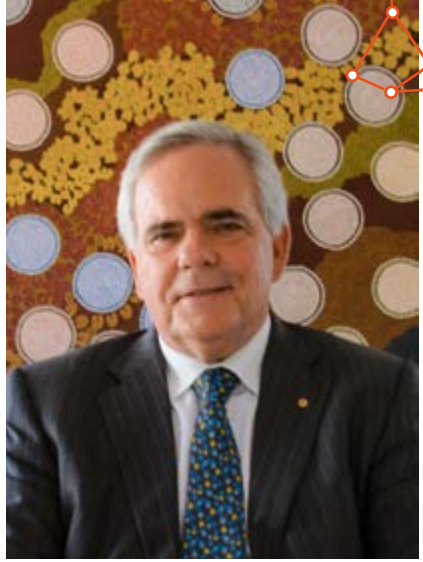
2014
2015

ANNUAL REPORT

PAWSEY
supercomputing centre


CSIRO
PAWSEY



It is with great pleasure that I open this Annual Report, covering the first year of the Pawsey Supercomputing Centre's full operation and the first full year of my tenure as Pawsey Board Chairman. As one of two national world class supercomputer centres funded under the NCRIS program, the Pawsey Supercomputing Centre is at the very forefront of Australia's scientific future.

The Pawsey Supercomputing Centre is a venture that has always been about vision, seeing the limits of scientific capability and pushing beyond them. While it is indeed the most advanced facility for scientific computing in the nation, arguably what is more important is what the Centre represents for the future.

As well as providing solutions for the Big Science issues facing Australian researchers, the Pawsey Supercomputing Centre creates the foundation for what is expected to make Australia the most scientifically significant nation on the planet.

Western Australia will play home to part of the world's greatest scientific undertaking – the Square Kilometre Array project – and the computational infrastructure required to manage it will be of a level beyond current comprehension.

The vision of Pawsey is to bridge that gap, to provide a solid support for what will be the most powerful computing infrastructure in human history.

While the world comes together to make the SKA a reality in a historical collaborative effort, the Australian Government has joined the Western Australian Government and the Pawsey Partners in a collaboration unique in Australia's scientific landscape.

I am proud to have overseen this first year of Pawsey, and to present you with this Annual Report.

John Langoulant
Chairman of
Pawsey Supercomputing Centre
September 2015

OVERVIEW

Pawsey Supercomputing Centre northern facade

The Pawsey Supercomputing Centre is a world class high performance computing facility representing Australia's commitment to the solution of Big Science problems. The Centre is leading the national drive to support research which secures Australia's economic, social and environmental future, by delivering the highest level of computational power available to tackle the biggest of issues.

Named in honour of Dr Joseph Pawsey, the father of Australian radio astronomy, the Pawsey Supercomputing Centre stands at the forefront of Australia's most important scientific disciplines by handling computational challenges of the highest scale. The Centre services key scientific areas such as radio astronomy, bioinformatics, resources science and energy research, ensuring Australia remains internationally competitive in sectors of national significance. Housing Magnus, the most powerful public research supercomputer in the Southern Hemisphere, the Pawsey Supercomputing Centre is a state-of-the-art facility delivering cutting edge science for Australia's future.

The Pawsey Supercomputing Centre is a joint venture that brings together the Federal Government, Western Australian Government, University Partners and collaborating organisations in a consortium that has been steadily producing outcomes for more than fourteen years. Rather than a single-service agency, the Centre is focused on providing integrated research solutions by giving users simultaneous access to world class expertise and infrastructure in supercomputing, data, and visualisation services.

Australia is home to a robust national research infrastructure network that provides researchers with an extensive array of tools and services to conduct their work to the same level or beyond their peers in any other nations. Within this diverse range of services the Pawsey Supercomputing Centre has defined itself by supporting projects that require the highest levels of raw computing power, allowing other organisations to handle smaller projects. This singular focus brings unique value to Australian researchers, allowing them to tackle issues of a scope beyond that manageable by many other nations.

The Pawsey Supercomputing Centre's priority research areas are radio astronomy, resources and mineral sciences, and energy research. As a uniquely West Australian facility, the Centre is able to capitalise on the local expertise in radio astronomy and earth sciences to allow researchers in these fields to lead the world in ground breaking scientific activities that return significant benefits to the State and the nation.

Positioned in the world's most heavily-populated timezone, the Centre takes a leading role in managing Australia's position in the Asia-Pacific high performance computing sphere and ensures knowledge transfer flow with neighbouring nations.

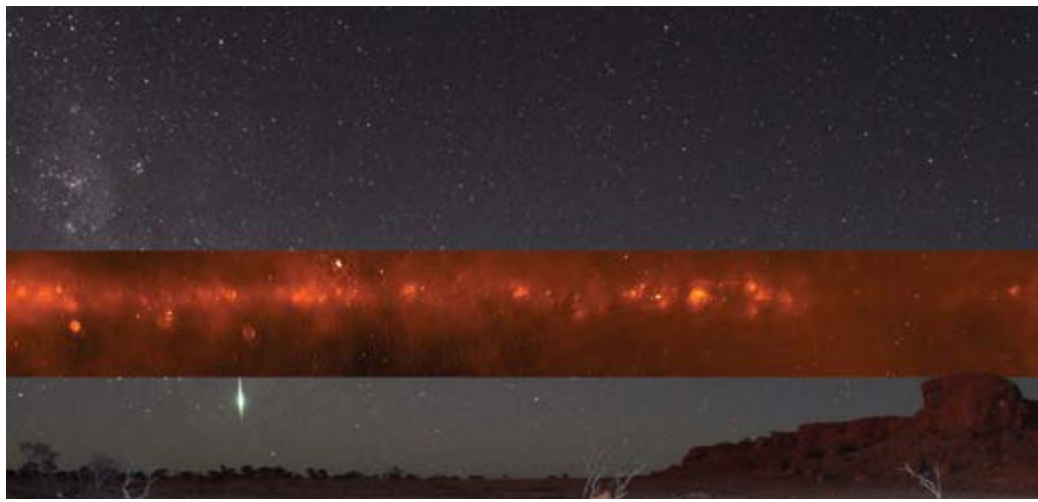
In recognition of the focus of the Centre, in the 2014-2015 period a 25% share of its supercomputing capability was devoted to the radio astronomy sector, in support of Australia's commitment to the SKA project, with a further 25% allocated to resources, energy and minerals research. Researchers across the nation are able to access 15% of capacity through the national merit allocation scheme with the remaining 30% and 5% committed to the Pawsey Supercomputing Centre's Partners and the Pawsey Supercomputing Centre Executive Director's share respectively.

The Government of Western Australia has committed approximately $21m over the next 5 years to enable the Centre to operate its facilities and develop Perth as one of the leading centres of supercomputing expertise in the region. The continuing long term investment by the Government recognises the vital role supercomputing plays in the future prosperity of the State across a broad range of research areas and reinforces the commitment of Western Australia to the SKA, the world's greatest science project.

The Pawsey Supercomputing Centre's Partner organisations - CSIRO, Curtin University, Edith Cowan University, Murdoch University and The University of Western Australia - all contribute significantly both in terms of operational support and providing access to expertise in key activity areas.

The Centre is a purpose-built structure, housing supercomputers and associated works, located in Kensington, Western Australia. The building is located on CSIRO-owned land adjacent to the Australian Resources Research Centre facility, approximately six kilometres from Perth's CBD. The facilities incorporate initiatives to minimise impact on the environment and employ best practice technologies to reduce energy usage.

Through a world-leading collaborative effort between Government and academic institutions, the Pawsey Supercomputing Centre leads Australia's most important high powered research activities and has made Western Australia a regional leader in high performance computing expertise.



Top: Murchison Widefield Array (MWA) image of the Milky Way galaxy, spanning a large fraction of the southern sky (credit: MWA consortium). Bottom: Artist's impression of the Bombora Wave Power flexible membrane energy generator.

2014-15 has seen the Pawsey Supercomputing Centre take its place as the Australian leader of high performance computing research services and expertise. Utilising the power of the most powerful public research computer in the Southern Hemisphere, we are enabling Big Science outcomes that are simply not possible anywhere else in the nation.

This has been the first year of the Centre's full operation and it has realised the potential created by years of hard work and investment of resources by many people. Bringing together diverse partners from across the nation, we have created an institution that will ensure Australia remains globally competitive in high performance science for decades to come.

Our drive has been the creation of a Centre that does not solely focus on providing local services, but recognises Australia's role in the global knowledge economy and works to maintain its primacy in key areas of endeavour.

This is reflected in our involvement in the Square Kilometre Array (SKA) Project which will see the eyes of the world on Western Australia as it hosts a significant portion of the greatest scientific project in human history. The SKA is attracting the world's finest minds in the fields of radio astronomy and computational science, and the Pawsey Centre acts as a central point with which to construct the critical mass of knowledge required for the SKA to succeed.

We are also devoting a significant portion of the Centre's capacity to research in the Energy and Resources sectors, recognising that this is an area of crucial global scientific importance where Australia is a key thought leader. Building on decades of research, we work to develop new, better ways of gaining access to these fundamental building blocks of advanced society and to explore new technologies that will provide a sustainable future for generations to come.

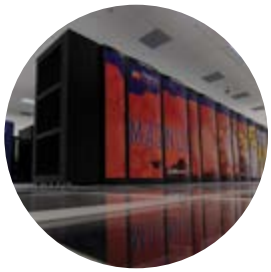
Moving forwards, we will build upon the spirit of unity that informed our creation, to work with the Western Australian and Australian Governments to ensure the finest science outcomes are achieved through collaborative practice between all areas of the research community.

The Pawsey Supercomputing Centre is the most advanced research facility of its type in the country, and I am proud to work with our talented staff and the most exceptional researchers to ensure the world is aware of Australia's unique place at the head of the global scientific community.

Neil Stringfellow
Executive Director of
Pawsey Supercomputing Centre
November 2015

July 2014

Magnus Phase 2 upgrade takes it to the Petascale.



November 2014

Magnus debuts at #41 on Top500 list, most powerful scientific supercomputer in the Southern Hemisphere.

SC14: Pawsey manages Australian Student Cluster Competition team for second year running.

December 2014

Hon Donna Farragher announces iVEC officially rebranding to Pawsey Supercomputing Centre and publicly launches Magnus Phase 2 upgrade.

January 2015

Pawsey Nectar node goes online.

February 2015

Bioinformatics Pawsey Petascale Pioneers projects begin.

April 2015

Pawsey manages Big Data Week in Perth for third year running.

May 2015

Pawsey Supercomputing Centre user Professor Julian Gale elected as one of the Australian Academy of Science's 2015 Fellows.

June 2015

Pawsey users Professor Steve Tingay and Dr Randall Wayth are recognised at the Thomson Reuters Citation and Innovation awards for MWA research.

BIG SCIENCE FOR AUSTRALIA'S RESEARCH FUTURE

The Pawsey Supercomputing Centre represents a unique recognition by Australia's government and research organisations that a single world class supercomputing facility is not sufficient to keep Australia globally competitive in areas of key endeavour.

In previous decades, the nationalised focus of research allowed greater concentration of advanced computational infrastructure. This saw Australian researchers build on a long history of achievements that includes the pacemaker, medical penicillin, Wi-Fi technology and the bionic ear.

However, globalisation and the spread of high speed internet connectivity has changed the international research landscape and the Pawsey Centre was born of a vision to ensure Australia remains at its forefront.

Researchers are now able to share and grow their knowledge at an unprecedented level and this information revolution has seen the birth of 'Big Science' – and the need for research solutions that can encompass it.

Where scientists may have previously been limited to working with data sets that were either locally sourced or procured at great difficulty from distant locations, they now can draw on vast amounts of information that can be delivered almost instantly from anywhere in the world.

The result is that the scale of research has increased exponentially in a brief historical timeframe and scientists are wrestling with how to manage this increase in scope and allow it to deliver commensurately greater benefits – 'Big Science', arising from the explosion of 'Big Data'.

Big Science challenges require the power of supercomputing and cutting edge data management technology, united to give researchers easy access to the best data and the computational power to make use of it.

The Pawsey Supercomputing Centre, and its sister centre, NCI in Canberra, represent Australia's response to the challenge of Big Science and the recognition that every coming year will see bigger and bigger projects undertaken.

Australia is in a race with other nations to deliver scientific solutions to global issues, and to deliver innovations which return social and economic dividends. Failing to be competitive means purchasing these advances from others and has a flow on effect towards the attractiveness of the nation for potential investors.

The hosting of two national supercomputing facilities recognises that in order to maintain this competitiveness, the correct technology and expertise mix is required. As high performance computational hardware has a lifespan of 3-5 years, a pair of facilities allows one to operate at peak global level while the other is re-tooling and acquiring new hardware. These roles are then traded back and forth to ensure Australia maintains sustained coverage and does not spend time utilising sub-optimal equipment.

The importance of Big Science in maintaining Australia's global competitiveness cannot be underestimated and will grow continuously. As the Southern Hemisphere's most powerful facility of its type, the Pawsey Supercomputing Centre is central to securing the nation's research future and is already delivering results in key scientific disciplines.

Two areas of scientific endeavour have been chosen as the primary focus for the Centre – Radio Astronomy and Resources and Energy Science. These are disciplines in which Australia is a global leader and the power of the Pawsey Supercomputing Centre is being used to ensure it remains so for years to come.

RADIO ASTRONOMY AND THE SKA

Outrigger tile (Credit, Kirsten Gottschalk, ICRAR).

Galaxy.

The Square Kilometre Array (SKA) is an international project to build a next-generation radio telescope, which will be 50 times more sensitive and able to survey 10,000 times faster than today's most advanced telescopes. A $2.3 billion joint effort between institutions from over 20 countries, the SKA will be co-hosted by southern Africa and Australia.

The SKA will help scientists answer fundamental questions about the origins of the universe, such as how the first stars and galaxies were formed.

