYDNEY

RESEARCH HIGHLIGHT

Reducing ship grounding risk off the coast of Australia

An image taken by DHI on a full scale field measurement campaign.

Global not-for-profit water and maritime engineering organisation DHI is using NCI to model currents and waves to understand the risks of ships coming aground on the Australian coast. Working with the Australian Maritime Safety Authority (AMSA), DHI is trying to help them understand where the risk of ships going aground is the greatest.

Simon Mortensen, DHI's Group Executive for Port and Navigation and one of Engineers Australia's Top 50 Most Innovative Engineers of 2016, says, "We need to forecast what waves and currents are doing in the ocean on a very large scale. These massive models that cover large sections of Australia sometimes need to simulate ocean conditions for several years. This requires a massive amount of computer power, which is where NCI fits in. Working with NCI has allowed us to model longer and wider than we ever have before."

Ships going aground often cause a lot of damage, have the potential to create oil spills and are expensive to rescue. By understanding where the waves, currents and winds might push them if they broke down close to shore, DHI and AMSA hope to dramatically reduce the risk of those events happening.

Based on the results of DHI's modelling, AMSA is now able to mitigate risks in ways that were previously impossible, for example by placing tugboats in areas that are known to present a higher risk to ships. With this new knowledge and modelling expertise, DHI is able to go all over the world to apply it to other coastlines too.

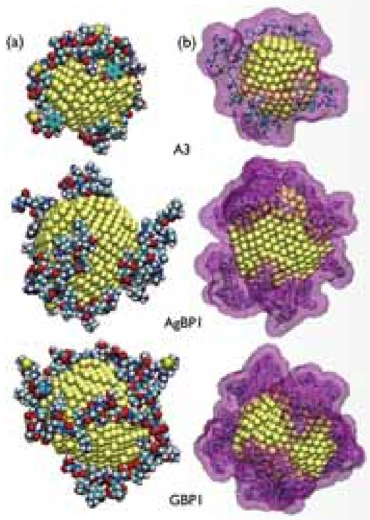
"DHI are envisioning an even stronger partnership with NCI in the future," says Mr Mortensen. "Our numerical Metocean models can provide much higher resolution results these days due to the access to the computer power provided by NCI. Overall, we've been extremely pleased with the collaboration. It's had an absolutely amazing impact on the problems we've been able to solve."

DHI

RESEARCH HIGHLIGHT

Nanoparticles for industrial catalysis

Professor Tiffany Walsh and her team from Deakin University are working with international collaborators to understand what makes certain kinds of nanoparticles good at catalysing chemical reactions. In industry, catalysts are pivotal to increasing the efficiency of production of commodity chemicals. Ideally, the catalysts themselves should be easy and safe to make, so a focus on environmentally benign production approaches for catalysts is preferable.



In this work, published in the *Journal of the American Chemical Society,* the combined experimental and modelling teams devised and tested a 'green', water-based approach to making catalytic gold nanoparticles. To do this, the team used biomolecules, namely peptides, as growth agents of the gold nanoparticles in water. The peptides wrap around the outside of the gold nanoparticles to stop their growth, which not only prevents the nanoparticles from aggregating in water and losing their catalytic potency, but, as the team found out, also helps to expose or cover up different sites on the nanoparticle surface that are relevant to catalysis.

Different peptides were found to produce gold nanoparticles with very different catalytic properties, and until now scientists were not sure of the reasons for this. By predicting the structure of the peptide/nanoparticle interface, Walsh's team were able to identify the peptide characteristics that led to enhanced catalytic performance.

Professor Walsh says, "One peptide sequence will do a pretty good job of lowering the energy barrier for the reaction, and a different one won't do anything to lower the energy barrier. Depending how the peptides arrange themselves on the particle surface, we thought this had something to do with their catalytic behaviour."

To investigate the effect of different peptide structures on the nanoparticles, the team at Deakin simulated the structure of the nanoparticle and associated peptides in liquid water, at the atomistic level. Advanced simulation approaches are essential for this work and meant that each simulation was modelled using 16-32 copies of each system at once. Because each system comprises between 50,000 and 100,000 atoms, this molecular modelling approach becomes highly computationally intensive.

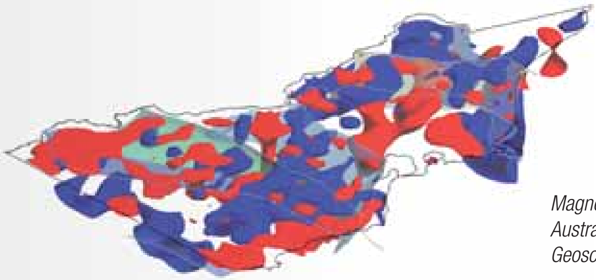
"That's where the need for lots of nodes on Raijin comes into play. We couldn't do these sophisticated simulations on such huge molecular systems without access to Raijin, otherwise it would be impossible. So for us to be able to make these connections between the catalytic behaviour and the structure of the peptide that we used, it was essential that we used the NCI," says Professor Walsh.

Next, the team will focus on replacing the gold in their studies with other materials such as iron oxide or copper sulfide. "Gold was the proof of concept, it has some useful properties from a physical and from a modelling point of view, but gold is expensive! Now that we've established a reliable way to tackle the problem using gold, we want to move to study transition-metal oxides. However, while they're cheap materials for industry, they're very challenging from a simulation point of view, so that's a major challenge for us."

This research is a first step in the 'green' production of new kinds of catalytic nanoparticles. Learning about the production, structure and behaviour of these nanoparticles is the start of a process to understand how to make cheaper and cleaner catalysts in the future.

RESEARCH HIGHLIGHT

Mapping the electric underground



Magnetotelluric imagery of Victoria, Australia, image courtesy of Geoscience Australia.

The National Computational Infrastructure has generated new optimisation solutions to help resolve important details emerging from magnetotelluric studies of the Australian continent.

Magnetotellurics (MT) is a process by which the measurement of the variations in the Earth's magnetic field and electric field can reveal the geological makeup of the underground. This information helps researchers to understand the composition of the Earth's interior and locate valuable resources.

A new study, the Australian Lithospheric Architecture Magnetotelluric Project (AusLAMP), led by Geoscience Australia (GA) will see the placement of 2,800 magnetotelluric instruments across Australia, allowing researchers to create a much more detailed map of the earth beneath our feet.

While past surveys have mapped the underground in 2D, the high-performance computing facilities at NCI will allow geophysicists to study the structure of the Australian continent in 3D. These new 3D models of the Earth's crust will help scientists generate valuable information about the Australian continental geodynamic framework, and will help identify characteristics in the crust and the upper mantle.

Although a three-dimensional approach has been available in the past, this is the first time we can compute a large-scale model. This is only possible by combining groundbreaking research by Geoscience Australia with the experience of high performance computing experts at NCI.

The software used to analyse the MT surveys data requires both the petaflop infrastructure at NCI as well as access to the datasets housed at the facility. However, there were critical bottlenecks in the code that limited both its performance and scalability. NCI's HPC Scaling and Optimisation team were then brought in to analyse the code and improve its scaling to the resolution needed to undertake this work.

Senior HPC Specialist Dr Dale Roberts was able to identify and adjust key components of the code to address these issues. "The key concern with this software initially was its high memory usage, which limited the ability to run even the smallest test cases. The examples we were given could only be run on the large memory nodes of Raijin, which make up 2 per cent of the system, meaning that full-scale jobs could not be run on Raijin at all," explains Dr Roberts. "By adjusting the way that the code used disk instead of memory during processing, we were able to both take advantage of Raijin's high-performance parallel filesystem and reduce memory usage."

"The modified code can now scale with more CPUs; which means that instead of taking a couple of weeks, we can now generate a solution in less than a week" explains GA Section Leader Tristan Kemp. "We couldn't run the large models required for AusLAMP without using NCI or the expert assistance from the HPC Scaling and Optimisation team."

Australian Government
Geoscience Australia

3

Our Infrastructure

Our vendors

HPC: Raijin

- Fujitsu Primergy cluster
- 1.37 Petaflops peak performance
- 57,864 Intel Xeon cores (Sandy Bridge, 2.6 GHz)
- 3,609 compute nodes
- 56 NVIDIA Tesla K80 GPUs
- Mellanox FDR 56 Gb/sec Infiniband full fat tree interconnect
- 162 TB main memory
- 12.5 PB disk storage
- Over 500 million core hours per year
- 314 software packages
- 29.9 PB of high-performance operational storage capacity

Raijin is NCI's peak high-performance computing system, providing over 500 million hours of calculations every year to researchers around the country. This year's introduction of Graphics Processing Units has added an extra dimension to the work that Raijin can do, boosting performance for specialised research projects in chemistry and deep-learning.

This year's uptime of over 99 per cent made Raijin a reliable source of computing infrastructure for hundreds of different research projects. Coupled with improvements to the job tracking and scheduling systems, Raijin has continued to offer the best possible computational service to every user.

NCI has begun planning for an expansion of Raijin funded through the NCRIS Agility Fund, to come online at the start of 2017. This new infrastructure will provide a much needed boost to Raijin's computing performance and alleviate some of the growing demand for HPC services at NCI.

Cloud

NCI has three different cloud facilities for research purposes: the Tenjin cloud, available to NCI's partner organisations; the NeCTAR cloud, available to all users; and the RHOS private cloud. The Tenjin and NeCTAR clouds are built to supercomputer specifications with the same hardware foundation and interconnect as Raijin, giving NCI the fastest cloud environment in the Southern Hemisphere.

Tenjin

Tenjin, NCI's supercomputer-grade cloud, was made available to the NCI partner organisations in September 2014. Since then, Tenjin, that comprises 1,600 cores, has been maintained at greater than 99.5 per cent uptime. Tenjin provides an OpenStack cloud environment that is tightly integrated with NCI's supercomputing and high-performance storage infrastructure. This provides a configuration which is fit-for-purpose for data-intensive research, such as earth system science, genomics, and geophysics. It is an ideal environment for research requiring access to the datasets held in NCI, which is why it is the home of the Virtual Desktop Infrastructure (see Case Study 1) allowing remote access to collections such as the Environmental Research Data Collection. Unlike the complementary NeCTAR cloud, described below, the service provided on Tenjin is a managed, rather than a self-service environment, providing privileged and secure access to NCI's global parallel filesystems.

NeCTAR Federation

NCI is one of the eight nodes of the Australian Government's National eResearch 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 and other organisations, the access for which is mediated through the Australian Access Federation (AAF). 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 sits 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.