The Australian component of the telescope will be located at the Murchison Radio Astronomy Observatory (MRO), the centre of a radio-quiet zone near Boolardy in Western Australia, 315km northeast of Geraldton. The Australian component covers the low-frequency range of the SKA.

In addition to delivering groundbreaking scientific results, the SKA also brings many other benefits to Australia.

As one of the two co-hosts, Australia's central involvement in the SKA will help to cement the nation's place at the forefront of the global scientific community.

By raising Australia's international profile as a scientific leader, the SKA will bring greatly increased international investment to the North West region of Western Australia as well as the entire nation.

The Pawsey Supercomputing Centre is one of around 20 members of the SKA Science Data Processing consortium (SDP). The consortium is responsible for designing the infrastructure, hardware and software necessary to process, archive and visualise the data produced by the SKA.

The Australian component of the Science Data Processor of the SKA is under consideration to be hosted at the Pawsey Supercomputing Centre.

The Pawsey Supercomputing Centre's cutting-edge resources and expertise will be crucial in processing the immense data products produced by this world-leading astronomy project.

The ambitious scope of the SKA presents a number of challenges, some of which the Pawsey Supercomputing Centre is uniquely positioned to help with.

When the SKA is completed, it will collect more data than is contained in the entire Internet today, representing a significant computing challenge.

The amount of data produced is expected to be too large to store for any reasonable period of time. This means the data must be processed in real-time, necessitating an immense amount of processing power.

Two pathfinder projects for the SKA, the CSIRO's Australian Square Kilometre Array Pathfinder (ASKAP) and the Murchison Widefield Array (MWA) were launched in late 2012 and are serving as important technological demonstrators for the SKA.

Both ASKAP and the MWA already make use of the Pawsey Supercomputing Centre's facilities, which represents an advantage in terms of hosting the SDP component.

The Pawsey Supercomputing Centre supercomputer 'Galaxy' is the Science Data Processor for the ASKAP and MWA projects. Data products from both projects are stored at and distributed from the Pawsey Supercomputing Centre.

With its experience in processing data from the pathfinders, the Centre has vital experience testing the technologies and potential problems the SKA may face.

As a member of the SKA SDP consortium, the Pawsey Supercomputing Centre can comment and advise on its experience in this field in a way that many other supercomputing centres that are involved cannot.

Pawsey staff are actively contributing to the Science Data Processor consortium. This includes system architecture, horizontal prototyping, data delivery, and data centre design. Since the Science Data Processor is a distributed international consortium, Pawsey staff have travelled to ASTRON in the Netherlands, Fremantle, and Cambridge England. Pawsey staff have also visited the LOFAR and Westerbork radio telescopes in the Netherlands.

The Pawsey Supercomputing Centre also holds key skills in the area of visualisation, which will allow the raw data from the SKA to be explored in new dimensions by the international community.

ENERGY AND RESOURCES

Australia's economic prosperity in recent decades has relied heavily on exports of mineral and energy resources. However, global expenditure for resources exploration has seen sharp declines, with a follow on effect to the Australian, and in particular Western Australian, economy.

Part of the reason behind this slump is the exhaustion of cheaply and easily accessed deposits and the difficulty of finding and exploiting more inaccessible deposits. To maintain this vitally important sector of the Australian economy, improved imaging and extraction techniques are needed across a wide scope of resources and energy sectors.

The Pawsey Supercomputing Centre is committed to enabling research into investigating and developing these new techniques, including enhanced identification, imaging and recovery methods. Not only do these technologies hold direct economic benefits for Australia that can be measured in billions of dollars, but they also help to place Australia firmly at the forefront of minerals and resource exploration in the global scientific community.

This commitment is signalled by the allocation of up to 25% of the total resources of Magnus, the most advanced research supercomputer in the Southern Hemisphere, to research in these areas. These resources are made available to researchers nationwide, with submissions assessed on their scientific merit and alignment with national and state science priorities.

Through this process, the Centre is enabling a concentrated portfolio of resources and energy research projects that is unmatched anywhere in the world. In accordance with the governmental priority areas, the projects supported include both more efficient means of conducting traditional energy and resources activities and the development of new methods aiming to introduce step change technologies.

The allocation of raw compute power is matched by the provision of specialist services that allows researchers to maximise their utilisation of the resources available. With over a decade of experience in supporting computational research projects in these sectors, the Centre has established a knowledge base of critical expertise that ensures tailored support solutions.

Beyond supercomputing power and expertise, users are supported with world-class data management, networking and visualisation technologies which allow a variety of research products to be output.

A full solution service is provided by the Centre, allowing users to run project calculations on Magnus, transfer to the Petabyte Data Store or remote locations via high speed networking, and output 3D visualisations that can be experienced firsthand in the fully equipped visualisation room.

With scientists across Australia engaged in world leading resources and energy projects made possible by its resources, the Pawsey Supercomputing Centre is acknowledged as a leading global hub for these research sectors.

SIMULATING THE FIRST GALAXIES

PROJECT LEADER: Doctor Alan Duffy
AREA OF SCIENCE: Astronomy
SYSTEM: Magnus
TIME ALLOCATED: 1,400,000 Hours

A team of researchers led by Dr Alan Duffy from Swinburne University's Centre for Astrophysics and Supercomputing is using the petascale power of the Pawsey Supercomputing Centre to uncover the secrets behind the birth of the Universe's first galaxies. The project is simulating the little-understood formation of these galaxies at an unrivalled level of detail, which is not only groundbreaking research in its own right, but will also help unlock the potential of next-generation radio telescopes.

Challenge

"We're now trying to understand the earliest moments of our universe's history," says Dr Duffy.

"It's challenging because we don't understand the physics of the early universe particularly well; we don't really know exactly how to 'build' a galaxy in detail."

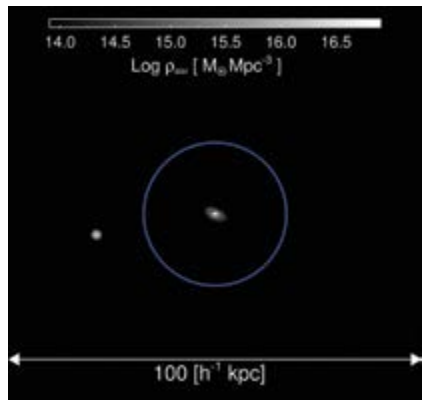
The processes behind the birth of these galaxies can be studied both through simulation using supercomputing, as in this project, or directly observed using telescopes such as the Australian Square Kilometre Array (SKA) precursor projects.

"However, we are limited in those observations, quite drastically at this stage. So, we have to infer from these tiny bits of information we have from these vast distances, essentially what the galaxies are doing," says Dr Duffy.

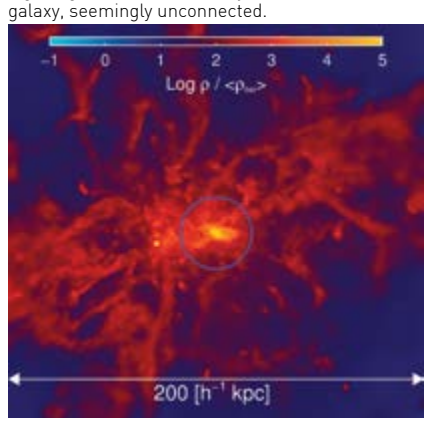
As these telescopes produce data sets in the form of raw statistical outputs, simulations like Dr Duffy's are essential to allow researchers to properly interpret the results of their projects – acting as a 'numerical laboratory' to make "...solid predictions for these first galaxies, and then to try to guide the interpretation of the observations as well."

However, this process is practically impossible to perform using traditional computing methods, according to Dr Duffy.

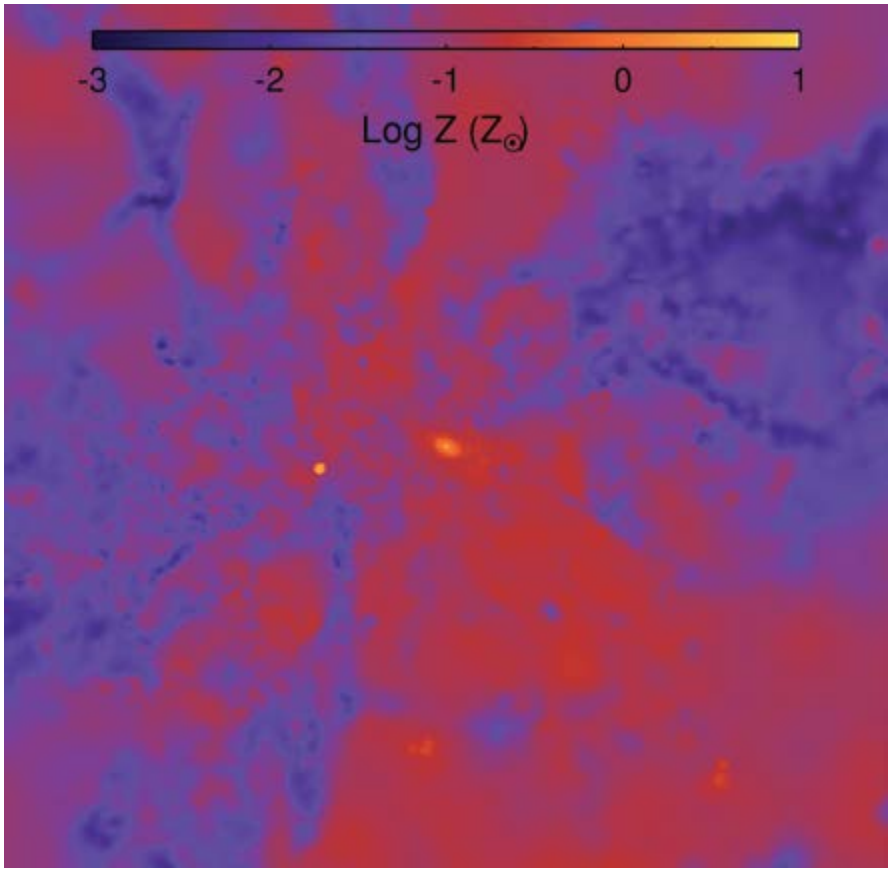
"You have to run the same simulation over and over again, tweaking the physics each time - it's extremely time-consuming, computationally speaking, to run one of these simulations even once. To do it over and over again, systematically varying your experiment, is only possible thanks to the extraordinary facility the Petascale Pioneers Program offered."



The stars in a galaxy forming ~1bn years after the big bang. There is a main object and a satellite galaxy, seemingly unconnected.



Tenuous filaments of gas connect the central galaxy more widely to the large structures around it in the early universe.



Heavier elements ejected from exploding stars into the 'pristine' gas around the forming galaxy. In the real universe these will one day find their way into forming planets and ultimately the iron in your blood and calcium in your bones.

Solution

Using highly optimised code running on the petascale 'Magnus' supercomputer, Dr Duffy and his team were able to simulate the formation of these galaxies at a scale previously unseen in Australia.

"The code we were using had been systematically improved over the years working on Pawsey's previous machines, Epic in particular, and then having the confidence to scale this up to the billion particle scale we are ultimately able to run on Magnus."

Dr Duffy and his team are also able to take advantage of Pawsey's world-class data storage resources and expertise to help archive and access the vast amounts of information produced by a project like this.

"It's one thing to crunch the numbers but an entirely different thing to actually store it and to analyse it," says Dr Duffy.

"What is also crucial is knowing the Petabyte storage facility had the capacity and the fast disk to take the data."

Outcome

Dr Duffy and his team are able to simulate the formation of some of the earliest galaxies in the universe at an "unsurpassed" resolution – over a billion particles.

"The results from this project are going to be used in interpreting the results from the Murchison Widefield Array telescope facilities in Western Australia. With the telescopes, you basically get a statistical description of the night sky, and to actually turn that into 'where's the galaxies, what are they doing?' that has to come through these simulations."

The vast amounts of data produced by this project are also spurring the development of next-generation software and infrastructure to transfer and analyse this data and allow practical sharing of the results of this project and others like it.

"This data set ended up being a test case for that," says Dr Duffy.