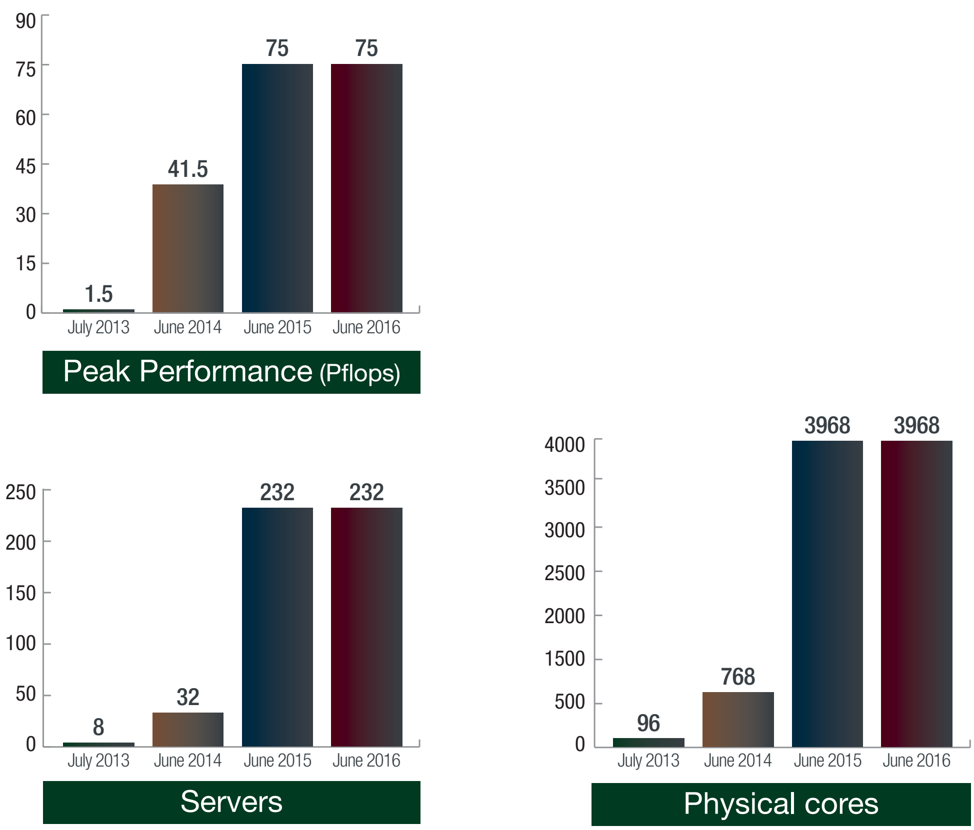
RHOS

The NCI Red Hat OpenStack (RHOS) cloud environment is NCI's first generation private cloud. It is in the process of being decommissioned after reaching end-of-life. All of its remaining projects are being migrated to Tenjin for more powerful and integrated cloud computing.

TABLE 4: 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	Centos (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
NeCTAR	Researchers affiliated with the AAF	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
RHOS	NCI partners	Red Hat OpenStack	4	32	768	Intel Xeon Westmere, 2.6GHz	Dell 10 Gb/sec Ethernet	4.6	12.8	Yes

FIGURE 5: CLOUD STATISTICS



Annual Report 2015-16

Data Storage

One strength of NCI's integrated e-research infrastructure comes from the colocation of large data collections with a high-performance computing system. NCI's persistent filesystems are among the fastest in the country, providing active projects with rapid access to data collections covering decades of observation, modelling and findings from all areas of research.

NCI's data storage infrastructure comprises four large Lustre filesystems for persistent, active data, and an archival data system as a long-term data repository. The Lustre filesystems are made up of Raijin's /short filesystem for rapid-access data, and three global persistent filesystems - /g/data1, /g/data2 and /g/data3.

Each of NCI's filesystems is made up of between 2,400 and 5,300 hard drives, communicating with each other and the Raijin supercomputer at an aggregate speed of 90 GB/second. The rapid communication between compute and data storage is essential to the efficient running of NCI's supercomputer. With the introduction of /g/data3 in 2015-16, NCI runs the two fastest sustained performance filesystems in Australia. Raijin's /short filesystem, its most active data repository for currently running jobs, has Australia's fastest filesystem performance at 151 GB/second.

The archival data system, Massdata, comprises a 29.9 petabyte magnetic tape library, made up of over 8,500 individual tapes.

The filesystems link NCI's compute and data resources via a high-speed 56 gigabit FDR Infiniband fabric, providing unparalleled service integration.

FIGURE 6: FILESYSTEM CONFIGURATION

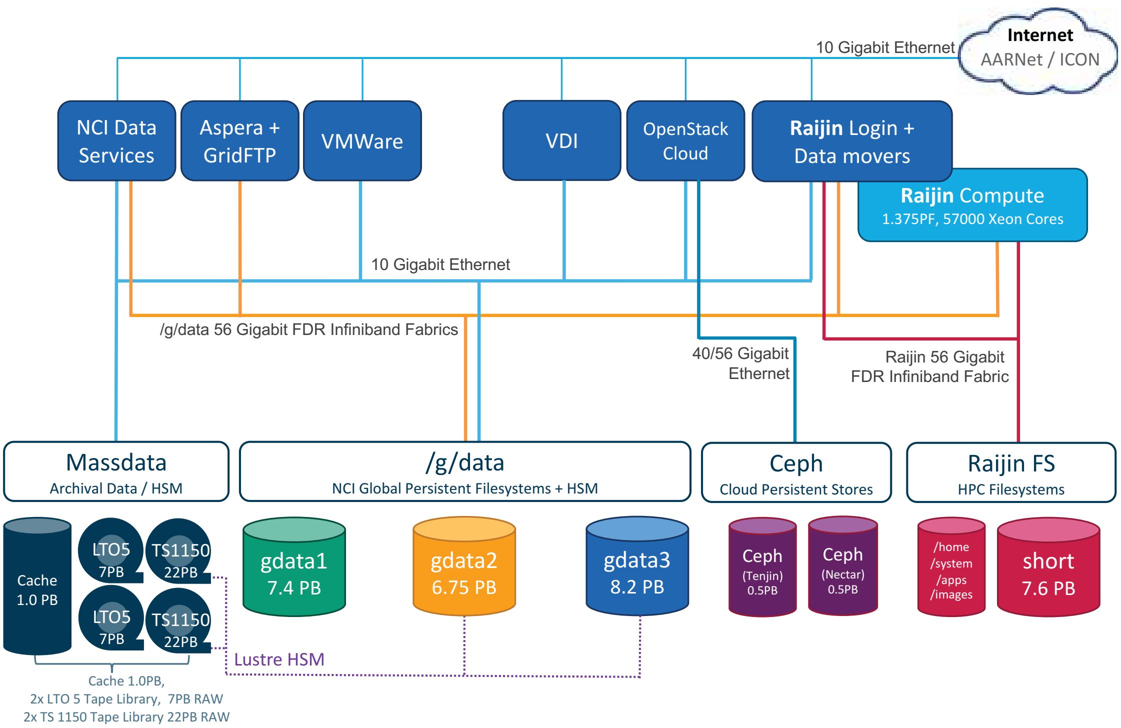
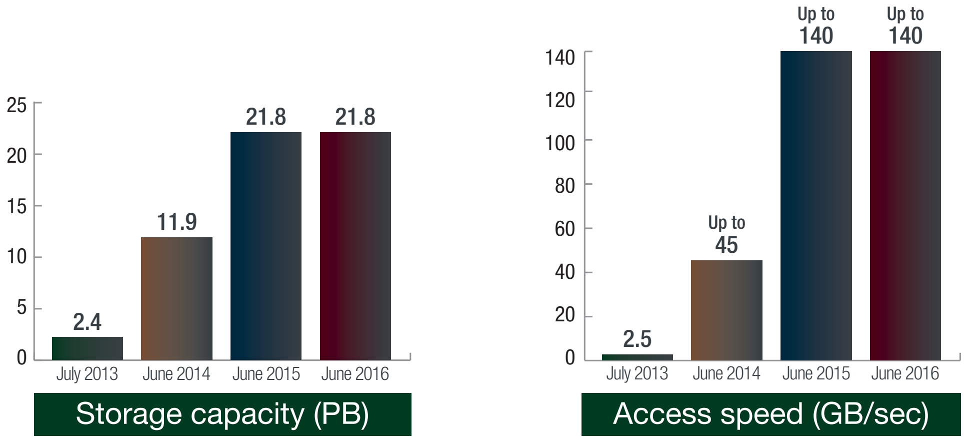
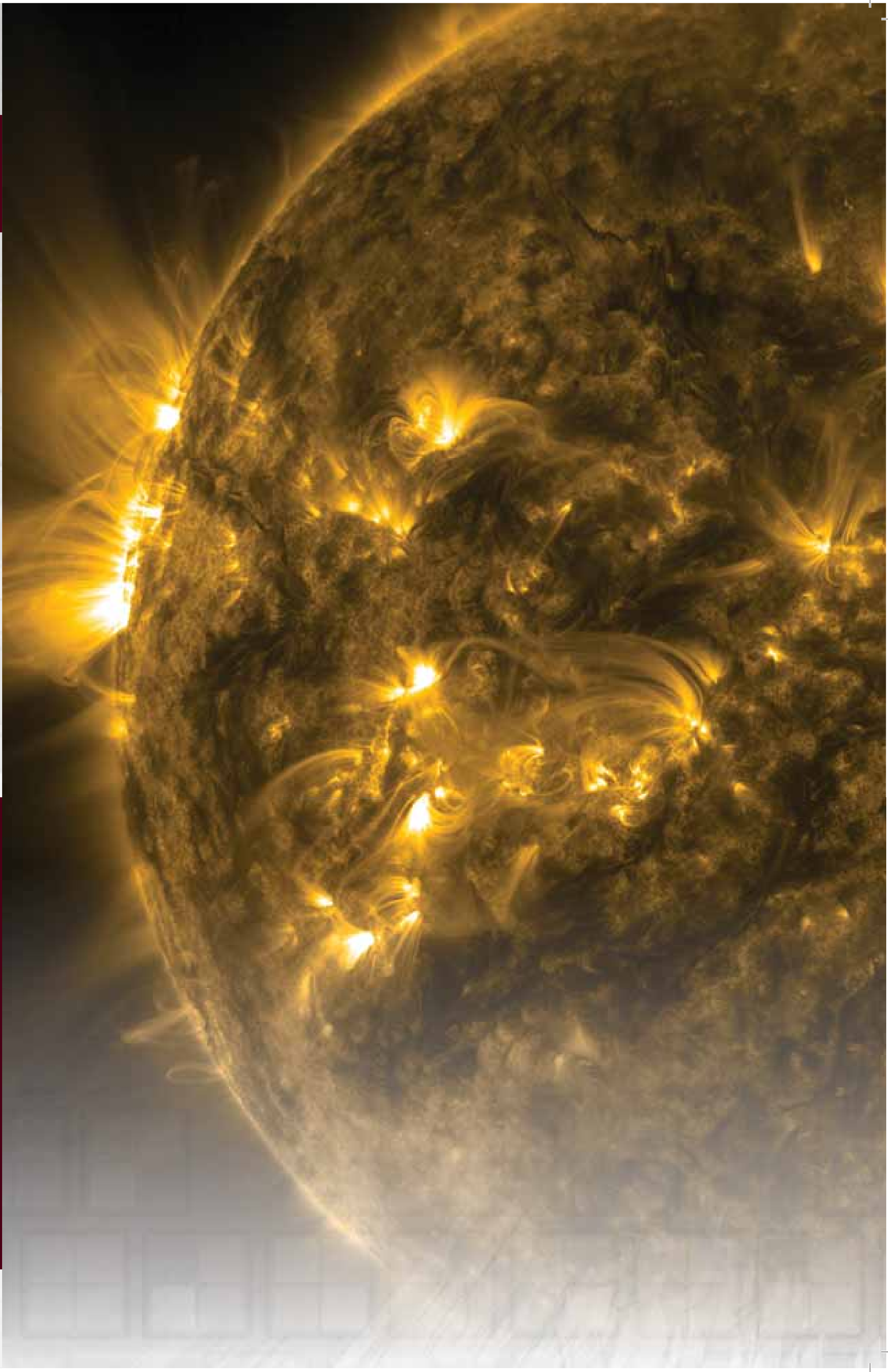


FIGURE 7: DATA STORAGE STATISTICS



	Lustre Filesystems (high-speed, parallel)		
	/g/data	**/short**	**massdata**
Speed	60-120 GB/s	150 GB/s	1TB/hr
Size	22 PB	7 PB	20 PB
Backup	No	No	Yes
Purpose	Datasets, Cloud, VDI	Scratch, processed data	Tape archive



4

Outreach

Active regions of the sun are shown in this image from NASA's Solar Dynamics Observatory, captured on April 20, 2015.