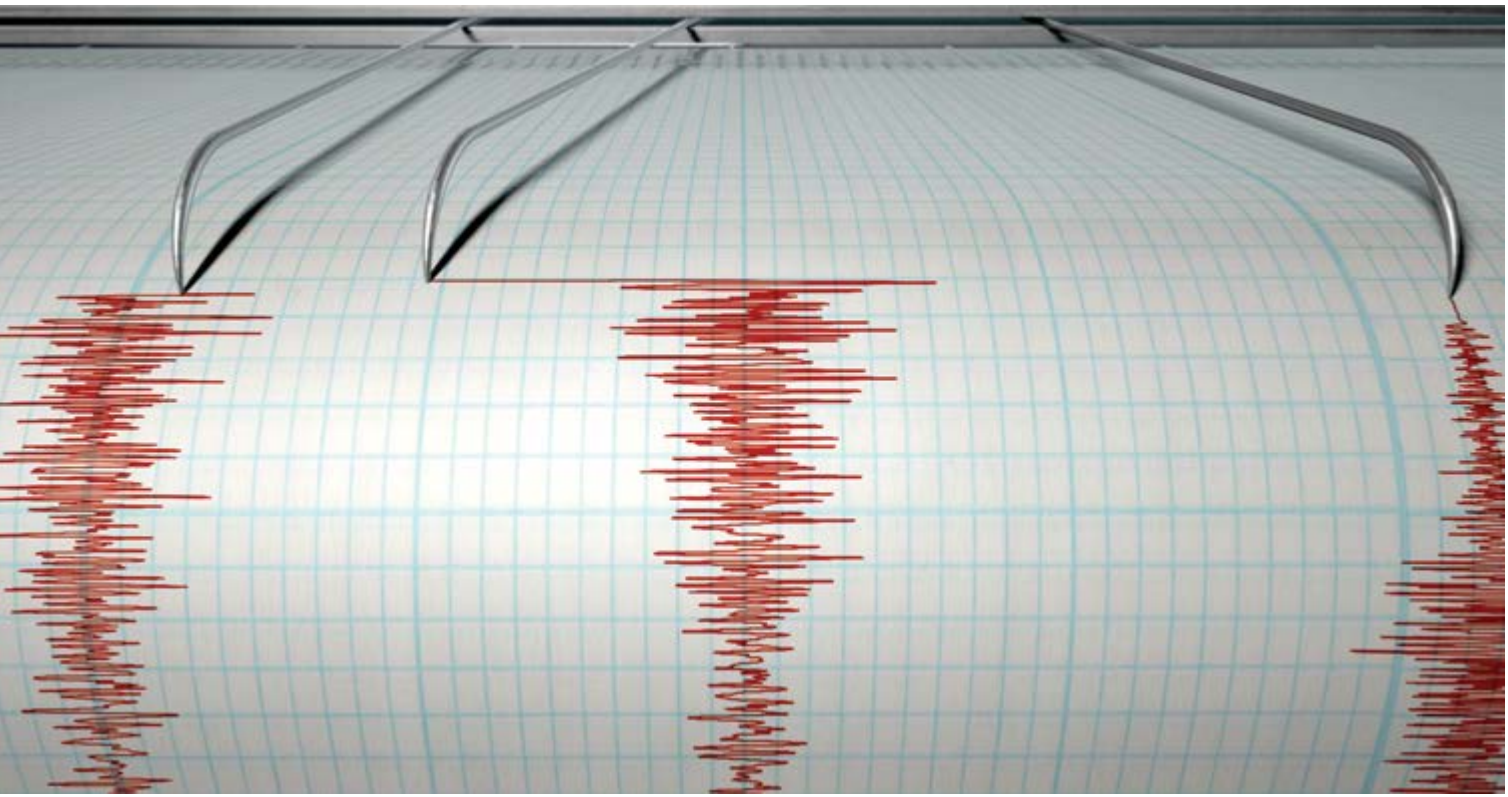
"That protocol has been widely used since – it's stupendously fast, orders of magnitude faster than anything else that was available. All in all it's been a challenge, but that challenge has inspired some amazing development."

SWINBURNE UNIVERSITY OF TECHNOLOGY

PRODUCING SAFER CARBON STORAGE OUTCOMES

PROJECT LEADER: Professor Jeff Shragge
AREA OF SCIENCE: Resources
SYSTEM: Magnus
TIME ALLOCATED: 10,000,000 Hours

Associate Professor Jeffrey Shragge, in collaboration with other researchers at The University of Western Australia, is using the Pawsey Supercomputing Centre's resources and expertise to perform large-scale simulation, imaging and inversion of 3D passive elastic seismic wavefields. 3D and time-lapse (4D) seismic imaging are central to the exploration and monitoring the production of Western Australia's hydrocarbon resources as well as achieving a better subsurface understanding in CO2 geosequestration projects.



Seismograph machine needle drawing a red line on graph paper depicting seismic and earthquake activity.

Challenge

Passive seismology, which uses continuously recorded ambient seismic wavefields without the explicit use of man-made sources, is increasingly becoming an important part of modern hydrocarbon and CO2 geosequestration projects. Passive seismic imaging and velocity inversion involves processing ambient recordings to determine the internal structure of the Earth and recover estimates of physical properties. Passive seismic monitoring over calendar time can be useful for imaging subsurface fluid flow and revealing subsurface geomechanical alteration.

"These waves have a lot of information about the structure of the Earth, the velocity and other material property parameters of the Earth," says Assoc. Prof Shragge.

According to Assoc. Prof Shragge, while the computation of a numerical solution to a individual wave equation is fairly straightforward, the compact 'stencil' operations used in these solutions have to be repeated many thousands of times over a large grid for industry-scale projects, making the process extremely computationally expensive.

"The key is, without supercomputing we're really inhibited by the scale we can work with.

"These complex 3D and 4D seismic wavefields are a large computational problem and a significant high performance computing issue because we're talking about very computationally expensive kernels, which have to be repeated up to tens of thousands of times."

Solution

Assoc. Prof Shragge and UWA collaborators Prof. David Lumley, Dr. Rie Kamei, Dr. Toby Potter and Dr. Taka Miyoshi are using a combination of existing and in-house codes on the Pawsey Supercomputing Centre's petascale 'Magnus' supercomputer.

"We represent our wave equations as very compact 'stencils', which can be shifted around all over our grid," says Assoc. Prof Shragge.

"Because we have these compact stencils combined with very large grids, we can really leverage the parallelism inherent in the Pawsey Centre computing architecture."

This approach, combined with the processing power of Magnus, allows researchers to simulate realistically sized 3D models.

"One of the key things is just the scale of the cluster is allowing us to move fully into 3D active- and passive-source imaging and inversion. In order to be really relevant to local industry, we have to be able to do these things in 3D, as the world is inherently 3D and complex," says Assoc. Prof Shragge.

Outcome

By being able to simulate realistically sized 3D models, Assoc. Prof Shragge and his collaborators can provide more detailed and accurate information to support projects like the National Geosequestration Laboratory (NGL), a collaboration between UWA, CSIRO and Curtin University that enables research and development of commercial-scale carbon storage options for Australia.

"The other thing is that we have a lot of partnerships through our UWA:RM (UWA Reservoir Management) Research Consortium consisting of industrial sponsors," says Assoc. Prof Shragge.

"A lot of the research that we do, we collaborate closely with our industrial partners in terms of solving advanced seismic imaging and inversion problems. Largely, this is focused on the North West Shelf of WA and the oil and gas fields there.

"A lot of the practical benefits come from working closely and the technology transfer to local, national and international industry."

Assoc. Prof Shragge says access to the Pawsey Centre allows public institutions like WA to deliver internationally competitive results.

"Machines like Magnus are enabling technologies that allow us to do what we know we need to."

PROJECTS
USING QUANTUM MECHANICS TO UNLOCK THE SECRETS OF CORAL

PROJECT LEADER: Professor Julian Gale
AREA OF SCIENCE: Chemistry
SYSTEM: Magnus
TIME ALLOCATED: 48,960,000 Hours

Biomineralisation is one of the most important processes for mineral formation in the natural world – taking place in everything from coral reefs to bones and teeth in the human body. One of the most widespread of these minerals is calcium carbonate. Despite being so widespread, relatively little is known about the formation of these minerals. Professor Julian Gale from Curtin University is leading a team of researchers to uncover the secrets of these common but little understood processes.

Challenge

"One of the most widespread minerals in the environment is calcium carbonate and its formation is especially important since it can be found everywhere from the limestone cliffs of the Nullarbor to scale in kettles & industrial pipelines. Closely related minerals are also being considered as candidates for long-term geosequestration," says Professor Gale.

Despite being so common, it is very difficult to directly study the formation process of biominerals like calcium carbonate due to the extremely small size of the species involved and their low concentration. Recently, supercomputing has helped researchers produce computer models to simulate the early stages of formation.

"The advent of petascale computing it has now become feasible to directly test some of the results of empirical force models against what should be, in principle, more reliably methods based on quantum mechanics, in which the interactions come from fundamental laws of physics," says Professor Gale.

However, these simulations can be extremely computationally intensive. Professor Gale says that while most simulations of this kind to date have involved tens of thousands of calculations, his team's project aims to model many millions of steps instead.

> "The challenge is not to be able to run a single calculation, but that the parallel scaling needs to be sufficient that each calculation would only take a few seconds to execute to make long runs feasible."

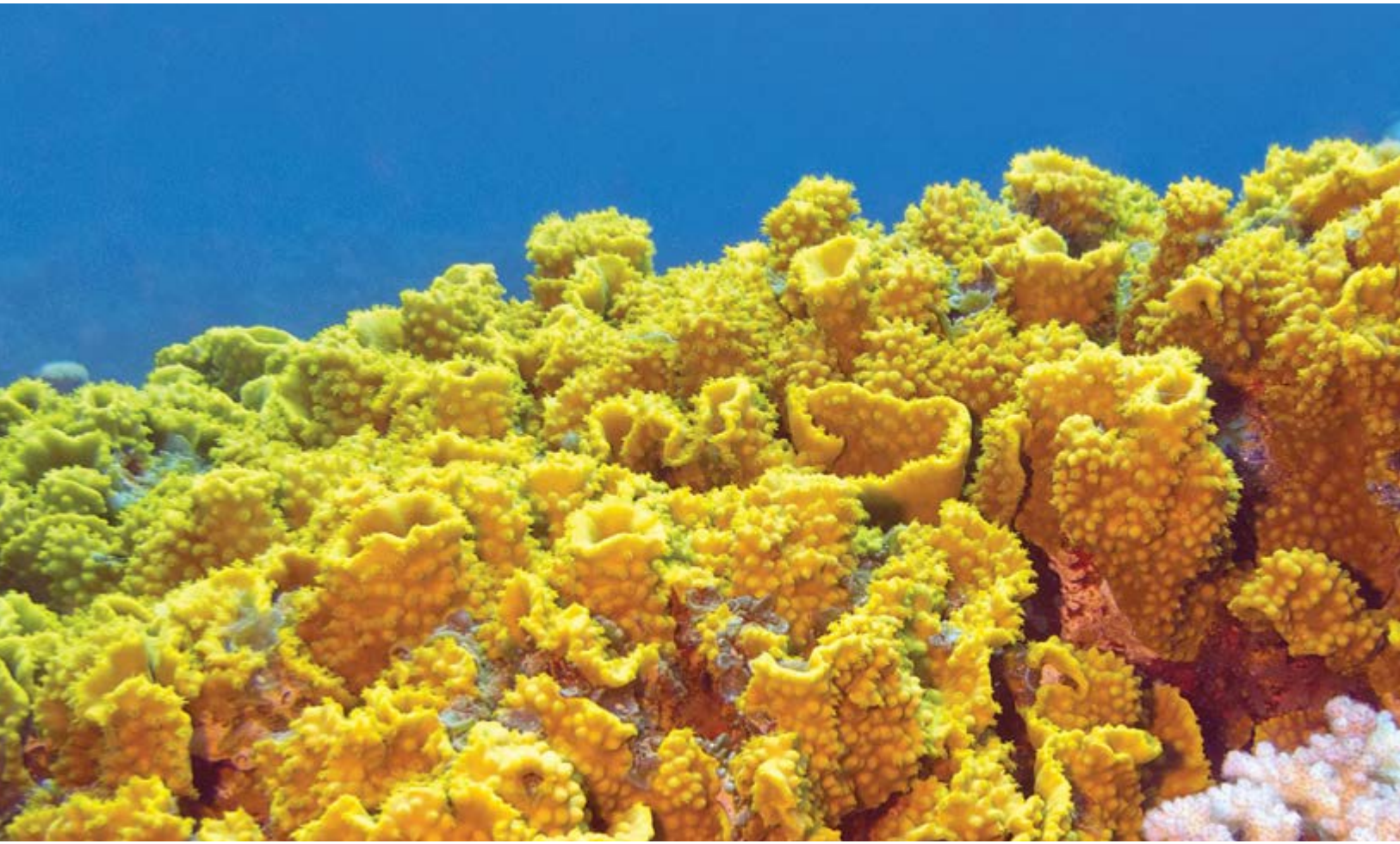
Solution

Using Magnus, Professor Gale and his team are able to perform the rapid parallel calculations needed to simulate millions of steps in a practical timeframe.

"Choice of algorithm and some of the unique features of CP2K in particular are key to being able to exploit the computing power of the Pawsey Centre and to achieve the objectives of our project," says Professor Gale.

"During the course of the project we have managed to tune the computational settings to gain in excess of an order of magnitude in productivity (i.e. time per step) without adversely affecting the quality of the results."

Combining supercomputing processing power with advanced codes and algorithms, Professor Gale and his team are able to model the binding of calcium and carbonate atoms at a realistically low concentration.



Coral reef with yellow coral turbinaria mesenterina at the bottom of a tropical sea.

Outcome

"Our simulation is one of the most extensive quantum mechanical molecular dynamics studies ever performed in the world to date," says Professor Gale.

The simulation highlights some significant differences between the quantum mechanical and empirical simulations that will now be explored.

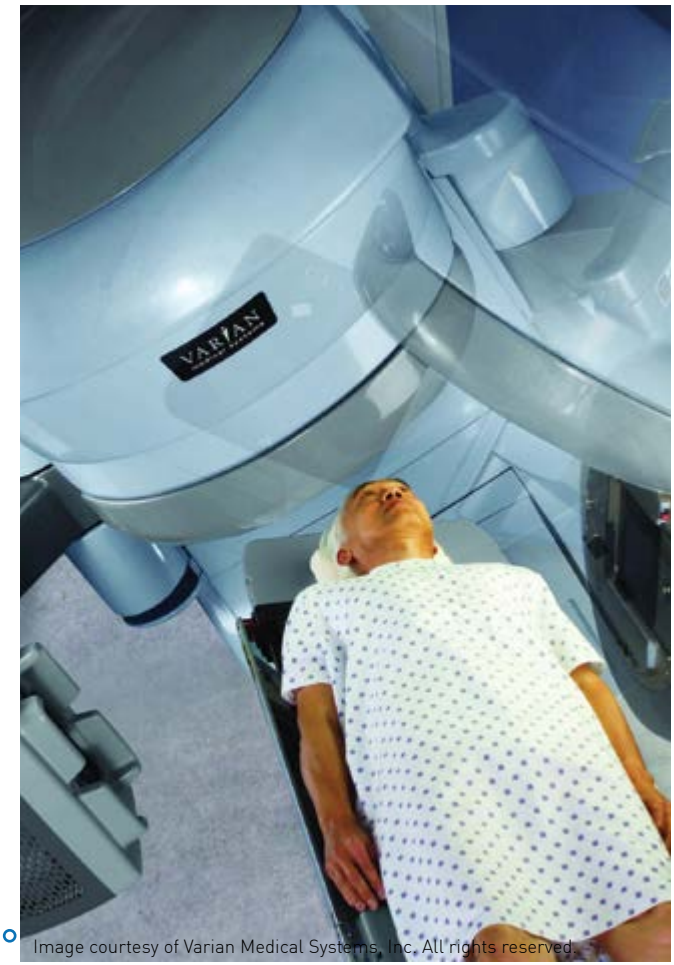
"The results from this project will lead to improved force field models that better capture some of the important features of the quantum mechanics."