FIGURE 8: MEDIA AND ONLINE ENGAGEMENT

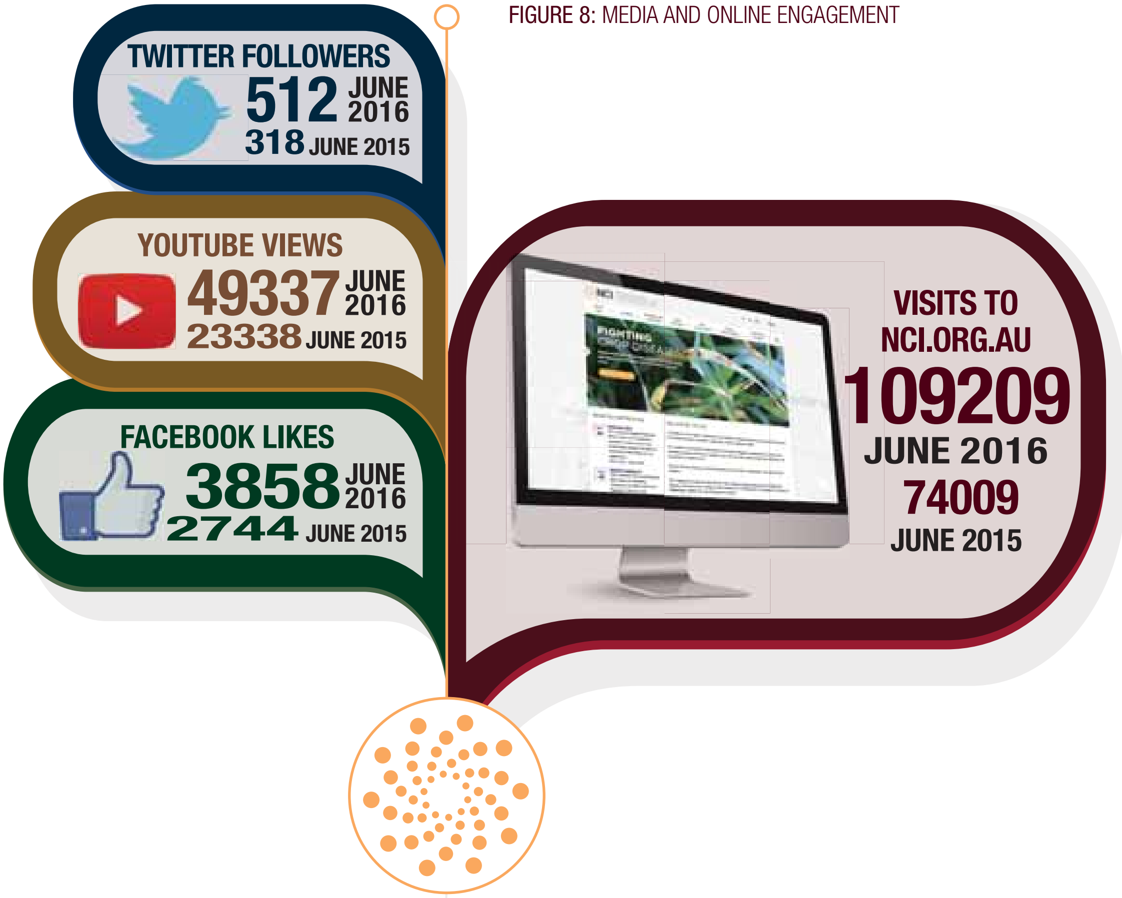


TABLE 5: BUILDING TOURS AND OUTREACH ACTIVITIES

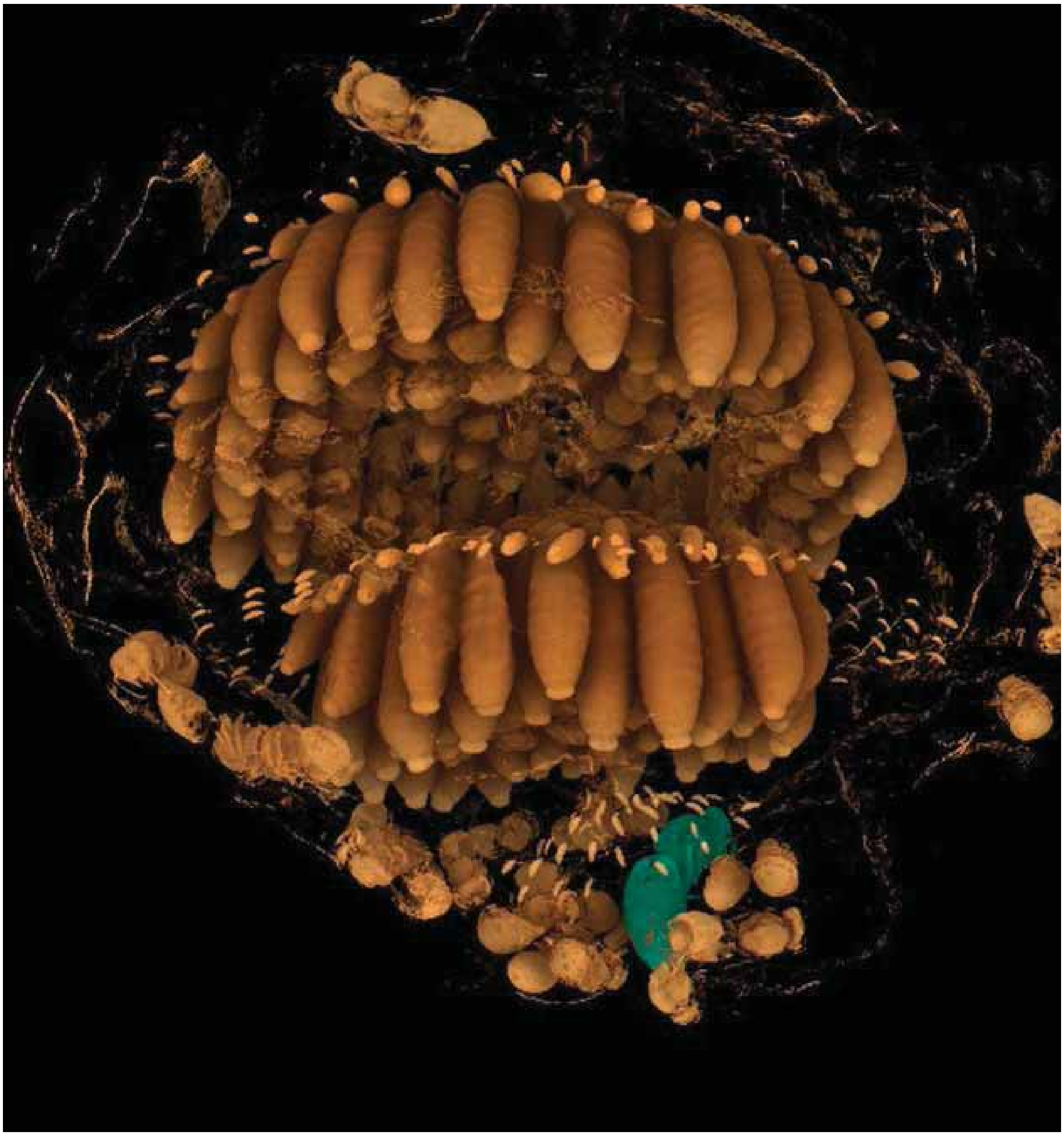
Group	Date
Staff from the Department of Environment	3 July 2015
Staff from Geoscience Australia	7 August 2015
Staff from Research Infrastructure Branch, Department of Education and Training	12 August 2015
MPs Paul Fletcher (Minister for Territories, Local Government and Major Project) and Karen Andrews (Assistant Minister for Science)	14 September 2015
ANU Computer Science students	27 October 2015
Dr Silke Schumacher, Director of International Relations at the European Molecular Biology Laboratory	10 December 2016
National Science Teachers Summer School participants	11 January 2016
National Youth Science Forum students	13 January 2016
BMBF (Federal Ministry of Education and Research) Delegation from Germany	5 February 2016
Chinese Delegation visiting ANU College of Engineering and Computer Science	17 February 2016
Committee on Earth Observation Satellites (CEOS) International Delegates	17 March 2016
Chief Scientist Dr Alan Finkel and President of Global Research Alliance Dr R.A. Mashelkar	27 April 2016
Girls in ICT Day	28 April 2016
ANU Computer Science students	20 May 2016
Geoscience Australia Graduates	15 June 2016
Staff from the Department of Education and Training	22 June 2016

TABLE 6: CONFERENCE PRESENTATIONS BY NCI STAFF

Conference	Country	Date
Lustre Community Conference	Australia	24-25 August 2015
PBS Works User Group Conference	USA	14-17 September 2015
2015 NCI/Nvidia Bioinformatics GPU Workshop and CUDA Programming Workshop.	Australia	17-18 September 2015
Coupled Modelling and Prediction: From Weather to Climate (CAWCR Annual Workshop)	Australia	19-22 October 2015
eResearch Australasia	Australia	19-23 October 2015
Geological Society of America Annual Meeting	USA	1-4 November 2015
EMN Meeting on Computation and Theory	Turkey	9-12 November 2015
Super Computing 15 (SC15)	USA	15-20 November 2015
OGC Technical Committee Meeting	Australia	30 Nov – 4 December 2015
OzViz 2015	Australia	1-2 December 2015
Conference of the Association of Molecular Modellers of Australasia	Australia	2-5 December 2015
IEEE/ACM 8th International Conference on Utility and Cloud Computing	Cyprus	7 December 2015
American Geophysical Union Fall Meeting 2015	United States	15 December 2015
APAN 41 Manila	Philippines	25-29 January 2016
RACI Phys Chem Conference	New Zealand	2-5 February 2016
AMOS/ARCCSS National Conference	Australia	8-11 February 2016
DMF User Group Meeting	Australia	11-12 February 2016
Golang-Syd Meeting-Go 1.6 Release Party	Australia	17 February 2016
Universities Australia Conference	Australia	9-11 March 2016
European Geosciences Union General Assembly	Austria	15 April 2016
OpenStack Australia Day	Australia	5 May 2016
EarthCube Advancing netCDF-CF for Geosciences Workshop	USA	24-26 May 2016
Consortium for Ocean-Sea Ice Modelling in Australia Meeting	Australia	26-27 May 2016
2016 Australian Government Scientific Computing Systems Meeting	Australia	27 May 2016
Australian Square Kilometre Array Pathfinder Conference 2016	Australia	6-10 June 2016
AMSI Computational Sciences Workshop	Australia	7-9 June 2016
Unified Model User Workshop	UK	11-15 June 2016
International Super Computing 2016 (ISC 2016)	Germany	18-22 June 2016

TABLE 7: DRISHTI PRAYOG INSTALLATIONS AROUND THE WORLD

Installation	Country	Date
Emerging Technologies Conference (EMiT)	UK	30 June – 1 July 2015
Science and Technology Facilities Council Daresbury Lab Visualisation Facility	UK	July 2015
Tomography For Scientific Advancement Symposium	UK	3-4 September 2015
Questacon The National Science and Technology Centre	Australia	24 Nov 2015 – 9 Oct 2016
Manchester X-Ray Imaging Facility Drishti Prayog Touchscreen Facility	UK	May 2016
Cheltenham Science Festival	UK	7-12 June 2016

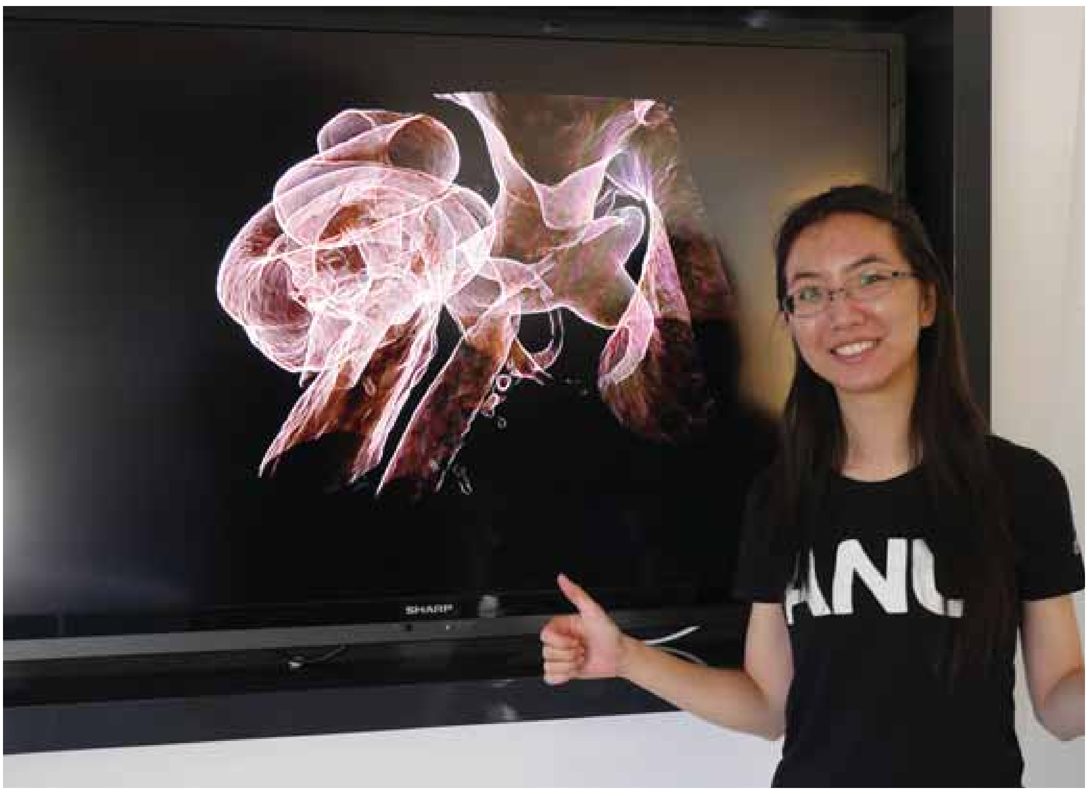


The inside of a wasp's nest, visualised using NCI's Drishti software. The queen is coloured in green.

National Youth Science Forum students visiting NCI in January 2016.

SuperComputing 15 (SC15) in Austin, Texas, USA

International SuperComputing 16 (ISC16) in Frankfurt, Germany.



5

Governance and Finance

The NCI Board

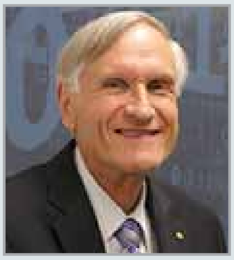
NCI is governed by The Australian National University on the advice of the NCI Board, which comprises:

- 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.

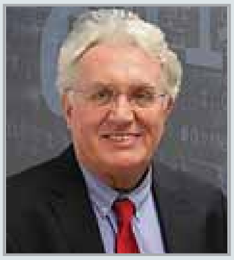
The Board is advised by:

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

Board Members



Emeritus Professor Michael Barber
Chair



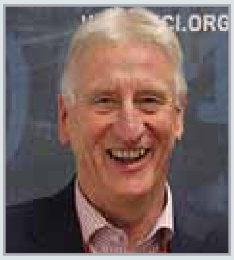
Professor Lindsay Botten
Director, NCI

FIGURE 9: ORGANISATIONAL STRUCTURE

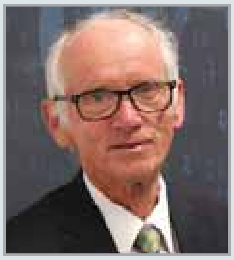
Professor Margaret Harding
Deputy Vice-Chancellor (Research),
Australian National University

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

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

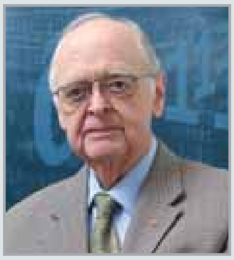


Dr Chris Pigram
Chief Executive Officer, Geoscience Australia



Emeritus Professor Robin Stanton
Independent Member and Deputy Chair

Dr Thomas Barlow
Independent Member
Research Strategist, Barlow Advisory



Dr Robert Frater
Vice-President (Innovation), ResMed
(retired June 2016)

Financial report

Preamble

NCI is an organisational unit of The Australian National University. 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, GA, and a range of other research intensive universities and consortia supported by the ARC) fund a significant proportion of NCI's operating costs. A small, but growing proportion of the NCI Collaboration income comes from the commercial sector.

NCI also administers a number of grants and contracts outside 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 research computing service, provides world-class, high-end services to Australia's researchers. In order to do this, NCI invests significant amounts of money in its expert team of staff and high-performance computing infrastructure. NCI has been constrained in its capacity to replace infrastructure approaching end-of-life due to the lack of external funding for this purpose. To maintain service quality NCI has invested in extending the useful life of its existing infrastructure through the renewal of maintenance contracts. This is reflected in NCI's expenditure profile, whereby the modest Capital expenditure is contrasted with the substantial spend on Utilities and Maintenance.

Review/Audit

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

This consolidated statement has been reviewed by ANU's Finance and Business Services Division.

The Chief Financial Officer certifies that:

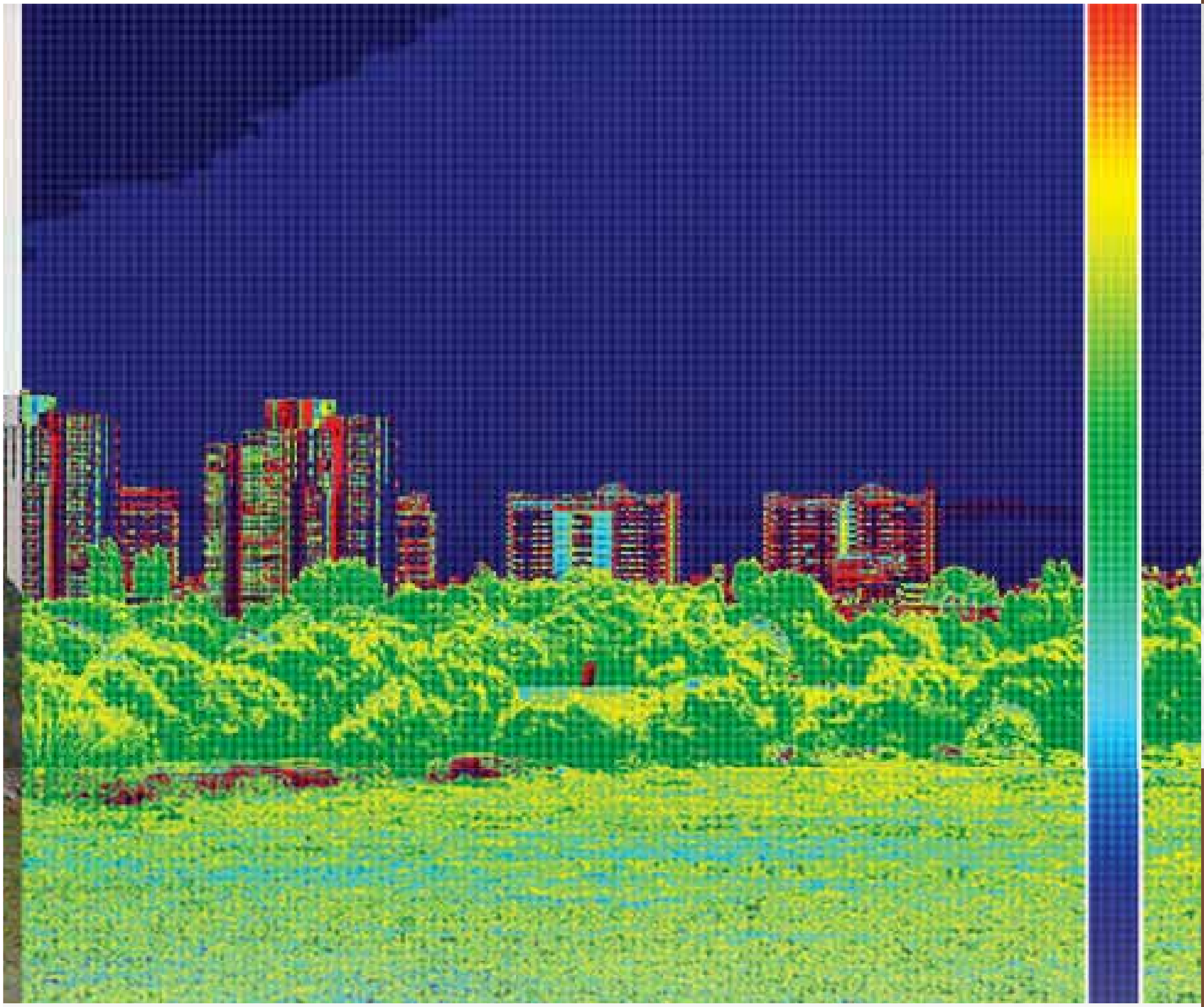
The statement accurately summarises the financial records of these grants and that these records have been properly maintained so as to accurately record the Income and Expenditure of these grants.

TABLE 8: FINANCIAL REPORT

STATEMENT OF INCOME AND EXPENDITURE
For the Period 01 July 2015 to 30 June 2016

For the NCI Collaboration and associated project accounts

	Current Period $
Balance as at 1 July 2015	**15,666,157**
Add	
NCI Collaboration Income	11,282,957
Other grant income	6,533,977
Investment Income	75,146
Total Income	**17,892,080**
Total Available Funds Before Expenditure	**33,558,238**
Less	
Salaries & Related Costs	6,897,932
Equipment - Capital	744,334
Equipment - Non-Capital	93,210
Utilities & Maintenance	6,442,195
Travel Field & Survey Expenses	418,697
Expendable Research Materials	362
Contributions	353,260
Consultancies	343,197
Consumables	1,092,322
Internal Purchases	157,923
Other Expenses	221,699
Transfers to other	47,449
Total Expenditure	**16,812,581**
Unspent Balance as at 30 June 2016	**16,745,657**