As a result of this project, one of the most common but least understood building blocks of the world is now being uncovered.

DEVELOPING SAFER CANCER RADIATION THERAPY

PROJECT LEADER: Professor Martin Ebert
AREA OF SCIENCE: Medicine
SYSTEM: Fornax
TIME ALLOCATED: 60,000 Hours

A team of researchers led by Professor Martin Ebert from The University of Western Australia and Director of Physics Research at Sir Charles Gairdner Hospital is using the Pawsey Supercomputing Centre's resources to develop safer and more efficient methods of cancer treatment through radiation therapy. The project is studying radiation detector response to high-energy X-ray beams used in the treatment to better determine potential risks and develop improved treatment technologies.



Challenge

Team member Mr Ben Hug says that recent advancements in cancer treatment technology have resulted in the ability to deliver radiation with a higher level of accuracy and precision than ever before.

However, the increase in complexity increases the risk of error and difficulties in verifying the treatment delivery, which could compromise patient safety.

According to Mr Hug, the main computational challenge is that a very large number of histories (treatment case examinations) must be simulated to render the required statistics. The time taken to analyse a history depends on the complexity of the geometry through which that history is being simulated and the different energy cut off values that can determine how long a particle is tracked before it is 'killed'. This research requires a large number of histories, specifically regarding lower energy particles and their associated energy deposition. Running these computational simulations on a desktop system would take an impractical length of time due to the amount of data and necessary software capabilities.

Solution

The proposed solution to this problem is to introduce a device located between the patient and the radiation source, which will monitor the radiation beam as it is treating the patient. This would comprise a flat-panel digital imager that can provide real-time images of the radiation passing through it.

"By comparing the resulting images against the expected image, the amount of radiation and its variation in time can be assessed against that planned," says Mr Hug.

"Any detected difference will indicate an error in the delivered treatment that can be corrected before the patient's next treatment."

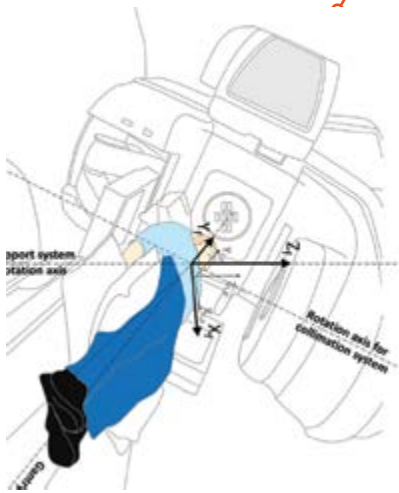
"The detector will also be simulated in a computational environment so that its response can be understood and methods selected to optimise its response over the range of measurement conditions," says Mr Hug.

Outcome

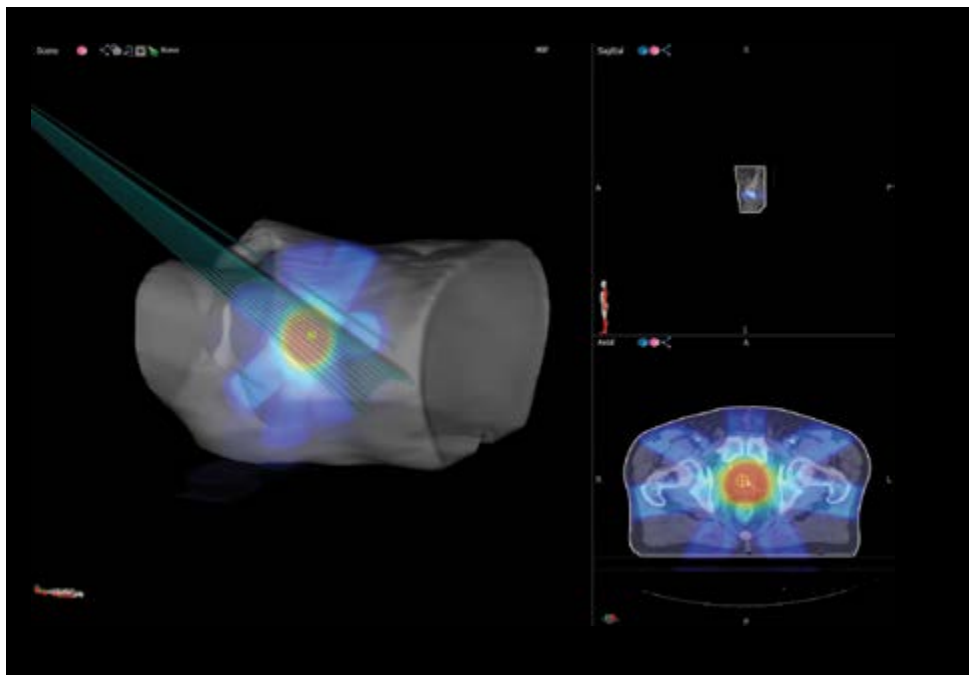
According to Mr Hug, the project involves acquiring a commercial flat-panel imaging system and undertaking measurements on clinical linear accelerators to characterise the system's response under typical conditions.

Ultimately, the end goal is to produce a well-characterised device that can be used to monitor the radiation beam in real time, reducing the quality assurance burden of these advanced techniques, and expand their safe and effective use across larger numbers of patients.

The novel scientific outcomes from this project have been proven to be invaluable, especially considering this type of research has not been done before. This work has aided in gaining an understanding of a fundamental physics concept, which can be challenging to measure. The Pawsey Supercomputing Centre helped both in terms of providing staff to get the code packages installed and running, and also by providing enough compute power to obtain the necessary results.



Conceptual diagram of a patient being treated on a medical linear accelerator.



Simulation of intensity modulated radiation therapy beams on patient from varying angles produced using Geant4 Monte Carlo package on Fornax. Image courtesy of Ben Hug.

PROJECTS

BETTER DISASTER PREDICTION FOR SOUTH EAST ASIA

PROJECT LEADER: Doctor Erdinc Saygin
AREA OF SCIENCE: Geoscience
SYSTEM: Magnus
TIME ALLOCATED: 1,900,000 Hours

Southeast Asia is a tectonically active region that sees many natural disasters such as tsunamis and earthquakes occur as a result of these specific conditions. A team of researchers led by Dr Erdinc Saygin from the Australian National University is using the power of the Pawsey Supercomputing Centre to employ advanced imaging techniques that will significantly increase understanding of the tectonic profile of the region. This work aims to develop processes that may provide early warnings in a broad range of threat areas, potentially saving immeasurable lives and resources.

Challenge

In 2014, the United Nations Statistical Yearbook for Asia and the Pacific ranked the area as the "world's most disaster prone region", with deaths from natural disasters in 2004-13 increasing over 300% over the previous decade. Many of these deaths occur as a result of disasters such as earthquakes, tsunamis and volcanic eruptions that are produced as a result of tectonic activity.

Full waveform inversion is a technique developed over the past decade that enables imaging of the Earth and its tectonic activity with an unprecedented resolution by utilising all of the information contained in seismic waveforms. However, it is extremely computationally intensive and requires use of a high performance computing facility like the Pawsey Supercomputing Centre.

Dr Saygin is working to estimate the seismic velocity structure of the Southeast Asian crust and uppermost mantle using large amounts of full seismic waveform data collected in Australia, Indonesia and neighbouring countries. The Australian tectonic plate is subducting underneath the Eurasian plate and this movement is causing large earthquakes and volcanism in the region.

Full waveform inversion will provide much higher resolution than traditional methods but requires considerably more computational resources and data storage, making it impractical for desktop or small cluster environments.

"Simulation of propagation of seismic waves in 3D is a computationally demanding problem," says Dr Saygin.

"It involves comparison of simulated and observed waveforms, and then updating the underlying model to increase the similarity between these waveforms."

Solution

Using the Pawsey Supercomputing Centre, Dr Saygin was able to draw upon the world-class computational resources required to conduct his research in an exponentially faster time frame.

"Without the facilities at Pawsey, this project could not be materialised," says Dr Saygin.

> "To give an idea, I would have needed 192 individual computers working at the same time to perform the same work, and each step producing over 3TB of data. This would have been impractical."

The work conducted at the Pawsey Supercomputing Centre can now be employed in developing a more comprehensive understanding of local tectonic conditions.

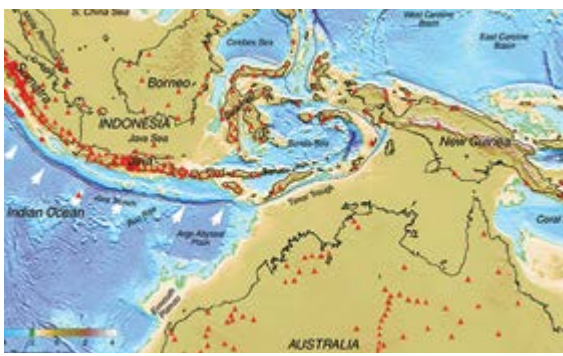
Outcome

The products of this research will reveal information about the 3D structure of the SE Asian crust, which is relevant to seismic hazard studies, regional tectonics and mineral exploration.

"We are currently simulating the waveforms and comparing them with the observed ones," says Dr Saygin.

"The next step is to incorporate a misfit minimisation scheme, which will perturb the model to generate simulated waveforms, which will match the observed ones. This is a multi-iteration approach, which will require many thousands of core hours."

The resulting models will be crucial in increasing understanding of the tectonic framework of the region and in improving the earthquake locations for nuclear test ban monitoring, rapid earthquake impact assessment, and tsunami warning systems.



Map showing distribution of seismic stations used to collect data.

Australian National University

CUTTING EDGE GLOBAL WEATHER SIMULATION

PROJECT LEADER: Dr Marcus Thatcher
AREA OF SCIENCE: Climate Science
SYSTEM: Magnus
TIME ALLOCATED: 15,000,000 Hours

Dr Marcus Thatcher from CSIRO's Ocean & Atmosphere Flagship is using the petascale power of the Pawsey Supercomputing Centre to create the most detailed single global climate run undertaken in Australia. The project explores new techniques that can help future research in high resolution climate models, as well as deliver practical benefits in areas such as extreme rainfall prediction, improved extreme weather management plans and developing better renewable energy technologies.

Challenge

"Essentially the problem is resolution," says Dr Thatcher. "Every time we halve the resolution, such as going from a 100km to 50km grid, the computational cost increases by roughly eight times."

However, these smaller grid sizes can produce vastly more accurate simulations due to better resolving key atmospheric processes, making them extremely valuable for research.

"Even though our computing is getting better all the time, the resources we need are enormous. It is very, very expensive in terms of computing to keep increasing resolution on a global model," says Dr Thatcher.

"You definitely need more powerful computers, because the computational problem you're trying to simulate – weather behavior that occurs over minute or second timescales being simulated over years or decades – generates a massive mismatch in timescales."

Solution

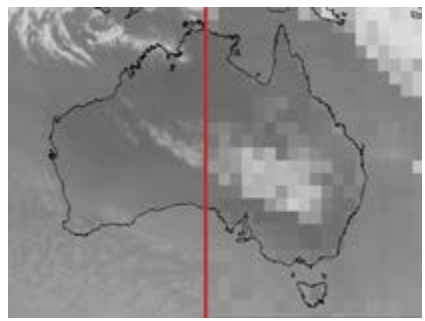
Dr Thatcher is using CSIRO's Cubic Conformal Atmospheric Model (CCAM) to experiment with different strategies to connect ocean and atmosphere models on the Pawsey Supercomputing Centre's petascale Magnus supercomputer. Magnus is the most powerful public research supercomputer in the Southern Hemisphere, providing Dr Thatcher with the raw computing power to run these high-resolution simulations.

"The big advantage with CCAM's design is it scales very well – meaning you can adapt it to the computing resources that you have. If you have a small computer, you can 'shrink' it down to match, and similarly if you have a powerful computer you can expand it fairly easily," says Dr Thatcher.