6

Appendix

COMPUTE PROJECTS SUPPORTED BY NCI IN 2015-16

Lead CI, Institution	Allocation (KSU)	Project title
Amanda Barnard, CSIRO	43266	Properties and Stability of Nanoparticles for Advanced Applications
Guo Liu, Bureau of Meteorology	25000	Seasonal Prediction Systems and Science
Michael Naughton, Bureau of Meteorology	21450	BoM ESM research at NCI
Daohua Bi, CSIRO	20769	ACCESS - AOGCM
Jill Gready, Australian National University	18000	Simulation and Phylogenetics to decipher Rubisco structure, function and evolution
Andrew Hogg, Australian National University	17000	The Dynamics of the Southern Ocean
Daohua Bi, CSIRO	16700	Joint project on ACCESS-CM2 development
Gary Brassington, Bureau of Meteorology	14300	BLUElink3 - Bureau
CSIRO	10859	Computational Design of Complex Materials
Ben Corry, Australian National University	8000	Simulation studies of biological and synthetic channels
Geoffrey Bicknell, Australian National University	7602	Astrophysical Accretion Disks, Jets and Winds and Interactions with the Surrounding Medium
Derek Leinweber, University of Adelaide	6700	Electromagnetic Structure of Matter
Xuebin Zhang, CSIRO	6583	Downscaling future climate change from CMIP5 climate models with an eddy-resolving ocean model
Matthew England, University of NSW	6492	Past, present and future climate variability and change in the Southern Hemisphere
Salvy Russo, Royal Melbourne Institute of Technology	6441	Quantum Modelling of Photo-Electrode Materials
Sean Smith, University of NSW	5280	Computational Nanomaterials Science and Engineering
Alan Mark, University of Queensland	5261	From molecules to cells Understanding the structural and dynamic properties of cellular components at an atomic level.
Robert Rees, CSIRO	5245	Molecular Simulations of Ionic Liquids for Energy Storage Applications
Commercial Partners	5141	Commercial Projects - not specified
Malcolm Sambridge, Australian National University	5000	Computational Earth Imaging
Andrew Hogg, Australian National University	4659	Mechanisms and attribution of past and future ocean circulation change
Anthony Rafter, CSIRO	4487	Regional-Scale Seasonal Prediction Over Eastern Australia and the Coral Sea
Dietmar Mueller, University of Sydney	4438	Geodynamics and evolution of sedimentary systems
Adele Bear-Crozier, Geoscience Australia	4427	Development of volcanic risk models
William Thurston, Bureau of Meteorology	4100	Weather and Environmental Prediction Specialised Forecasting Systems (WEPSFS)
NCI-BoM-Fujitsu Collaboration	4100	NCI-Fujitsu ACCESS Model Optimisation
Christoph Federrath, Australian National University	4000	Modelling the formation of galaxies, star clusters and binary-star systems
Aaron Thornton, CSIRO	3346	CO_2 conversion in catalytic MOFs
Manolo Per, Royal Melbourne Institute of Technology	3343	Development and Application of Quantum Monte Carlo methods
Jack Katzfey, CSIRO	3190	High-resolution Downscaled Climate Runs
Vincent Wheatley, University of Queensland	3096	Performance Enhancement in Access-to-space Scramjets
Evatt Hawkes, University of NSW	3090	Direct Numerical Simulations of Turbulent Combustion
Alexander Heger, Monash University	3042	The Last Minutes of Oxygen Shell Burning in Supernova Progenitors
NCI Internal (System, Training, Development)	3034	NCI Internal Projects
Julian Gale, Curtin University of Technology	3000	Atomistic Simulation for Geochemistry and Nanoscience

Lead CI, Institution	Allocation (KSU)	Project title
Shin-Ho Chung, Australian National University	3000	Action of Toxins from Venomous Animals on Biological Ion Channels Molecular Dynamics Studies
Michelle Coote, Australian National University	3000	A Quantum-Chemical Approach to Understanding and Controlling Chemical Processes
Martin Asplund, Australian National University	3000	3D magneto-hydrodynamical stellar modelling and 3D non-equilibrium radiative transfer
Aurel Moise, Bureau of Meteorology	2900	Climate Change Science and Processes
Ekaterina Pas, Monash University	2872	Development and application of quantum chemistry methods for the prediction of physicochemical properties of ionic materials
Catherine Stampfl, University of Sydney	2868	First-Principles Investigations of Processes and Properties in Catalysis, Coatings, and Devices
Todd Lane, University of Melbourne	2845	Atmospheric and oceanic processes and dynamics
Tiffany Walsh, Deakin University	2692	Molecular simulation of carbon fibre composites
Michael Ferry, University of NSW	2630	Bulk metallic glasses
Andrew Hogg, Australian National University	2400	The Dynamics of the Southern Ocean
Adam Smith, Bureau of Meteorology	2250	Water Information Services
Rhodri Davies, Australian National University	2200	From Plume Source to Hotspot
Phil Cummins, Geoscience Australia	2150	Geohazard Modelling for the Asia-Pacific Region
Aibing Yu, Monash University	2122	Simulation and Modelling of Particulate Systems
Leo Radom, University of Sydney	2036	Structural and Mechanistic Chemistry
Johnathan Kool, Geoscience Australia	2000	Modelling biophysical connectivity in Australia's territorial waters
Martin Asplund, Australian National University	2000	3D magneto-hydrodynamical stellar modelling and 3D non-equilibrium radiative transfer
Benjamin Galton-Fenzi, University of Tasmania	1915	Research, development and production computing for Antarctic Climate & Ecosystems CRC under the ACE-CRC/AGP/AAD-NCI partnership
Michael Kramer, CAASTRO	1900	A search for highly accelerated binary pulsars
Matthew Chamberlain, CSIRO	1892	ACCSP Dynamical Ocean Downscaling of Climate Change Projections
Christoph Arns, University of NSW	1800	Integration of conventional and digital core analysis
Adrian Sheppard, Australian National University	1800	Understanding petrophysical and multiphase flow properties of rock through experiment, 3D imaging and modelling
Claire Carouge, University of NSW	1786	Terrestrial modelling within the Centre of Excellence regionalising land surface processes
Serdar Kuyucak, University of Sydney	1700	Molecular Dynamics Simulations of Ion Channels and Transporters
Wenjun Wu, Geoscience Australia	1700	AGDC Operations and code repositories (Public and private)
Julio Soria, Monash University	1678	Investigations of transitional and turbulent shear flows using direct numerical simulations and large eddy simulations
Chenghua Sun, Monash University	1678	Computer-Aided Materials Design for Clean Energy
Ben Thornber, University of Sydney	1627	Mix in high-acceleration implosions driven by multiple shocks
Zhe Liu, Monash University	1626	First-principles computational designs for advanced structural and functional materials
Patrice Rey, University of Sydney	1612	Modelling the formation of sedimentary basins and continental margins
Michelle Coote, Australian National University	1600	A Quantum-Chemical Approach to Understanding and Controlling Chemical Processes
Louis Moresi, University of Melbourne	1600	Instabilities in the convecting mantle and lithosphere
Benjamin Galton-Fenzi, University of Tasmania	1515	Research, development and production computing for the Antarctic Gateway Project under the ACE-CRC/AGP/AAD-NCI partnership
Edoardo Tescari, University of Melbourne	1500	The Interplay Between Galaxies and Intergalactic Gas At High Redshift, part III

Lead CI, Institution	Allocation (KSU)	Project title
Jason Evans, University of NSW	1500	Regional Climate Modelling in South-east Australia
Evatt Hawkes, University of NSW	1500	Direct Numerical Simulations of Turbulent Combustion
Jing Huang, CSIRO	1433	Hi-res mapping of renewable energy from meteorological records for Australia
Hugh Blackburn, Monash University	1412	High-Order Methods for Transitional and Turbulent Flows
Debra Bernhardt, University of Queensland	1390	New materials and fluids for catalysis, battery technologies and sensors.
Kerry Hourigan, Monash University	1365	Advanced Modelling of Biofluid and Fluid-Structure Interaction Flows
John Young, UNSW Canberra	1315	Low Reynolds Number Aerodynamics of Flapping Wings
James Goodwin, Geoscience Australia	1310	Geophysics
Thomas Huber, Australian National University	1300	Protein structure calculation using pseudocontact shifts
Gregory Sheard, Monash University	1268	High-magnetic-field liquid-metal flows for fusion power and big-data cooling solutions
Mark Ragan, University of Queensland	1247	Comparative Analysis of Completely Sequenced Genomes of Diverse Environments
Toby Allen, Royal Melbourne Institute of Technology	1228	Mechanisms of charge-membrane interactions and transport.
Nathan Bindoff, University of Tasmania	1200	Turbulence and mixing in the Southern Ocean
Ivo Seitenzahl, Australian National University	1200	Hydrodynamical explosion simulations and radiative transfer for thermonuclear and core-collapse supernovae
Luz Garcia, Swinburne University of Technology	1200	Diagnosing Hydrogen Reionisation with metal absorption line ratios.
Aijun Du, Queensland University of Technology	1200	Nanomaterials for Energy, Nanoelectronics and Environmental Applications: Contribution from Modelling towards Rational Design
Kevin Walsh, University of Melbourne	1200	South Pacific High-resolution Climate Model Simulations
Katrin Meissner, University of NSW	1200	Abrupt climate change events in the past, present and future
Daohua Bi, CSIRO	1199	ACCESS preparation for IPCC AR5
Suresh Bhatia, University of Queensland	1152	Interfacial Barriers for the Transport of Nanoconfined Fluids
Andrew Greentree, Royal Melbourne Institute of Technology	1128	Atom-photon interactions in biologically relevant media
Mark Thompson, Monash University	1118	Transition, stability and control of bluff body flows
Dan Taranu, Western Australia Research Institution not elsewhere defined	1100	UWA Modelling and simulating the evolution of spiral galaxies
Wenjun Wu, Geoscience Australia	1100	AGDC Development and Science (GA internal)
James Wurster, Monash University	1078	What Regulates Star Formation?
Adrian Sheppard, Australian National University	1050	Computational Mesoscale Physics, Probing Complex and Hierarchical Material Structure
Benjamin Galton-Fenzi, University of Tasmania	1030	Research, development and production computing for the Australian Antarctic Division under the ACE-CRC/AGP/AAD-NCI partnership
Tim Pugh, Bureau of Meteorology	1020	Unified Model porting
David Chalmers, Monash University	1007	The dynamics of drug behaviour in the human body
Ananthanarayanan Veeraragavan, University of Queensland	1001	Numerical Simulations of Microcombustors
Alistair Rendell, Australian National University	1000	Computer Science Undergraduate Course
Jill Gready, Australian National University	1000	Simulation of Enzyme Mechanisms, and Protein Dynamics, Structures and Properties
Tiffany Walsh, Deakin University	1000	Development and application of bio/nano interfacial simulations

Lead CI, Institution	Allocation (KSU)	Project title
Jason Sharples, University of NSW	1000	Modelling and simulation of dynamic bushfire propagation
Ingo Stotz, Australian National University	1000	Modelling the Australia-Antarctica divorce: quantifying controls on plate motions
Warren Kaplan, Garvan Institute of Medical Research	1000	Garvan Genome Pilot
Benjamin Galton-Fenzi, University of Tasmania	1000	Modelling of the interaction between Antarctica and the Southern Ocean
Russell Boyce, UNSW Canberra	1000	Physics of the interactions between high-speed craft and their environment
Amanda Barnard, CSIRO	1000	Theory and Simulation of Nanomorphology and the Environmental Stability of Nanostructures
Ross Griffiths, Australian National University	1000	The role of convection in ocean circulation
Justin Borevitz, Australian National University	1000	TraitCapture: An Open Source, High Throughput Phenomics pipeline
Rong Chen, Australian National University	1000	Animal toxins as novel analgesics and pesticides
Gregory Metha, University of Adelaide	988	Metal Nanoclusters as Catalysts for Photoreduction of CO2
Benjamin Powell, University of Queensland	940	Computational approaches to organic photonic and electronic materials: from strongly electronics to device engineering
David Gildfind, University of Queensland	921	Simulation of hypersonic flows in expansion tubes
Michael Reeder, Monash University	920	Predicting and understanding Australia's regional rainfall distribution in a changing climate
Megan O'Mara, Australian National University	920	Investigating membrane protein dynamics, substrate recognition and transport
Ashish Sharma, University of NSW	910	Dynamical downscaling hydro-climatic simulations for water resources planning and management in a changing climate
Sean Li, University of NSW	860	Investigating electronic properties of novel oxide materials for spintronic and energy applications
Simon Ringer, University of Sydney	851	Exploring structure–property correlations in advanced materials Nexus between computational simulation and atomic resolution microscopy
Christoph Rohmann, University of Queensland	850	Computer-aided materials design for metal matrix composites reinforcements.
Pascal Elahi, University of Sydney	843	SSimPL-ACS The Survey Simulation PipeLine - Alternative Cosmologies Study
Elizabeth Krenske, University of Queensland	836	Theoretical modelling of protein-inhibitor interactions and chemical reactivity
Jeffrey Reimers, University of Sydney	812	Modelling of Chemical Systems Including Molecular Excited States, Photosynthesis, and Molecular Electronics Applications
Meredith Jordan, University of Sydney	812	Molecular Interactions
Sheena McGowan, Monash University	808	Structural characterisation of malarial drug targets
Shin-Ho Chung, Australian National University	800	Computational Studies of Poplypeptide Toxins from Venomous Animals Targeting Cationic Membrane Channels
Amir Karton, University of Western Australia	800	Mimicking nature: computational design of better antioxidants
Salvy Russo, Royal Melbourne Institute of Technology	800	Prediction of the Properties of Materials and Nanomaterials
Robert Stranger, Australian National University	800	Computational Studies of the Mn/Ca Cluster in Photosystem II
Haibo Yu, University of Wollongong	800	Molecular Simulations of Enzymatic Catalysis
Nikhil Medhekar, Monash University	797	Atomistic Simulations for Electronic, Chemical amd Mechanical Properties of Nanoscale Materials
Tianfang Wang, University of the Sunshine Coast	788	Bioinformatics, molecular dynamic simulation of biofunctional proteins and mass spectrometric fragmentation mechanisms
David Karoly, University of Melbourne	780	Mechanisms and attribution of changes in Australian climate extremes