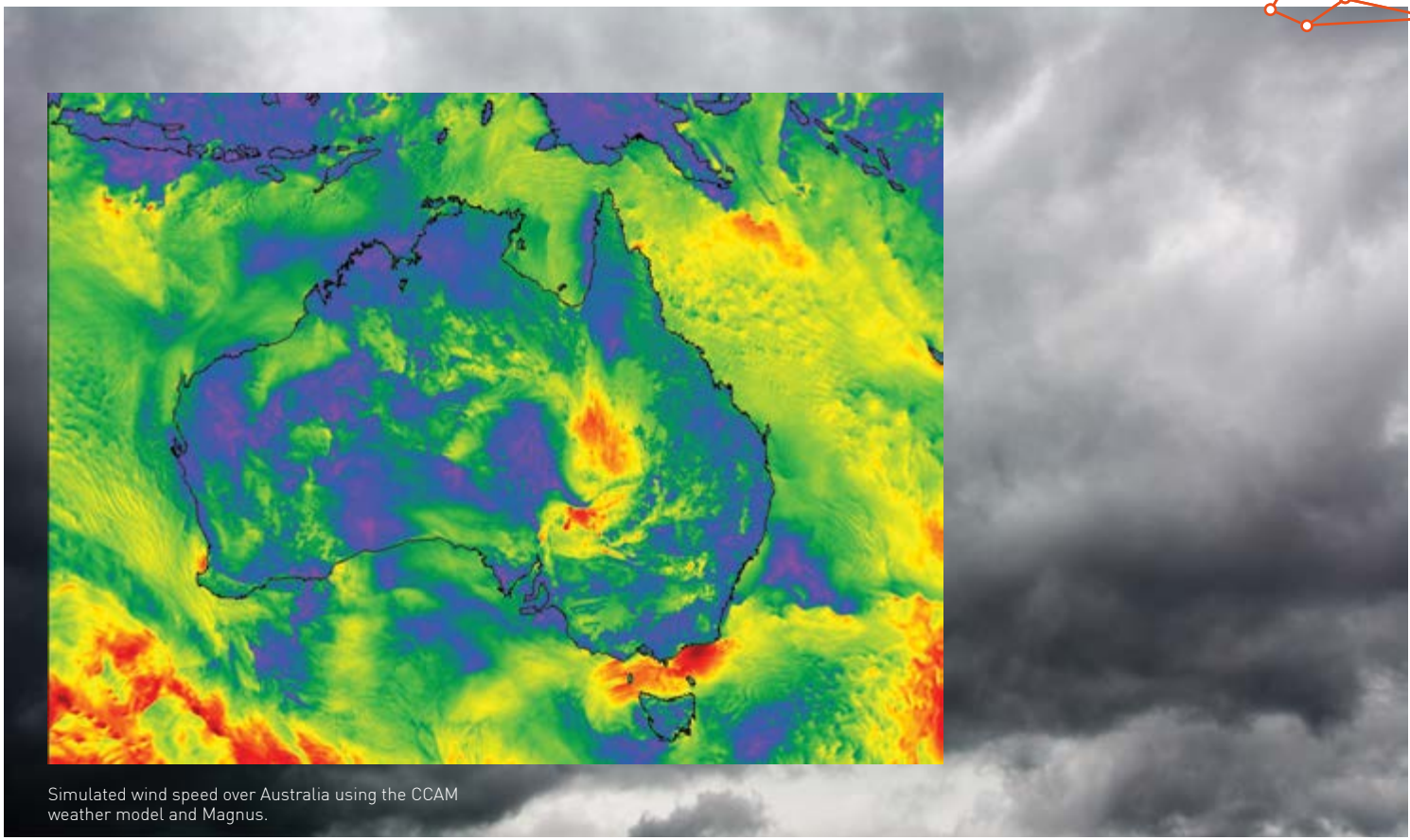
Due to this scaling, and Magnus' efficient architecture, Dr Thatcher is able to achieve internationally competitive results using a fraction of the compute size and cost traditionally required.

"We got performance that was not only competitive in terms of simulating many years at a time at a very high resolution, but we were also able to achieve this on the order of 10-20,000 cores whereas overseas groups are using 200,000 cores."

"Pawsey also helped in terms of configuring the machine, with optimisation tools and on the file I/O side. You can do a lot of calculations quickly, but there's almost no point if you can't get your output down on disk so you can see the results."



Depiction of simulated clouds in terms of longwave radiation L: Dr Thatcher's simulation. R: Example of old simulation.



Simulated wind speed over Australia using the CCAM weather model and Magnus.

Outcome

Using CCAM and the power of petascale supercomputing, Dr Thatcher was able to produce the most detailed single global climate run in Australia.

"We were able to achieve a 13km resolution at 5 simulation years per day, which is up there with the best of them."

Being able to model these high resolutions over a long timescale can bring a range of practical benefits for Australia.

These include more accurate methods for extreme weather prediction, which can lead to improved management and protection strategies.

The project also benefits the work being done on renewable energy

"These technologies are strongly affected by the climate, and more accurate modeling means you can design these systems to more reliably deliver energy into cities despite the fluctuations due to weather."

Dr Thatcher says the Pawsey Supercomputing Centre's petascale resources and the results of this project are a "step change" in climate modeling.

"This was all possible because of this level of computing power."

COMBATING ALZHEIMER'S AND DEMENTIA

PROJECT LEADER: Dr Neha S. Gandhi
AREA OF SCIENCE: Medicine
SYSTEM: Epic
TIME ALLOCATED: 2,000,000 Hours

Thanks to advances in medical science, life expectancy has greatly increased in developed nations like Australia. However, an unwanted side effect of this is a rise in neurodegenerative diseases like dementia and Alzheimer's, with the number of Australians with dementia predicted to rise almost 500% by 2050. Tau protein aggregation is a common pathological process in many of these diseases. Researchers from Curtin University are using the power of the Pawsey Supercomputing Centre to simulate and model protein aggregation to help better understand these debilitating diseases, and develop new management strategies.

Challenge

Dr Gandhi's project is focused on increasing the fundamental understanding of the molecular mechanisms that lead to the abnormal formation of Tau protein in neurodegenerative diseases like Alzheimer's. These diseases, which are progressive and can affect all areas of the brain, are thought to be responsible for up to 70% of all cases of dementia.

Advanced molecular simulation methods can be used to help researchers develop a better understanding of the ways in which these proteins form in neurodegenerative disease cases.

However, this simulation work is extremely computationally intensive.

Dr Gandhi's project worked with representative systems, containing 100,000 atoms.

Using traditional computing methods, simulating the formation of these proteins over just a one microsecond timescale could take an entire year. This makes supercomputing necessary to perform these simulations in a practical timeframe.

Similarly, visualising the data produced by these simulations is very memory intensive, and can only be done using the type of cutting-edge visualisation tools provided by the Pawsey Supercomputing Centre.

Solution

Advanced molecular dynamics simulations were performed using AMBER14, the world's fastest molecular dynamics program, as well as other applications. These applications scaled extremely well on the Pawsey Supercomputing Centre's advanced systems.

"I was able to simulate up to 50 nanoseconds per day," says Dr Gandhi.

This means Dr Gandhi and her team of researchers were able to simulate in 20 days what would take an entire year using normal methods.

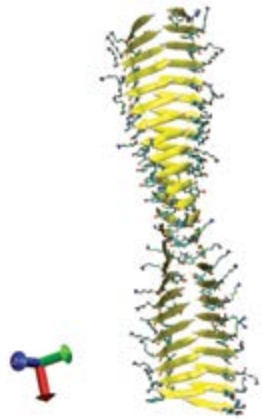
Outcome

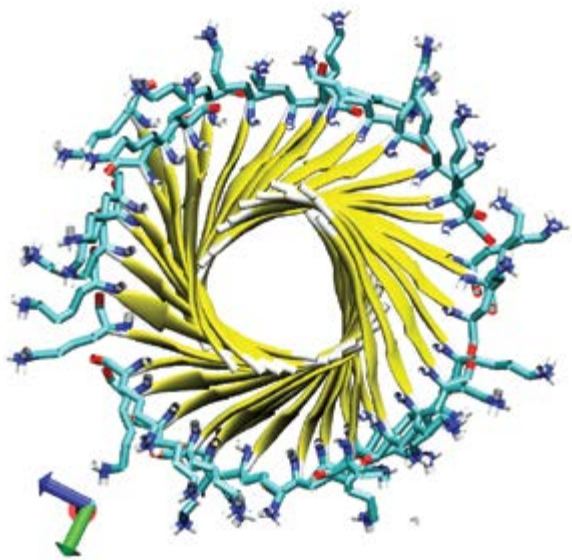
The world-class resources provided by the Pawsey Supercomputing Centre were able to process the immense amounts of data produced by this project efficiently and in a practical timeframe.

This gives researchers more time to interpret their data and deliver practical results.

Dr Gandhi says this project will help to further the understanding of how the Tau protein is formed, and how it contributes to diseases like Alzheimer's.

"The outcomes of this project will create opportunities for the development of new therapeutic interventions that can inhibit protein aggregation and halt the progression of these diseases," says Dr Gandhi.





A model of the Tau protein generated using the Pawsey Supercomputing Centre's resources.

SERVICE HIGHLIGHTS FROM THE 2014-15 PERIOD

The Pawsey Supercomputing Centre works across three main service areas – Supercomputing, Data and Visualisation. Together, these provide Pawsey users with a unified suite of research support resources on par with any in the world.

Supercomputing team

The Pawsey Supercomputing Centre's Supercomputing team is drawn from the international community and has a combined, scientific-computing experience in excess of 50 years. The team's activities are focused on growing the uptake of supercomputing within the Australian science community. This is about more than just porting a researcher's work flow: it is about helping researchers to understand how a petascale system allows them to consider a new class of problem. The supercomputing team is about upscaling researchers' ambitions as well as their applications.

The Supercomputing team engages with the Pawsey Supercomputing Centre community in a range of ways, developing and delivering training materials to grow the base of understanding, providing one-on-one consultations to tackle specific problems, and being embedded into research groups for longer term projects.

ACADEMIC PROJECTS

• Curtin University (Wei Hu): Reloaded Option Pricing -implementing shared-memory parallelisation techniques to extend the capabilities of option pricing models for financial-market simulations.

• CSIRO (Amanda Barnard): Migration of SIESTA models from Epic to Magnus.

• The University of Western Australia (David Glance): Scientific computing in the cloud - A comparison of cloud-based scientific-computing services, such as NeCTAR and Amazon EC2, with conventional HPC systems for modest-scale computations and simulations.

• Edith Cowan University (Maria Albertson): Epigenetic regulation of alternative splicing - porting of a neonatal genetic study onto supercomputing resources in order to extend the level of detail that may be considered.

• University of Western Australia (Linqing Wen): Gravitational Wave Observatory – deployment and optimisation of the analysis pipeline that will consume data streamed from, for example, the LIGO detector aiming to be the first to detect gravitational waves.

• Curtin University (Ben Mullins): Simulation of the human respiratory cycle – deployment and tuning of a moving-mesh CFD simulation aiming to achieve the most detailed simulation ever of the human respiratory system. This work was present in a paper at the HPC in Asia meeting (Leipzig, Germany, June 2014).

• ICRAR (Cormack Reynolds): Migration of VLBI image-processing pipeline and data cache from aging infrastructure within ICRAR onto the Pawsey Galaxy supercomputer.

• Curtin University (Gary Madden): Analysis of Finnish mobile phone trends - tuning and parallelisation of a statistical analysis of the trends in mobile-handset features and functionality.

• Edith Cowan University (Shane Henderson): Render Farm 2015 - Set up of high-performance render-farm environment for ECU students to create ambitious CG animations.

• Murdoch University (Julia Andrys): Set up of the climate simulation tool Planet Simulator, to support a novel approach to educating people about the effects of climate change through computer gaming.

• Curtin University (Ranjeet Utikar): Migration of the commercial application, Fluent, from Epic onto Magnus.

• The University of Western Australia (Laura Boykin): Studying the Whitefly and its effects on agriculture.

• CSIRO (Thomas Poulet): Port of the MOOSE geosciences modelling code to Magnus, along with user training.

• University of Queensland / University of Western Australia, (Kenneth Chan and Juan Montenegro): Port of the groups De

Novo Gene Assembly workflow for the wheat genome from the Barrine life-science facility in Queensland onto Zythos.

• Curtin University/ University of New South Wales/ The University of Western Australia: Remote Visualisation using the Zeus Cluster - Pilot data-intensive visualisation projects to guide the deployment and configuration of visualisation software on the Zeus cluster.

• Murdoch University (Paula Moolhuijzen): Upscaling Wheat Genome Analysis to the Petascale - Attempting to reformulate the way gene-analysis of the wheat genome is undertaken in order to significantly reduce the turn-around time.

• University of Western Australia (George Milne and Joel Kelso): Disease Spread Modelling: working with researchers in the UWA team to implement and prove a more realistic model of how Dengue fever spreads, and how vaccination programs may be optimised to contain outbreaks.

• University of Queensland (Dion Wetherley): Installing and tuning the ESysParticle DEM model on Magnus to support optimisations of the block-cave mining technique.

GOVERNMENT / INDUSTRY PROJECTS

• Department of Parks and Wildlife (Kym Ottewell and Tara Hopley): Migration of key workflows for the department onto Zythos, aiming to exploit the potential improvements and speedup possible with large-memory computing resources.

• Carnegie Wave Energy: Working in collaboration with researchers at Curtin University to set up simulations of the CETO technology, alongside field trials off Garden Island.

• Bombora Wave Power: Working in collaboration with researchers from Curtin University to set up virtual models of the tidal-membrane mechanism.

• Landgate (Aaron Thorn): Advanced Remote Sensing Methods for 3D Vegetation Mapping from Digital Aerial Photography - guidance and support during setup phase of project on Magnus.

• DHI Group (Perth office): training and support for the use of MIKE software, on Epic, to enable accurate flood-management strategies for Gold Coast Water.

• The DNA Bank (Tegan McNab): Magnus migration support.

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Data team

Scientific computing places new demands on a researcher to curate and share their data, to ensure the value, accuracy and longevity of their results. Data is everywhere – for example, the output of a computer simulation, the readings from a sensor network, or the output of a piece of apparatus. The volume, diversity, and variability of data that is being generated translates to both opportunities and challenges for the Pawsey Supercomputing Centre community.

The Data team provides hardware, services and expertise to help researchers improve their management of research data. Managing data involves storing the physical data sets, managing or adding metadata to make datasets discoverable and controlling access to the data.

The Data team is also the Pawsey Supercomputing Centre's interface to the Research Data Services (RDS) project and the National eResearch Collaboration Tools and Resources (NeCTAR) Project Cloud service.

ACADEMIC PROJECTS

• Compressing NetCDF data format (Tom Lyons, Murdoch University) – assisting researchers at Murdoch University to improve effectiveness of their use of Data Stores at Pawsey.

• Use of data stores (Dr Khady Ibraham-Didi, ECU) – assisting researchers at ECU to overcome local security issues.

• Supporting NeCTAR Natural Hazards Virtual Laboratory (Ryan Fraser, CSIRO) – 10 research groups and researchers to request EOIs to use a VL.

• Desert Fireballs Network (DFN) ingestion (Phil Bland, Curtin University) – Continued and extensive support to bring the DFN project to the state of being ready to begin ingesting field data into the production server. This work included the development of several scripts and metadata documents to facilitate this. The Data team has also supported the DFN Project by providing a live demonstration to DFN personnel on the use of a simple scripted approach to ingest some of their data. Additional scripts have been developed by Pawsey to facilitate searching and retrieval of data, in anticipation of the demands of the next phase of this project.