Lead CI, Institution	Allocation (KSU)	Project title
Valentijn Pauwels, Monash University	759	Bias removal in data assimilation systems for flood forecasting
David Parkinson, University of Queensland	750	Numerical simulations of stochastic galaxy formation in modified gravity theories
Jared Cole, Royal Melbourne Institute of Technology	748	The materials science of decoherence in quantum devices.
David Huang, University of Adelaide	744	Multi-scale modelling of soft condensed matter in functional materials and biology
Jason Evans, University of NSW	740	Precipitation-groundwater interactions over eastern Australia climate change impacts at multiple scales
Peter Oke, CSIRO	734	Bluelink developments
Andy Pitman, University of NSW	730	Land Surface Science
Marcela Bilek, University of Sydney	688	Harnessing the bioactivity of protein fragements and peptides
Luming Shen, University of Sydney	670	Atomistic simulations of nanoscale liquid flow on solid surface
Carola Vinuesa, Australian National University	650	Computational identification of medically relevant, personal genetic variation from the largest volumes of human genome sequences.
Irene Yarovsky, Royal Melbourne Institute of Technology	637	Theoretical Investigation of novel materials for industrial and biomedical applications
Anthony Murphy, CSIRO	620	Modelling of the Plasma Production of Nanostructures
Jingxian Yu, University of Adelaide	620	Peptronics: Understanding the Relationship between Structures and Properties
Yan Jiao, University of Adelaide	619	Modeling electrocatalytic energy conversion reactions on carbon-based materials by DFT for optimal catalyst design
Dietmar Dommenget, Monash University	610	Global scale decadal climate variability in an ACCESS hierarchy of climate models
Jason Monty, University of Melbourne	601	LES of high Reynolds number turbulent wall bounded flows
Igor Bray, Curtin University of Technology	600	Atomic Collision Theory
Iwan Jensen, University of Melbourne	600	Exact Enumerations in Statistical Mechanics and Combinatorics
Andrew Ooi, University of Melbourne	600	Computational Fluid Dynamics Studies of Buoyant Channel and Rough Pipe Flows
Todd Lane, University of Melbourne	600	Large-eddy simulation of atmospheric turbulence
Ting Liao, University of Wollongong	600	Density Functional Theory Design of Carbon Based Materials for Energy Application
Daniel Argueso, University of NSW	599	The future climate extremes of Australian cities
Wouter Schellart, Monash University	598	Geodynamic models of episodic mountain building
Orsola De Marco, Macquarie University	580	Common envelope interaction and stellar outbursts in the era of time-domain Astrophysics
Evelyne Deplazes, University of Queensland	551	Understanding peptide-membrane interactions at the molecular level
Lars Goerigk, University of Melbourne	545	Theoretical Quantum Chemistry Including Quantum Refinement, Development of Computational Methods and Computational Materials Science
Ravi Jagadeeshan, Monash University	534	The Mechanical Properties of Bio-Macromolecules
Richard Yang, University of Western Sydney	530	Multiscale modelling of Advanced Engineering Materials and Structures
Christoph Arns, University of NSW	509	Integration of conventional and digital core analysis
Paul Webley, University of Melbourne	500	First-principles computation study of Zeolite for gas separation: novel molecular sieving mechanism and rational design
Leon Majewski, Bureau of Meteorology	500	Remotely sensed observations for Earth system modelling
John Lattanzio, Monash University	500	Convective nuclear burning in 3D - Fixing the weak link in stellar models
Shahab Joudaki, Swinburne University of Technology	500	Testing Gravity on Cosmic Scales with Weak Gravitational Lensing and Redshift Space Distortions
Chris Power, University of Western Australia	500	Connecting the Local Universe to the EoR Insights from Galaxy Formation Models
Peter Rayner, University of Melbourne	500	Assimilation of Trace Atmospheric Constituents for Climate

Lead CI, Institution	Allocation (KSU)	Project title
Sylvain Foret, Australian National University	500	Coral genomics, transcriptomics and epigenomics
Gavin Huttley, Australian National University	500	Genomic analysis
Kim Chi Nguyen, CSIRO	496	Solar Rain
Michael Moore, Geoscience Australia	490	Mitigation of Site Specific Errors from Geodetic Time Series
Martin Bell, University of Sydney	490	Transients and Variables with the MWA
Xiao Hua Wang, UNSW Canberra	490	Oceanic Nepheloid Layers and Their Role in Coastal Oceanography
Emlyn Jones, CSIRO	471	eReefs EnKF Data Assimilation
Abhnil Prasad, University of NSW	460	The effects of tropical convection on Australia's climate
Peter Steinle, Bureau of Meteorology	453	Strategic Radar Enhancement Project
Serdar Kuyucak, University of Sydney	445	Computational investigation of voltage-gated sodium channels
Judy Hart, University of NSW	432	Design and development of new inexpensive photocatalysts for efficient hydrogen production and cancer treatment
David Edwards, University of Western Australia	430	Analysis of complex genomes
Xiaolin Wang, University of Wollongong	421	Searching for highly conductive molecules for future molecular circuits and sensors
Narjes Gorjizadeh, University of NSW	420	First-principles study of reaction between complex carbon-bearing materials and metallic phase towards a novel approach for recycling waste polymers for sustainable environment
Sergiy Shelyag, Monash University	418	Radiative magneto-hyrdrodynamic modelling of interconnected solar interior and atmosphere
Robert Stranger, Australian National University	410	DFT and TD-DFT Studies of Organometallic and Metal Cluster Systems
Serdar Kuyucak, University of Sydney	408	Free Energy Simulations of Ion Channels and Transporters
Asaph Widmer-Cooper, University of Sydney	408	Interactions and self-assembly of colloidal nanorods: Establishing design rules for creating new nano-structured materials
Chris Ling, University of Sydney	408	A combined experimental and computational approach to understanding and developing solid-state ionic conductors
Oliver Warschkow, University of Sydney	408	Chemistry at Semiconductor and Oxide Surfaces
Adam Phipps, Victor Chang Cardiac Research Institute	400	VC Dunwoodie
Daniel Chung, University of Melbourne	400	Direct numerical simulation of wall-bounded and buoyancy-driven turbulent flows
Alejandro Di Luca, University of NSW	400	Influence of sea surface temperatures and orography on the development of East Coast Lows.
Ben Corry, Australian National University	400	Simulation studies of biological and synthetic channels
Maria Forsyth, Deakin University	400	Computational investigation of new selective transport materials
Jason Bragg, Australian National University	400	Phylogenetic inference using genome-scale data: methods and applications
Adam Phipps, Victor Chang Cardiac Research Institute	400	VC Martinac
Jingming Duan, Geoscience Australia	390	Magnetotelluric and Electrical data inversion
Peter Jones, University of Technology Sydney	385	Allosteric Control of ATP Hydrolysis in the ABC Transporter Catalytic Cycle.
Zhimin Ao, University of Technology Sydney	380	Density functional theory calculation studies on two-dimensional and hybrid materials for a sustainable environment
Daniel King, University of Technology Sydney	375	Investigation of High Entropy Alloys for use in advanced nuclear applications
Fabio Capitanio, Monash University	366	4-D Numerical Models of Plate Tectonics Subduction with an Upper Plate

Lead CI, Institution	Allocation (KSU)	Project title
Katherine O'Brien, University of Queensland	356	Impacts of environmental change on coastal ecosystem health: application of the eReefs coupled hydrodynamic-biogeochemical model
Kris Ryan, Monash University	349	The evolution and stability of vortex rings and synthetic jets moving parallel to a flat plate
Ailie Gallant, Monash University	348	Mesoscale modelling of urban landscapes for assessing heat adaptation and mitigation strategies with climate change
Joseph Lai, UNSW Canberra	347	Disc Brake Squeal
Prabhakar Ranganathan, Monash University	340	Biology needs rheology.
Marlies Hankel, University of Queensland	340	Nanoporous membranes for energy applications
Nicolas Flament, University of Sydney	330	The geodynamics of past sea level changes
Jason Evans, University of NSW	325	Will East coast lows change in frequency or intensity in the future?
Kei-Wai Kevin Cheung, Macquarie University	320	Numerical Study of Extreme Weather Systems and Climate Variability associated with Monsoons
Chennupati Jagadish, Australian National University	320	Nanostructured optoelectronic devices
Michelle Spencer, Royal Melbourne Institute of Technology	315	Modelling Nanoscale Materials for Sensing and Device Applications
Luke Barnes, University of Sydney	310	Lyman Alpha and stellar emission from high redshift galaxies
Gleb Beliakov, Deakin University	300	Large-scale high accuracy computations for studies of Riemann's zeta function, as part of the 8th Hilbert problem
Randall Wayth, University of Melbourne	300	Advanced Processing of the GaLactic and Extragalactic All-sky MWA Survey (GLEAM)
Anh Pham, University of NSW	300	Theoretical study of 2D and 3D topological materials
Paul Tregoning, Australian National University	300	Analysis and interpretation of mass redistribution on Earth derived from space gravity observations
Robyn Schofield, University of Melbourne	300	Atmosphere-Ocean Coupled Chemistry Climate Modelling of Stratospheric Ozone and Aerosols
John Pye, Australian National University	300	Modelling of high-temperature concentrating solar thermal energy systems
Terry Frankcombe, Australian National University	300	Efficient chemical dynamics in gas phase, solid phase and heterogeneous systems
Michael Reeder, Monash University	290	The dynamics of subtropical anticyclones and the connection to drought, heatwaves and bushfires in southern Australia
Marie Ekstrom, CSIRO	289	Mesoscale Modelling of Rainfall for Sea
Nicholas Williamson, University of Sydney	281	Purging and destratifying of thermal and saline pools in Australia's inland rivers
Steven Siems, Monash University	278	Simulations of wintertime storms across Southeast Australia, Tasmania and the Southern Ocean
Lexing Xie, Australian National University	272	The Anatomy of Social Media Popularity
James Goodwin, Geoscience Australia	270	External Geophysics Users
Dougal McCulloch, Royal Melbourne Institute of Technology	268	Electronic structure of boron nitride and other novel coating systems
Michael Hewson, Central Queensland University	265	ARC Linkage Wind Generation Project - WRF Wind Climatology
Dino Spagnoli, University of Western Australia	262	Modelling surface electrochemistry-transport coupling in AlGaN/GaN-based sensors
Catherine Stampfl, University of Sydney	260	First-Principles Investigations of Processes and Properties in Catalysis, Coatings, and Devices
Magda Guglielmo, University of Sydney	260	The Milky Way and the Magellanic System: Interactions of gaseous halos and angular momentum transfer