• Access and use of data stores (Laura Boykin, Plant Energy Biology ARC Centre of Excellence, UWA) – assisting researchers at UWA to access to Pawsey Data Stores.

• Human Genetics (Philip Melton, UWA) - These data comprise next-generation sequence data, representing genetic data analysed by the Centre for Genetic Origins of Health and Disease Staff for both national and international collaborators. The Data team has been assisting this group with their application to ensure it can be stored on Pawsey infrastructure safely.

• ARC Centre of Excellence in Plant Energy Biology (Hayden Walker, UWA) – the Data team has been supporting the ARC PEB with the ingestion of data for the Next Generation Sequencing (NGS) pipeline.

• Surface Reflectance Data (Mark Broomhall, Curtin University) – This collection contains swath and gridded reflectance data for all MODIS (Aqua and Terra) bands that reflect from the Earth's surface. There is temporal coverage from 2000 to 2012. The Data team has been assisting the transfer of existing collections from Cortex to the new data stores.

• Australia-China Centre for Wheat Improvement (Rudi Appels, Murdoch University) - This data collection includes large datasets used in the course of research by the Australia-China Centre for Wheat Improvement at Murdoch University. The data collection includes both in-house data generated by Murdoch University, as well as datasets from the international wheat research community. Upon completion and publication of research, datasets in this collection will be made publicly available. The Data team has been assisting Murdoch researchers to use Pawsey Data Stores.

• Genomics on fungal plant pathogens (Jonathan Anderson, CSIRO) – The Data team has been involved with assisting the ingest of Next Generation Sequencing (NGS) raw data. This will be used to analyse fungal pathogenesis on plants by CSIRO.

GOVERNMENT / INDUSTRY PROJECTS

• GSWA State Geophysical Compilation Grids (David Howard – Department of Mines and Petroleum). A project that included data workflow, storage and publishing needs was scoped. The Data Team developed simple routines for NetCDF4 and GeoTIFF conversion from ER Mapper data format and tested data with LiveARC ingest. This data will be integrated with NeCTAR Virtual Geophysics Lab (VGL) developer for data publishing integration. The Data team has complete the work needed to integrate with the VGL.

• Pilbara Marine Conservation Partnership (Dirk Slawinksi, Department of Parks and Wildlife, DPaW). The Project scope has been developed and data has been ingested via Pawsey's new web interfaces for LiveARC.

• DPaW Imagery Katherine Zdunic (DPaW, Remote Sensing). The Data team has directly assisted upload/download of data from DPaW facilities.

• Canning Stock Route (Mollie Hewett, Curator FORM) The Data team has directly assisted upload/download of data from FORM on the Canning Stock Route, a major historical data archive for WA and Australia more generally.

In quarter two, the Data team also assumed some responsibility for supporting government uptake. Specifically this included a Western Australian based consortium of university, industry and government partners led by Dr Michael Meuleners from Ocean Systems Engineering. This consortium will develop a 20 year hind-cast solution of the complex surface wave and surface and subsurface ocean circulation and properties of the waters off Australia's South West coastline focusing on the Geographe Bay region. Coordinating with Dr Meuleners, Pawsey staff are examining the suitability of adapting the CATAMI code-base to be used as a basis for a data portal for the hind case solution results. This data portal would ingest model outputs in NetCDF format and output image products in on-demand manner. Finally Pawsey staff will implement the designed data system as a public data portal including integration with LiveARC.

Tape cell - Pawsey Supercomputing Centre

Visualisation team

Visualisation is the process of applying advanced algorithms and computer graphics to data to provide research insights. Data visualisation has a number of outcomes that include allowing researchers to learn something new, to work faster than using simpler techniques to more rapidly identify problems, and to communicate with peers or with a wider audience using visual displays. A petascale supercomputer enables a researcher to generate and subsequently analyse data of unprecedented size and complexity, so visualization plays a key role in understanding this data.

The Pawsey Supercomputing Centre Visualisation team provides a package of hardware, software and expertise, to tackle the whole range of visualisation activities that are relevant to the Pawsey Supercomputing Centre user community. As with supercomputing, a crucial contribution of the program team is to inform researchers of new ways to present and interpret their results.

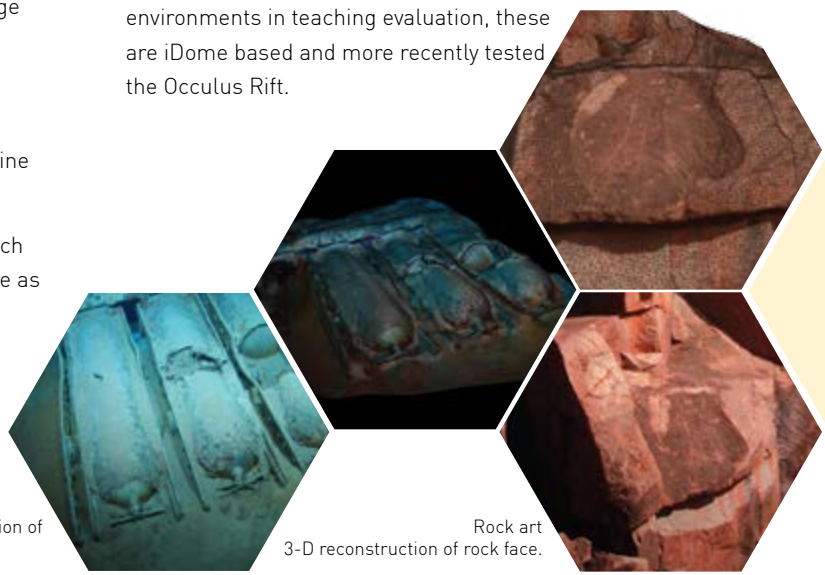
- Network visualisation in diverse fields from business project management to metabolic networks in plant energy biology.
- 3D reconstruction from photographs, a core research activity with applications largely in digital recordings in archaeology and geoscience.
- Volume visualisation and analysis, typically from a range of 3D scanning technologies such as CT (computerised tomography).
- General imaging, this includes but is not limited to gigapixel digital image capture, segmentation and machine vision image/video analysis.

There are almost 50 video productions created each year which include research focused teaching videos. A few examples are as follows:

- "Feeding the world" raises awareness of the rapidly growing population and how a UWA scientist's research helps solve the problem.
- "Seeds of Life" raises awareness of the East Timorese food shortage and shows how a UWA scientist guides the East Timorese people to grow their own food.
- "The biggest biochemical reaction that runs our world" Winthrop Professor Harvey Millar, from the ARC Centre of Excellence in Plant Energy Biology presents the importance of Energy Biology, the biggest biochemical reaction that runs our world.

GOVERNMENT / INDUSTRY PROJECTS

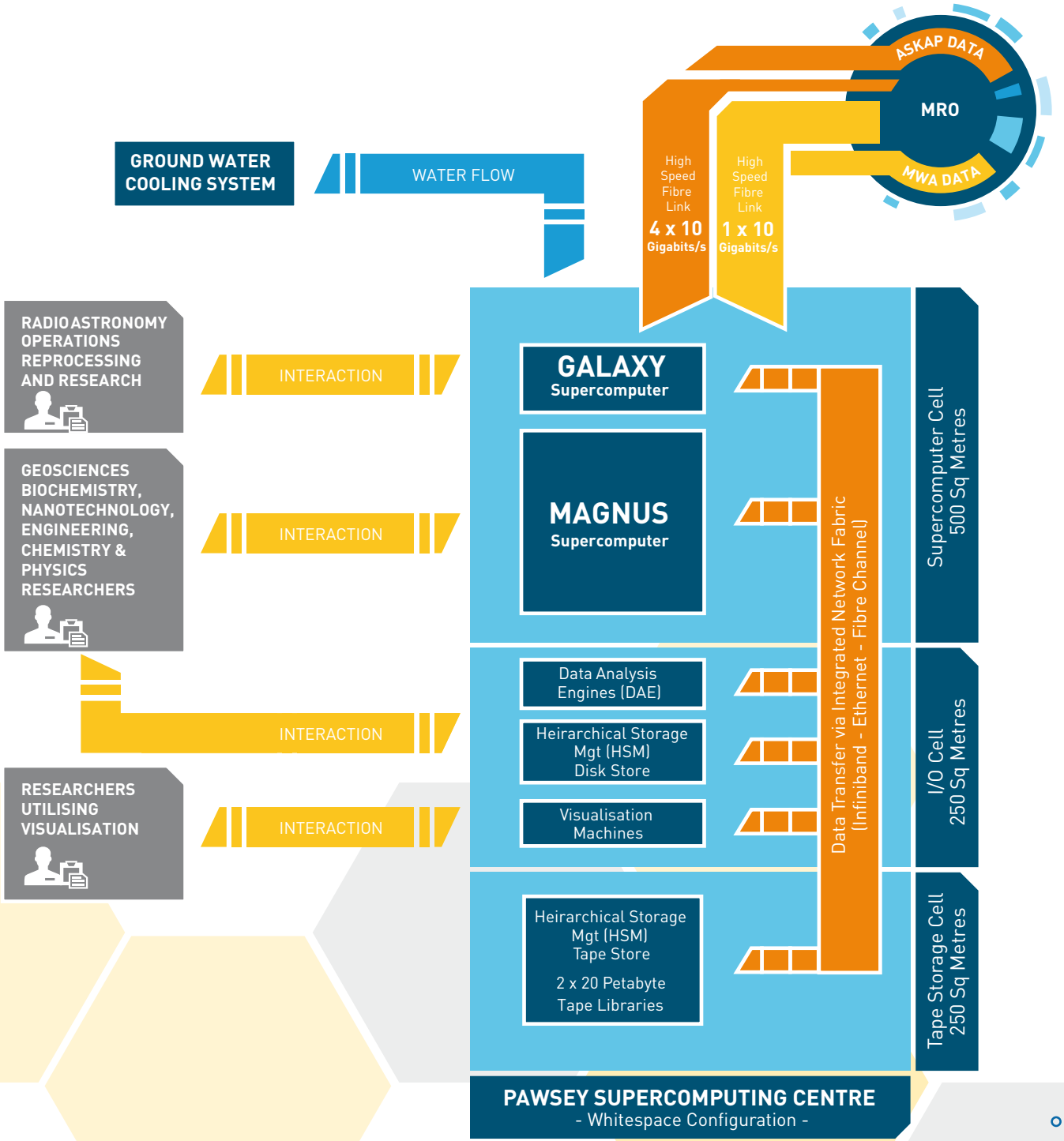
- Geological modelling for Ivan Zibra from DPM, collaboration on visualisation projects with the WA Maritime Museum, image mosaic generation of historic shipwreck sites for the WA Maritime Museum using techniques develop for 3D reconstruction.
- Discussion with the new director of the Scitech Horizon planetarium on possible future visualisation outreach projects.
- Assistance to new Avizo users to obtain access to and operate Avizo on workstations at ARRC and UWA.
- Participation in weekly SeeVogh meetings with QCIF and Evogh about SeeVogh features and technical issues.
- Continuing to work with researchers at ECU on immersive environments in teaching evaluation, these are iDome based and more recently tested the Occulus Rift.



Photograph and 3D reconstruction of HMAS Sydney 's torpedo tubes.

Rock art
3-D reconstruction of rock face.