Lead CI, Institution	Allocation (KSU)	Project title
Craig Arthur, Geoscience Australia	260	Severe Wind and Coastal Inundation Modelling
Alister Page, University of Newcastle	252	Quantum Chemical Modelling of Nanoscale Chemical Processes
Mohammednoor Altarawneh, University of Newcastle	252	Fundamental Understanding of the Role of Singlet Molecular Oxygen in Spontaneous fires
Simon Middleburgh, ANSTO	252	Developing a materials understanding of the silicide accident tolerant fuels - an atomic scale study
Jiabao Yi, University of NSW	252	Mechanism of ferromagnetism and spin manipulation in oxide and 2D-based diluted magnetic semiconductors (DMSs)
Paul Tregoning, Australian National University	252	Analysis and interpretation of space gravity observations
Petra Heil, University of Tasmania	250	(East) Antarctic sea ice: Ice-ocean interactions and ice kinematics in a changing climate.
Roger Amos, Australian National University	242	Ab initio calculations for large systems
Christopher Blake, Swinburne University of Technology	240	Swinburne Testing the cosmological model at low redshift: Mock catalogues for the 6dF and Taipan surveys
LiangChi Zhang, University of NSW	239	Multiscale mechanics of metal/semi-conductor/bulk metallic glass (BMG) systems, mixed lubrication and fibre-reinforced composites
Ian Dance, University of NSW	231	Computational Bio-inorganic and Supramolecular Chemistry
Duong Do, University of Queensland	210	Novel Characterisation of Porous Structure and Surface Chemistry of Carbon by means of Monte Carlo computer simulation
Andrea Schaller, University of Queensland	205	Molecular Dynamics Investigation of Epitopes and Biosurfactant Structural Stability
Timothy Kam, Australian National University	201	Liquidity Traps and Forward Guidance Monetary Policies: a new computational dynamic game perspective
Brian Yates, University of Tasmania	200	Designing Better Catalysts
Matthew Garthwaite, Geoscience Australia	200	Geodetric research to measure surface deformation of the Australian continent
Ross Griffiths, Australian National University	200	The role of convection in ocean circulation
Jiri Cervenka, University of Melbourne	200	Functionalised graphene for next generation nanoelectronics
Aaron Oakley, University of Wollongong	200	Dynamics of DNA Clamps and Clamp Loaders
Rosalie Hocking, James Cook University	200	Catalysts for Clean Energy from experimental data to reaction mechanisms
Andrew Neely, UNSW Canberra	200	Fluid-thermal-structural interactions for high-speed flight and propulsion
Andrew Chew, Australian National University	200	Raijin computing services for the ANU Mathematical Sciences Institute 2014
Alexander Heger, Monash University	200	The First Supernova
Robert Elliman, Australian National University	200	Resistive Random Access Memory
Joseph Horvat, University of Wollongong	200	GaAs 1-x-y P y Bi x mixed crystals with tunable bandgap, ab initio calculations and experiment
Nikolai Petrovsky, Flinders University	200	Computer Aided Design of Ebola Vaccines and Therapeutics
Thomas Plantard, University of Wollongong	200	Security Analysis of Lattice-based Cryptosystems
Thomas Welberry, Australian National University	200	Computation of X-Ray Diffraction Patterns for 3D Model Systems
Yun Wang, Griffith University	200	Theoretical understanding and computational design of perovskite solar cells
Alistair Rendell, Australian National University	200	Large scale online learning with a mixed regularisation model
William Foley, Australian National University	192	Whole genome analysis of Eucalyptus - Australia's foundation tree
Hareth Mahdi, University of Sydney	180	Gravitational Lensing in Coupled Dark Matter - Dark Energy Cosmologies
Rika Kobayashi, Australian National University	180	Chemistry Porting Project

Lead CI, Institution	Allocation (KSU)	Project title
Hamid Valipour, University of NSW	171	Engineering Materials simulation
Gleb Beliakov, Deakin University	170	Large scale high accuracy computations for studies of Riemann's zeta function
Craig O'Neill, Macquarie University	165	Tracking mantle slab dewatering using ASPECT
Ante Bilic, Curtin University of Technology	164	Small molecules for organic photovoltaics and light emitting diodes
Justin Freeman, Bureau of Meteorology	162	Marine Virtual Laboratory (BoM)
Stefano Bernardi, University of Queensland	160	Separation of ions and small molecules using Molecular Dynamics simulations
David Kent, Bureau of Meteorology	160	Extended Hydrological Prediction modelling
Ingo Jahn, University of Queensland	160	Supercritical CO2 Turbomachinery and Heat Exchangers
Anatoli Kheifets, Australian National University	160	Theory of multiple atomic ionisation
Timothy Garoni, Monash University	156	Design, analysis and application of Monte Carlo methods in statistical mechanics
William Church, University of Sydney	154	Structural and functional simulations of protein drug targets
Steven Armfield, University of Sydney	152	Direct simulation of transition for natural convection flow in inclined differentially heated cavities
Qing-Hua Qin, Australian National University	152	Piezoelectric bone remodeling analysis by finite element method
Scott Medling, Australian National University	152	Locating defects in doped semiconductor lattices
Stephen Williams, Australian National University	152	Computer Simulation of Glassy Materials out of Equilibrium
Eric Kennedy, University of Newcastle	150	Non-equilibrium plasma conversion of toxic halogenated compounds and waste halogenated refrigerants to value added polymers
Luis Azofra, Monash University	150	Electrochemical Conversion of CO2 and N2
Junfang Zhang, CSIRO	142	Molecular Dynamics Study of Gas Storage and Transport in Coals
Dorian Hanaor, University of Sydney	141	Understanding the Origins of Enhanced Photocatalytic Activity in doped TiO2 Nanostructures Using Density Functional Theory
Riyan Cheng, Australian National University	140	A powerful mixed effect model approach for novel genetic discoveries using joint analysis of multiple complex traits
Marcel Cardillo, Australian National University	140	Understanding patterns of evolutionary and ecological diversification
Wenju Cai, CSIRO	138	Climate Change Impact on Southeast Queensland Water Supply
Edward King, CSIRO	136	National Remote Sensing Processing Facility
Elmars Krausz, Australian National University	130	Vibrational Frequency changes in carboxylate ligands coordinated to manganese as a function of the metal oxidation state
Patrice Rey, University of Sydney	125	Understanding the Aegean-Anatolia Collisional System
Leo Radom, University of Sydney	121	Structural and Mechanistic Chemistry
Adam Phipps, Victor Chang Cardiac Research Institute	120	VC Stock
Dillon Hunt, University of Queensland	120	DSTO Pilot Project
Kenton Prindle, Australian Commercial Organisation	120	Woodside Energy Project
Robert Wittenmyer, University of NSW	118	Studying the Dynamics of Multiple Planetary Systems
Suresh Bhargava, Royal Melbourne Institute of Technology	114	An investigation on the interaction of heavy metal ions (As and Hg) with Surface Enhanced Raman Spectroscopy materials
Haibo Yu, University of Wollongong	111	Computer simulations of biomolecular systems
Nerida Wilson, Geoscience Australia	108	SRTM DEM processing
Maria Forsyth, Deakin University	101	Computational investigation of new selective transport materials

Lead CI, Institution	Allocation (KSU)	Project title
Snjezana Tomljenovic-Hanic, University of Melbourne	101	Diamond-based quantum devices
Andrew Rohl, Curtin University of Technology	100	Realistic Modelling of the Effects of Solvent and Additives on Crystallisation
Adam Phipps, Victor Chang Cardiac Research Institute	100	VC HO
Thomas Poulet, CSIRO	100	Tackling the unconventional resources challenge with multiphysics simulations
David Wilson, La Trobe University	100	Quantum Chemical Molecular Properties
Peter Strazdins, Australian National University	100	Performance Analysis and Optimisation of Large-scale Scientific Simulations
Nerilie Abram, Australian National University	100	Testing the drivers of Southern Annular Mode changes over the last millennium
Joe Hope, Australian National University	100	BEC manipulation through pulse sequences and quantum feedback control
Johannes Zuegg, Australian National University	95	Modulating the function and structures of bio-macromolecules by small molecules
Zongyan Zhou, Monash University	94	Flow and Heat Transfer Behavior in Fluid Bed Reactors
Madeleine Beekman, University of Sydney	92	The evolution of the mitochondrial genome
Martin Cope, CSIRO	92	Future Air Quality Projection
Zbigniew Stachurski, Australian National University	90	Scale Resolving Turbulence Simulations of Multi-layer Orthogonal-offset Plate Arrays
Zdenka Kuncic, University of Sydney	87	Insulin-IR complex
Tim McVicar, CSIRO	85	Developing an Australian Landsat-MODIS Blending Infrastructure (ALMBI)
Ashley Buckle, Monash University	83	Conformational regulation of enzyme function
Balazs Csaba, Monash University	82	Dark Matter Discovery
Michael Paddon-Row, University of NSW	80	Computational Quantum Chemical Studies of Stereoselectivity of Organic Reactions
Xuming He, Australian National University	80	Large-scale Holistic Scene Understanding in Video
Ian Dance, University of NSW	80	Computational Bio-inorganic and Supramolecular Chemistry
Uta Wille, University of Melbourne	80	Free radicals in organic chemistry: Mechanistic insight into radical and non-radical processes using computational methods
Alan Chaffee, Monash University	80	Computational Quantum Chemistry
David Henry, Murdoch University	80	Nanoscale materials and Nanoscale Interactions - From Catalysts through to Hydrophobic Soils
David Lescinsky, Geoscience Australia	80	Assessing geothermal energy potential for the Australian Continent
Bradley Evans, University of Sydney	80	Primary production in space and time
Mike Ford, University of Technology Sydney	79	Hybrid 2D Materials
Matthew Arnold, University of Technology Sydney	78	Optimisation of plasmonic nanoantennas and metamaterials
Alan Ley, CSIRO	77	Inversion AEM data
David Lescinsky, Geoscience Australia	75	Multiphase fluid flow and heat transport modelling with Tough2-MP
Yingping Wang, CSIRO	74	Using ACCESS to assess the biophysical consequence of a greening earth
Curt Wentrup, University of Queensland	71	Theoretical calculations on reactive molecules, intermediates and prebiotic chemistry pathways
Karol Czarnota, Geoscience Australia	70	Epeirogeny and basin dynamics of Australia
Stephen Hyde, Australian National University	70	Self-assembly of Polyphiles via Espresso Simulations
Aaron Sedgmen, Geoscience Australia	70	EODS Web Services Delivery

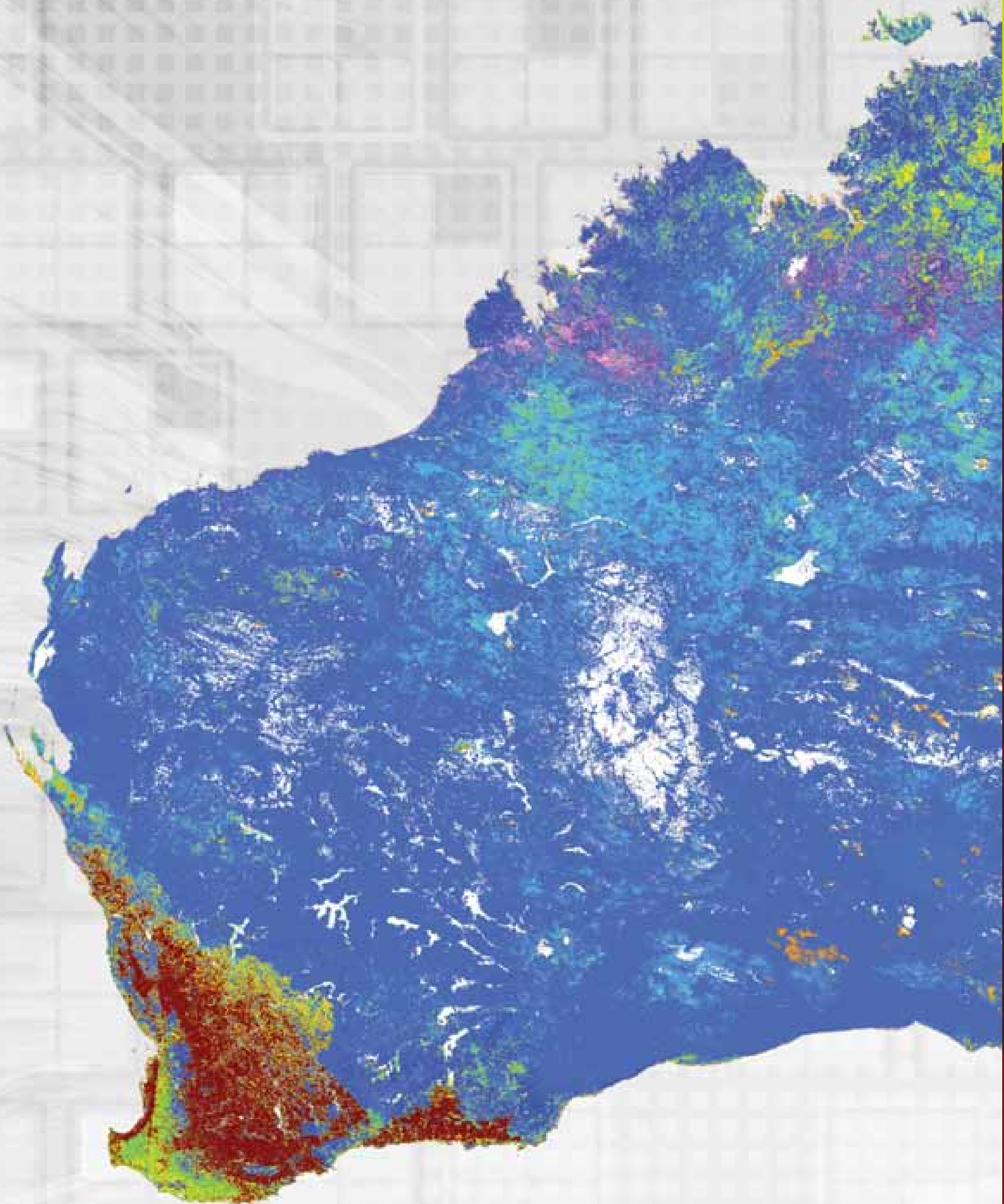
Lead CI, Institution	Allocation (KSU)	Project title
Tony Vassallo, University of Sydney	66	Modelling the interactions and influences of organic compounds in zinc-bromine redox flow battery systems
Robert Bell, CSIRO	65	General Share for User Code Development and Testing
Chunguang Tang, University of Sydney	65	Materials Design for Self-toughening Bulk Metallic Glasses
Naomi Haworth, Australian National University	64	How does insulin work?
Ahmad Jabbarzadeh, University of Sydney	63	Multiscale Simulations of Polymeric Systems
Tapio Simula, Monash University	62	Quantum Turbulence
Alejandro Montoya, University of Sydney	61	Modelling Dehydroxylation of Clay Structures for CO2 carbonation applications
Adam Phipps, Victor Chang Cardiac Research Institute	60	VC Suter
David McGuinness, University of Tasmania	60	Production of Linear Alpha Olefins Mechanistic and Applied Investigations
Allan Canty, University of Tasmania	60	Catalysis and Organometallic Chemistry
Kenneth Crozier, University of Melbourne	60	Nanophotonic devices based on semiconductor and plasmonic materials
John Webb, University of NSW	60	Measuring the laws of Nature across the Universe
Christian Wolf, Australian National University	60	SkyMapper and the Southern Sky Survey
Leo Lymburner, Geoscience Australia	60	AGDC Experimental (External)
Benjamin Schwessinger, Australian National University	60	The Evolution of stripe rust virulence
Peter Gill, Australian National University	57	Development and application of new quantum chemistry algorithms
Terry OKane, CSIRO	55	The AUStralian community ocean model ReAnalysis project (AURA)
Geoffrey Webb, Monash University	52	Learning from big data with generative and discriminative strategies
Duk-Yong Choi, Australian National University	52	Simulation of Photonic Nanostructures
Varghese Swamy, Monash University	52	First-Principles Modeling of Functional Titanium Dioxides and Hybrid Metalorganic Perovskites
Antonio Tricoli, Australian National University	52	Simulation of Nanoparticle Films Self-Assembly for Breath Analysis and Non-Invasive Medical Diagnosis
Weifa Liang, Australian National University	52	Efficient Algorithms for Finding Influential Communities in Large-Scale Networks
Andrew Kiss, UNSW Canberra	51	Nonlinear Dynamics of Ocean Currents
Terry Bossomaier, Charles Sturt University	50	Information flow in Vicsek Models
Debra Bernhardt, University of Queensland	50	Mechanisms for hydrogenation and dehydrogenation of complex aluminium hydrides and borohydrides
Mark Baird, CSIRO	49	eReefs Marine Modelling GBR1
Graham Ball, University of NSW	49	DFT and Ab Initio Studies of Inorganic and Organometallic Complexes and Drug DNA complexes
Dave Penton, CSIRO	48	Australian Water Resource Assessments Calibration Tes
Michael Collins, Australian National University	48	Molecular Potential Energy Surfaces and Properties of Large Molecules
Fangbao Tian, University of NSW	47	Fluid-structure Interactions and Complex Flows in Biological and Biomedical Systems
Mark Holzer, University of NSW	45	Decadal Changes in Southern Ocean Ventilation
Ross Brodie, Geoscience Australia	45	Potential Field Modelling in Spherical Coordinates
Tracie Barber, University of NSW	41	CFDMECH
Adam Trevitt, University of Wollongong	40	Computational Investigation of the Chemistry of Reactive Intermediates

Lead CI, Institution	Allocation (KSU)	Project title
Elena Pasternak, University of Western Australia	40	Deformation and failure of constrained fragmented structures
Cedric Gondro, University of New England	40	Evolution, Selection and Estimation of Polygenic Epistatic Networks in Quantitative Traits
Paul Hancock, University of Sydney	40	Scintillation and the structure of turbulent gas in the Milky Way
Michael Terkildsen, Bureau of Meteorology	40	Space weather modelling
Evan Gray, Griffith University	40	DFT studies of structure-function relationships in materials containing hydrogen
Gujie Qian, University of South Australia	40	Effect of Na and K on solar cell absorber materials Cu(In1-x,Gax)Se2: A first-principles study
John Wilford, Geoscience Australia	40	Data mining and geostatistical modelling for geoscience applications
Cedric Simenel, Australian National University	40	Microscopic and Macroscopic Studies for Nuclear Reactions
Mark Leonard, Geoscience Australia	40	EQRM
Andrey Sukhorukov, Australian National University	40	Active Control of Light in Photonic Nanostructures
Amanda Karakas, Australian National University	40	The heavy element composition of post-AGB stars and planetary nebulae
Matthew Hole, Australian National University	40	Computational Applications in Equilibrium and Instabilities of Advanced Plasma Confinement Geometries
RMIT	39	RMIT reserved allocation
Wei Wen, University of NSW	38	Joint Analysis of Imaging and Genomic Data to Study the Structure and Function of the Human Brain
Guobin Fu, CSIRO	38	Improving hydrological processes in CABLE land surface scheme
Alexie Papanicolaou, University of Western Sydney	37	CSIRO comparative genomics pap056
Hussein Abbass, UNSW Canberra	37	Transportation Modelling and Automation Group (TMAG)
Tony Vo, Monash University	36	From Saturn's hexagon to Earth's polar vortex elucidating shear-layer instability in rotating flows
Gregory Wilson, CSIRO	36	Electronic Structure of Organic/Inorganic Dyes for Photovoltaic Applications
Adrian Pudsey, Royal Melbourne Institute of Technology	35	Aerothermodynamics of Hypersonic Flight and Enabling Technology
Bijan Samali, University of Western Sydney	32	Intersect project
Brendan McKay, Australian National University	32	Extremal graph theory
Pierre Loos, Australian National University	32	Spherical geometry in chemistry and physics
Michelle Dunstone, Monash University	31	The structure of the MACPF/CDC giant pores
Joachim Mai, Intersect	30	Intersect project 10
Nicolas Cherbuin, Australian National University	30	Brain structure, cognition, and ageing a magnetic resonance imaging investigation
Amin Heidarpour, Monash University	29	The Structural Behaviour of Hollow Fabricated Columns with High Strength Steel Tubes and Double Skin Concrete-Filled Columns with Corrugated Steel Skins
Michael Banner, University of NSW	28	Computational study of 3D breaking deep water, shallow water and shoaling water waves
Saeed Masoumi, University of NSW	25	Molecular dynamics simulation of polymers
Thomas Loridan, Macquarie University	25	WRF simulations of Tropical Cyclones
Andrey Molotnikov, Monash University	24	Nacre inspired structures based on ceramic/polymer composites
Weimin Gao, Deakin University	24	HPC for fluid dynamics and molecular dynamics

Lead CI, Institution	Allocation (KSU)	Project title
Qijun Zheng, Monash University	24	Finite-element and discrete study of pipe belt conveyors
Monash University	24	4D Numerical Models of Lithospheric and Mantle Interaction
Malin Premaratne, Monash University	24	Plasmonic-based components for Nanotechnology
Stephen Gould, Australian National University	24	Machine Learning for Computer Vision
Wenyi Yan, Monash University	23	Optimisation and structural analysis for additive manufacturing and maintenance
Jim Smitham, CSIRO	23	Accurate activation energies for aqueous CO2/amine reactions
Ross McPhedran, University of Sydney	21	Nanostructures for Advanced Photovoltaic Applications
Quentin Parker, Macquarie University	21	Kinematic study of Galactic bulge planetary nebulae
Kylie Catchpole, Australian National University	20	Nanoplasmonic Solar Cells
Shankar Kalyanasundaram, Australian National University	20	Finite Element Modelling of Engineering Systems
Various researchers	800	Small Allocations - not specified

DATA COLLECTIONS STORED AT NCI IN 2015-16

Collection Name	Research Data Collections (TB)
Astronomy	
Skymapper	227
Social Sciences	
Australian Data Archive	4
Biosciences	
BPA Melanoma Dataset	569
Plant Phenomics	2
Climate Change and Earth System Science	
ACCESS Models	3,742
Coupled Model Intercomparison Project (CMIP5)	1,687
Seasonal Climate Prediction	618
Reanalysis	207
Year Of Tropical Convection	90
Ocean General Circulation Model (Earth Simulator)	27
CABLE Global Evaluation Datasets	3
CORDEX Int	2
Environment, Geodesy, Elevation and Bathymetry	
Satellite Earth Observation (Landsat, etc)	1,391
IMOS+TERN Australasian Satellite Imagery (NOAA/AVHRR, MODIS, VIIRS and AusCover)	560
Synthetic Aperture Radar	115
Digitised Australian Aerial Survey Photography	74
Australian Bathymetry and Elevation reference data	37
Australian Marine Video and Imagery Collection	7
Global Navigation Satellite System (GNSS) (Geodesy)	5
Satellite Soil Moisture Products	5
Earth Observation	
BoM Observations	369
BoM Ocean-Marine Collections	273
National CT-Lab Tomographic Collection	118
TERN eMAST	50
TERN eMAST Data Assimilation	30
Australian Natural Hazards Archive	27
Models of Land/Water Dynamics from Space	22
CSIRO/BoM Key Water Assets	20
Australian Geophysical Data Collection	10
Australian 3D Geological Models	3
TERN Phenology Monitoring: Near Surface Remote Sensing	2
Total	**10,296**



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