PAWSEY CENTRE SUPERCOMPUTER: KEY COMPONENTS

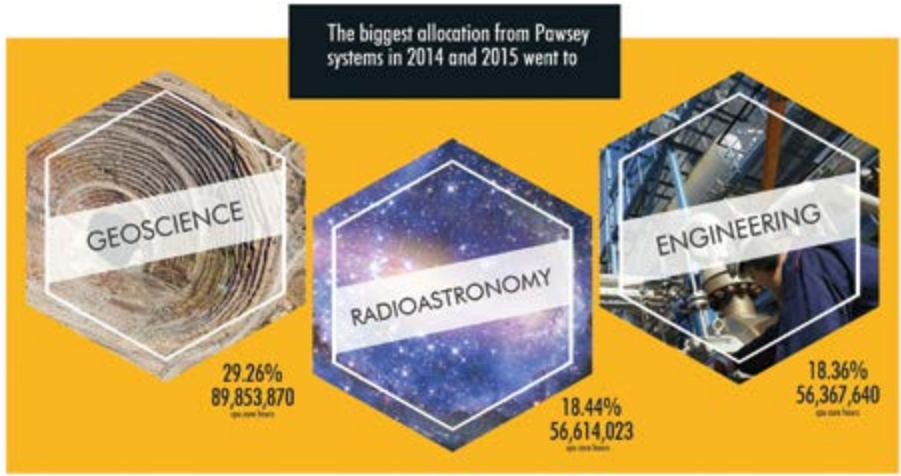


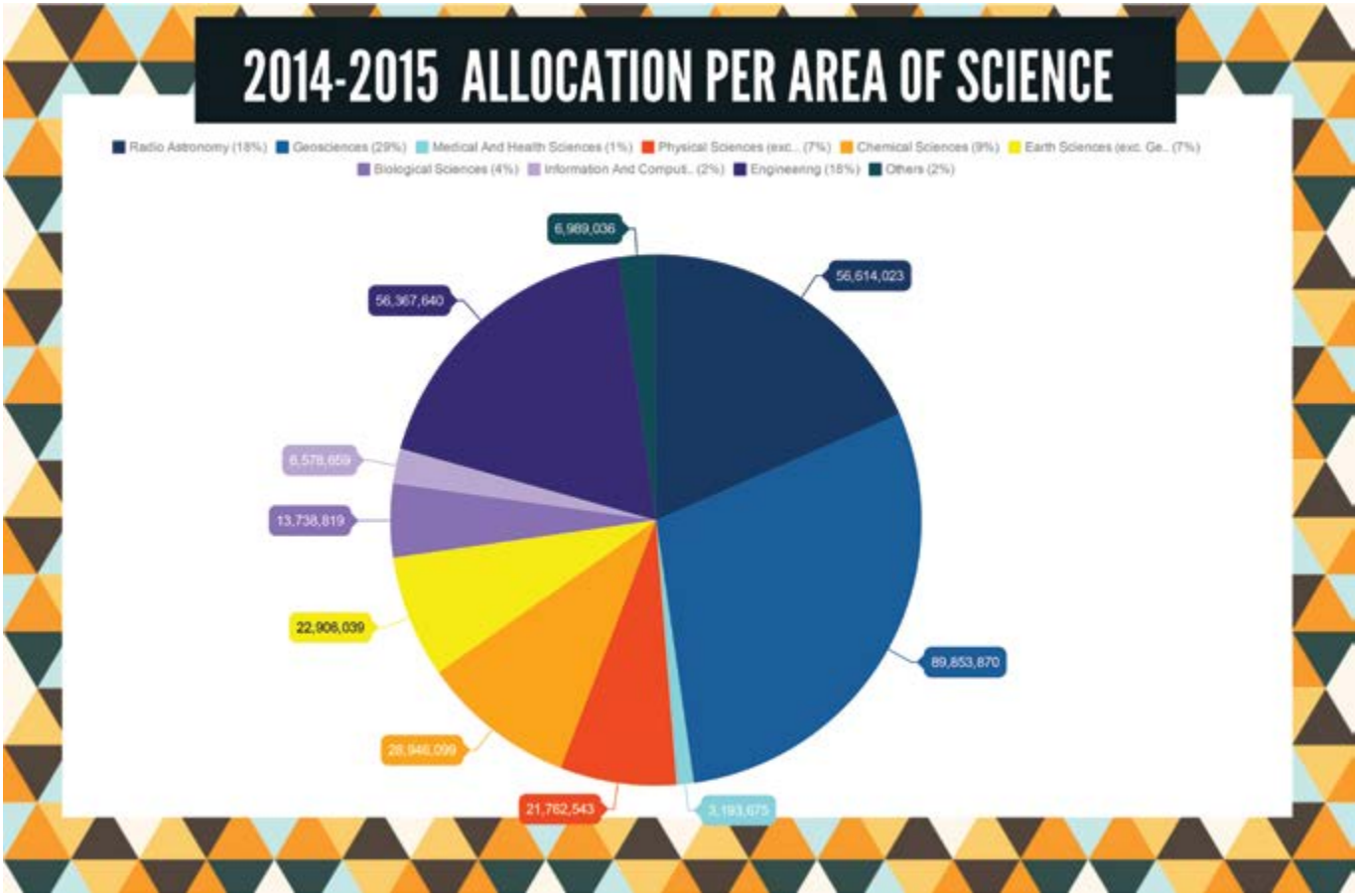
ALLOCATION

The Pawsey Supercomputing Centre provides access to its supercomputing resources through a number of national and local merit allocation schemes.

These schemes are summarised as follows for the 2014-15 period:

• National Computational Merit Allocation Scheme (NCMAS) – 15% of resources allocated. Annual call in September/October each year, with large, 12-month allocations, budgeted quarterly. Projects must be research-focused and the Principal Investigator





must be employed at an Australian university or research institution.

• Geosciences Merit Allocation Scheme – 25% of resources allocated. Six-monthly calls (in Q2 and Q4 of each year) with large, 12-month allocations, budgeted quarterly. Projects must be research focused on Geosciences and the Principal Investigator must be employed at an Australian university or research institution.

• Pawsey Partner Merit Allocation Scheme – 30% of resources allocated. Six-monthly calls (in Q2 and Q4 of each year) with large, 12-month allocations, budgeted quarterly. Principal Investigator must be employed at a Pawsey Partner institution.

• Pawsey Director's Allocation Scheme – 5% of resources allocated. Responsive-mode process, available most of the year with small (←0.1% of available resource time), 3-month allocations. Principal Investigator must be employed at an Australian university or research institution.

• Radio Astronomy operational commitment – 25% of Pawsey resources allocated (100% of Galaxy). Projects must support MWA/ASKAP operations and the Principal Investigator must be employed at an Australian university or research institution.

A list of supercomputing projects run on Pawsey resources in 2014 - 2015 can be found in this book beginning on Page 50.

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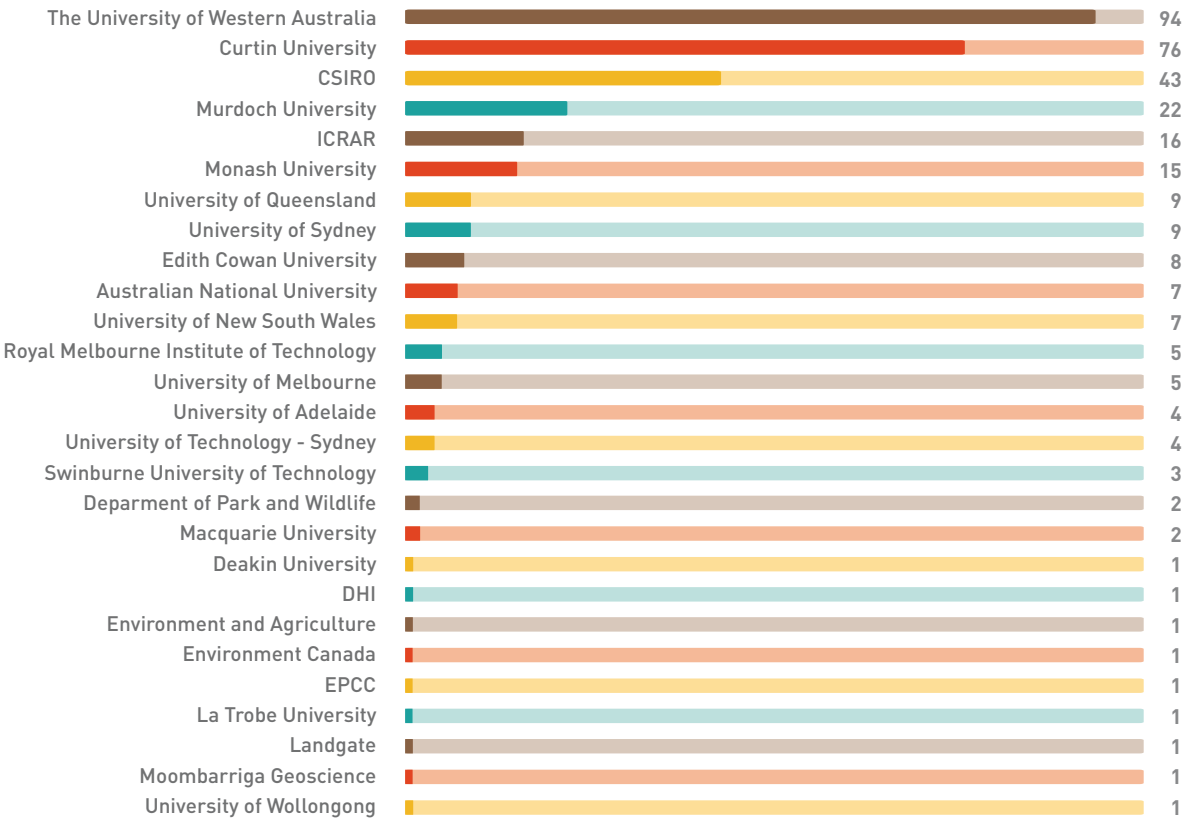
2014- 2015 NO. OF PROJECTS



Magnus

Magnus, from the Latin 'Great', is a latest-generation Cray XC40 system that is used for elite supercomputing projects across the entire range of scientific fields serviced by the Pawsey Supercomputing Centre, including geoscience and general research. Final installation of Magnus was completed in September 2014, providing researchers across Australia with access to over 1 PetaFLOP of processing power – the equivalent of over one quadrillion computations per second. On its debut, Magnus was ranked #41 in the November 2014 global Top500 list of supercomputers. This was updated in June 2015 to #58, making Magnus the most powerful public research supercomputer in the Southern Hemisphere at the time of writing.

The Magnus system provides users with over 35,000 cores, using the cutting edge Intel® Xeon® processor E5-2690 v3 'Haswell' processors that communicate amongst themselves over Cray's high-speed, low-latency Aries interconnect. Magnus is one of the first supercomputers in the world to make use of these latest generation processors. Magnus also provides users with three petabytes of scratch file system space, connected via 56 Gbit/s FDR Infiniband.

This architecture is specifically designed to allow parallel processing of extremely large, computationally intensive data sets. In order to demonstrate this capability and test Magnus prior to its availability to general researchers, Pawsey ran the Petascale Pioneers Program in late 2014. This program allocated almost 90 million CPU hours to fourteen grand challenge projects from local, national and international researchers spanning priority research areas including geoscience, astrophysics, chemistry and bioinformatics. Altogether, from its fully operational launch to June 2014, allocations on Magnus totalled over 318 million CPU hours.

The arrival of Magnus prompted the withdrawal of the previous generation Pawsey supercomputer, Epic, which it superseded with an order of magnitude greater capability and capacity. In order to ensure a smooth transition to Magnus for researchers, Pawsey ran a six-month migration program including a promotional campaign for the new system, targeted training for existing Epic-based research teams, and dedicated support for those projects that were identified as at risk of losing momentum in the transition period.

Galaxy

Galaxy is a Cray XC30 system that supports high-end radio astronomy activities within the Australian research community. It fulfils the real-time processing requirements of the Australian Square Kilometre Array Pathfinder (ASKAP) telescope, as well as providing for the reprocessing and research needs of the wider Australian radio-astronomy community, including those of the Murchison Widefield Array (MWA) telescope. In the context of ASKAP, Galaxy runs the Central Science Processor, allowing pseudo-real-time processing of data delivered to the Pawsey Supercomputing Centre from the Murchison Radio astronomy Observatory (MRO).

Galaxy consists of three cabinets, containing 118 compute blades, each of which has four nodes. Each node supports two, 10-core Intel Xeon E5-2960 'Ivy Bridge' processors operating at 3.00 GHz, for a total of 9,440 cores delivering around 200 TeraFLOPS of compute power. Galaxy local storage is provided by a Cray Sonexion 1600 appliance, providing 1.3 Petabyte of capacity via an FDR Infiniband network.

Data Analysis Resources (Zeus and Zythos)

In 2014-15, the Pawsey Data Analysis Engine service called Zeus was successfully brought into production, including the introduction of a very-large-memory SGI UV2000 system called Zythos. Zeus is heterogeneous with 39 nodes in various configurations. Zythos is the largest node and boasts 6TB shared memory, 264 Intel Xeon processor cores and 4 NVIDIA K20 GPUs.

Zeus, together with other infrastructure in Pawsey, allows a diverse range of workflows to be undertaken. Zeus and Zythos provide complementary capabilities to Magnus, including support for pre- and post-processing, data-intensive computations, and scientific visualisation.

Given the specialised nature of the Zythos system, an early-adopter program was executed to explore the different applications that could benefit from access to the 6 Terabytes of memory that it hosts. This program highlighted significant opportunities in bioinformatics and engineering, based on which Pawsey refined the configuration and access model for the service, including the deployment of a Centre-wide, high-performance project file system to facilitate exchange of data between Magnus, Zeus and Zythos.

NeCTAR Research Cloud

The Pawsey Supercomputing Centre is part of the national NeCTAR Research Cloud Federation, with the Pawsey node being launched in October 2014. The Pawsey Research Cloud provides researchers with a service that effectively bridges the gap between traditional desktop computing and the supercomputing resources provided by the Centre. This ensures Pawsey is able to provide a comprehensive range of services to meet the diverse needs of national researchers.

The Pawsey Research Cloud consists of 46 IBM System X 3755 M3 servers as compute nodes. Each node has 64 compute cores running at 2.3GHz, 256GB of RAM and 6 x 10Gbps links for storage and external access. Altogether, this provides researchers with 2,944 cores and 11.5TB of memory.

It also includes 31 IBM System X 3650 M4 servers as Ceph storage nodes. Each storage node has 24TB of raw SATA disk, which adds up to 216TB of short-term storage.

PAWSEY PATHFINDER SYSTEMS

2014-15 saw the retirement of the two Pawsey Supercomputing Centre pathfinder systems – Epic at Murdoch University and Fornax at The University of Western Australia. These systems were acquired as part of the Pawsey Centre Project in order for staff and users to develop the expertise required to make best use of the petascale system to be installed in the Pawsey Centre.

Epic was a general purpose machine, housed in a 'plug and play' shipping container, and saw most of its userbase successfully migrated to "Magnus" following the opening of the Centre.

Fornax was a machine focused on processing large data sets and was superceded by "Galaxy" as the Pawsey Supercomputing Centre's main radio astronomy processing machine.

Both machines saw intense use during their operational span and helped Australian researchers break new ground in hundreds of research projects across a vast array of scientific areas.

Epic and Fornax were exceptional machines whose legacy lives on in Magnus, and will be seen in the computational systems developed to support the Square Kilometre Array.

EPIC

Manufacturer: HP
Model: Commodity Linux Cluster
Compute Processors: Intel Xeon X5660 "Westmere"
Computing Power: 107 teraFLOPS
Nodes: 800 dual-socket compute nodes
Memory: 18 terabytes (24 gigabytes of PC3-10600 DDR3 per compute node, at 1,333 MHz)
Interconnect: QDR InfiniBand, at 40 gigabits/sec per node Network Topology: Fat Tree
Power consumption: 400 kW (peak)
Local storage: 500 terabytes Lustre filesystem

FORNAX

Manufacturer: SGI (USA)
Model: SGI water chilled Cluster
Compute Processors: Intel Xeon X5660 'Westmere' (6-core, 2.66 GHz)
GPU Processors: NVIDIA Tesla C2075
Computing Power: 62 teraFLOPS
Nodes: 96 (each with one GPU, two CPUs and 72GB memory, 7TB local Disk space)
Memory: 6.9 TB RAM (96 nodes with 72GB RAM per node)
Interconnect: 2 x QDR InfiniBand at 40 gigabits/sec per node
Local storage: 672 terabytes Lustre filesystem

The core network infrastructure connecting the Pawsey Centre itself with Pawsey facilities, staff and researchers requiring high-bandwidth access located at Pawsey member sites was upgraded in the 2014-15 period. This involved replacing the aging border and core routers with next-generation Cisco Nexus 7000 series devices supporting higher density 10 Gbs interfaces and non-blocking backplanes required to support large-scale data transfers such as those required for the creation and study of data products from the radio telescopes at the Murchison Radio-astronomy Observatory, both by researchers at Pawsey member sites and by researchers more far flung. Pawsey now has its own dedicated link to the new AARNet 4 core for internet connectivity, with failover through CSIRO's connection to AARNet 4 in WA (Pawsey also provides a failover path for CSIRO into AARNet 4). The old switch infrastructure servicing Pawsey staff was also upgraded, as was the wireless network, which involved a move to more secure 802.1x authentication as well as better coverage and higher capacity through the use of controller-based lightweight access points. Pawsey staff also served on the WA National Research Network (NRN) Steering Committee, which successfully completed its MRO and Perth fibre ring projects in 2014. These projects allowed the physical Wide Area Network (WAN) infrastructure connecting the Pawsey members CSIRO, Murdoch and ECU to be upgraded, moving from the old Uecomm fibre to the NRN fibre, offering greater resiliency by virtue of its ring configuration, and greater longevity into the future as the Indefeasible Right of Use (IRU) agreement with Uecomm approaches expiration. The Pawsey facilities at UWA are planned to be connected also via the NRN fibre in the near future, and a direct peering with UWA has been established so that traffic between Pawsey and ICRAR does not impact UWA's internet connection. This is similar to the configuration that exists between Pawsey and Curtin's radio-astronomy groups. Also in this period, networking was put in place to support the CSIRO Groundwater Cooling Visualisation facility, and the visualisation facilities at UWA and CSIRO ARRC.

PAWSEY CENTRE BUILDING FEATURES

The Pawsey Supercomputing Centre building incorporates a number of best practice features and solutions. These features include:

- A 'dual skin' building construction to ensure the most effective insulation of the supercomputing environment from external temperature extremes.
- Fibre optic high speed networks linking researchers from Australia and overseas. This includes a dedicated high-speed link to the Murchison Radio Astronomy Observatory, some 800km north of Perth.
- Scalable cooling and electrical services which will enable flexible supercomputer expansion within the 1,000 square metre computer hall.
- A unique groundwater cooling system for removing heat from the supercomputer and reinjecting and dissipating this heat into the aquifer, 140m below the Pawsey Supercomputing Centre, with no net loss of groundwater.
- A photovoltaic system has been incorporated into the building's shaded facade plus an extensive PV array on the roof of the building. This PV installation generates 140kWs of electricity onsite, which acts to offset the electrical and CO2 footprint of the Supercomputing Centre.
- The Pawsey Supercomputing Centre is an automated, secure, 'intelligent' building with real-time monitoring to facilitate efficient operation and support fine tuning of operations to reduce overall power costs.

Overall, the facility has been designed to be as future proof as possible, allowing Pawsey to anticipate and accommodate the high power, cooling and physical requirements of the next generation of supercomputers.

140kVA Pawsey's solar PV array.

View inside the Pawsey Supercomputing Centre plan room. Photo courtesy PS Structure copyright Brian Smyth Photography.

Geothermal Cooling System

CSIRO has developed an innovative geothermal solution for cooling the Centre's supercomputing systems. The system is known as groundwater cooling and was funded by the Australian Government as part of the CSIRO Geothermal Project.

The process involves pumping water with an ambient temperature of around 21°C from the Mullaloo aquifer through an above-ground heat exchanger to provide the necessary cooling effect for the supercomputer, then reinjecting the water back into the aquifer. CSIRO estimates that using groundwater cooling to cool the supercomputer will save approximately 14.5 million litres of water per year in the first two years of operation compared to using conventional cooling towers. The system is designed to have the capacity to scale with additions to the supercomputing hardware. Part of this upscaling is already under way, with Pawsey in the process of purchasing and installing a new, more efficient water chiller. This new, low-load chiller will enable more granular control of cooling according to temperature to job ratio – ensuring the system is running at optimum efficiency as much as possible.

VISITATION AND OUTREACH

As a nationally significant facility the Pawsey Supercomputing Centre generates a high-level of interest in visitation from local, national and international groups. In the 2014-15 financial year alone, over 330 visitors toured the Centre.

These visitors, including international delegations, industry groups, researchers and representatives from local, State and Federal Governments, are able to see first-hand Pawsey's resources, expertise and infrastructure that are enabling cutting-edge research for Australia's future, firmly placing Western Australia and the nation at the forefront of the global scientific community.

Visitation highlights from 2014-15 include:

- Premier of Western Australia and Minister for Science Colin Barnett touring the Centre to announce $21.6m of funding for Pawsey to accompanying media.
- Representatives from the Western Australian Water Corporation and The West Australian newspaper.
- Western Australian Chief Scientist Professor Peter Klinken.
- Technology media representatives as part of iiNet's "0-Week."
- Federal Minister for Defence Kevin Andrews and Senator Linda Reynolds.
- A delegation of international Consuls General with the WA Department of State Development, including the United States of America, China, Indonesia and Vietnam.
- Western Australian Government representatives from Departments including Food and Agriculture and Education.
- Industry groups including Consolidated Minerals and Chevron.
- International delegations including groups from Kazakhstan, South Africa, Uganda, the United States of America, India and the European Union.

Premier Colin Barnett.

WA Chief Scientist Professor Peter Klinken and Ms Jennifer McGrath.

Minister for Defense, the Hon. Kevin Andrews MP and Senator Linda Reynolds.

VISITING PAWSEY

INDUSTRY HIGHLIGHTS

- CHEVRON
- TELSTRA
- CONSOLIDATED MINERALS
- IINET

GOVERNMENT HIGHLIGHTS

- DEPARTMENT OF FOOD AND AGRICULTURE
- GENERAL CONSULS (US, China, Indonesia, Italy, Vietnam and Croatia)
- KAZAKHSTAN DELEGATION


Telstra delegation.


Kazakhstan delegation.


EU Economic and Commercial Councillors & Research, Innovation and Education Councillors Joint Mission to WA.


Consuls General.

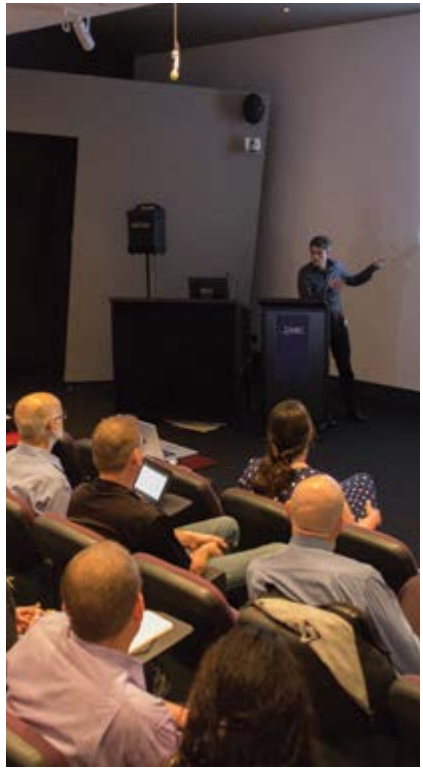
Developer training.

Training

In order to allow researchers to take best advantage of the resources provided, the Pawsey Supercomputing Centre engages in a wide range of training activities to ensure optimal knowledge flow. As a full service centre as opposed to a purely computational facility, training activities are integrated into all aspects of business.

From 2014 to 2015, the Centre provided 67 training sessions in supercomputing, data services and visualisation, attracting approximately 700 attendees.

In addition to pure training courses, a series of Data Clinics, Profiling Parties and Merit Allocation Workshops were conducted at the Centre and at Pawsey Partners sites – with a total of 15 such service support events during the period.



Andre J. Aberer during his presentation at the Bioinformatics Symposium.

Experts in Residence

The Pawsey Experts-in-Residence program aims to inject expertise and energy into the research community. Expert visitors in 2014-2015 included Cody Permann, Idaho National Laboratory, USA (MOOSE workshop and mentoring meetings); Andre J. Aberer, Research Associate, Heidelberg Institute for Theoretical Studies, Germany (Bioinformatics Symposium and mentoring); Evatt Hawkes, UNSW; and Tony Rafter, CSIRO (Annual Symposium).

Bioinformatics Petascale Pioneers group after August's workshop.

Communities of Interest

In order to best service users, the Pawsey Supercomputing Centre is engaged in a Communities of Interest program to encourage knowledge exchange between researchers and develop supportive communities. The intention is to work with user groups to determine common issues and concerns and provide shared solutions that are developed in cooperation with Pawsey staff. The Bioinformatics Community has been chosen as a test bed for the program and has already seen positive activity with the Bioinformatics User Group (BUG) formed at the inaugural Bioinformatics Symposium. The first activity for the group was a Bioinformatics Petascale Pioneers Program, which saw seven groups migrate their science onto the Magnus supercomputer. A series of community events have been run through 2015, and will culminate in an end of year event.

Pawsey interns during a tour in the Whitespace.

Internship Program

The Pawsey internship program helps to grow the next generation of computational scientists by placing top students with researchers using Pawsey resources. Over 100 students have gone through the program since its inception, working on leading edge projects and gaining experience in research. In 2014-2015, fifteen intern students were selected to work with researchers from the Pawsey Partners, including students from Curtin, ECU, Murdoch and UWA. Four of the interns were part of the joint Pawsey/ICRAR internship program, two from UWA, one from ANU and one from the University of Adelaide. They gave their final presentations on 17th February 2015, and have submitted papers and podcasts to report on their results. Student posters were displayed at the Pawsey Annual Symposium.

Part of 2014 SCC team with Dr. Rebecca Hartman-Baker (right centre).

Student Cluster Competition

In November 2014, Senior Supercomputing Team member Rebecca Hartman-Baker coached and organised Pawsey's second Student Cluster Competition entry at Supercomputing 2014 in New Orleans. The Student Cluster Competition is an annual highlight of the convention, a way to showcase the expertise of the next generation of the HPC community. Student teams from around the world engage in a non-stop 48-hour challenge to design and build a supercomputing cluster from commercially available components and demonstrate the greatest sustained performance across a series of applications.

The six-member team was made up of students from Curtin and UWA and all learned valuable skills for building and using supercomputers as part of the preparation for the contest.

Home to Australia's most advanced computational research resources, the Pawsey Supercomputing Centre plays a central role in Australia's scientific community. The Centre has a strong commitment to its relationships with several other significant scientific and ICT organizations and works to ensure Australian researchers can obtain the highest level of support, no matter their needs.

Pawsey Partner Organisations

The Pawsey Supercomputing Centre is a joint venture between CSIRO and the four public WA universities. Being founded in 2000, the Centre is the longest running and most successful organisation of this type in Australia.

This long-lasting success is a tribute to the exceptional possibilities that can be achieved thanks to these organisations' dedication to enhancing collaboration in Australian science.

National Computational Infrastructure (NCI)

The Pawsey Supercomputing Centre actively cooperates with its sister facility, NCI in Canberra, in order to provide Australia with consistent, globally competitive supercomputing power across all areas of science.

Together, the Pawsey Supercomputing Centre and NCI are the two most powerful scientific supercomputing facilities in the Southern Hemisphere. Moving forward, this relationship will only continue to strengthen, allowing the Pawsey Supercomputing Centre and NCI to evolve and meet Australia's future scientific needs.

Research Data Services (RDS)

The RDSI (Research Data Storage Infrastructure) was a $50 million Australian Government project designed to create a national system to collect and preserve historic Australian research for future generations. The Pawsey Supercomputing Centre was chosen in a competitive process to serve as one of

the eight RDSI facilities around Australia.

The RDS is the NCRIS-funded project that builds upon RDSI to optimise the value it provides to Australian researchers and support the infrastructure by focusing on data as a service.

National eResearch Collaboration Tools and Resources (NeCTAR) Project

A $47 million Australian Government initiative, NeCTAR connects researchers around Australia, helping them work together to discover groundbreaking new possibilities. This is achieved by providing cutting-edge technologies like Virtual Laboratories, national servers and research clouds.

The Pawsey Supercomputing Centre Research Cloud is the only Western Australian NeCTAR facility. By providing over 3,000 cores, the Pawsey Supercomputing Centre is allowing Australian researchers to unlock new avenues of research.

International Centre for Radio Astronomy Research (ICRAR)

ICRAR is an Australian collaboration that achieves world-class research in astronomical science and engineering. It also plays a key role in the Square Kilometre Array (SKA), the largest scientific project in human history.

These research achievements would not be possible without the sizeable contributions of the Pawsey Supercomputing Centre, which provides state-of-the-art resources and expertise to ICRAR and the SKA precursor projects.

Australian Academic Research Network (AARNet)

AARNet is a national resource, providing researchers and institutions across Australia with a world-class high-speed communications network infrastructure.

As part of its relationship with AARNet, the Pawsey Supercomputing Centre is connected nationally to other users and facilities across Australia. This allows research excellence produced at the Pawsey Supercomputing Centre to be shared quickly with all of Australia.

Antennas of CSIRO's Australian SKA Pathfinder (ASKAP) telescope, at the Murchison Radio-astronomy Observatory (MRO) in Western Australia. Credit Pete Wheeler, ICRAR.

Overview

Each year a survey is distributed to the Pawsey Supercomputing Centre userbase to elicit feedback about overall performance, and what additional services or activities users are interested in.

In 2014 the survey was announced on 24 November and closed on 17 December. There are approximately 600 users on the user mailing lists.

Areas of interest

Overall opinion of services, competence and professionalism was high; with 80-90% of respondents rating them as good or very good. These ratings have been consistent over the last four years and most saw slight improvements compared to the previous year.

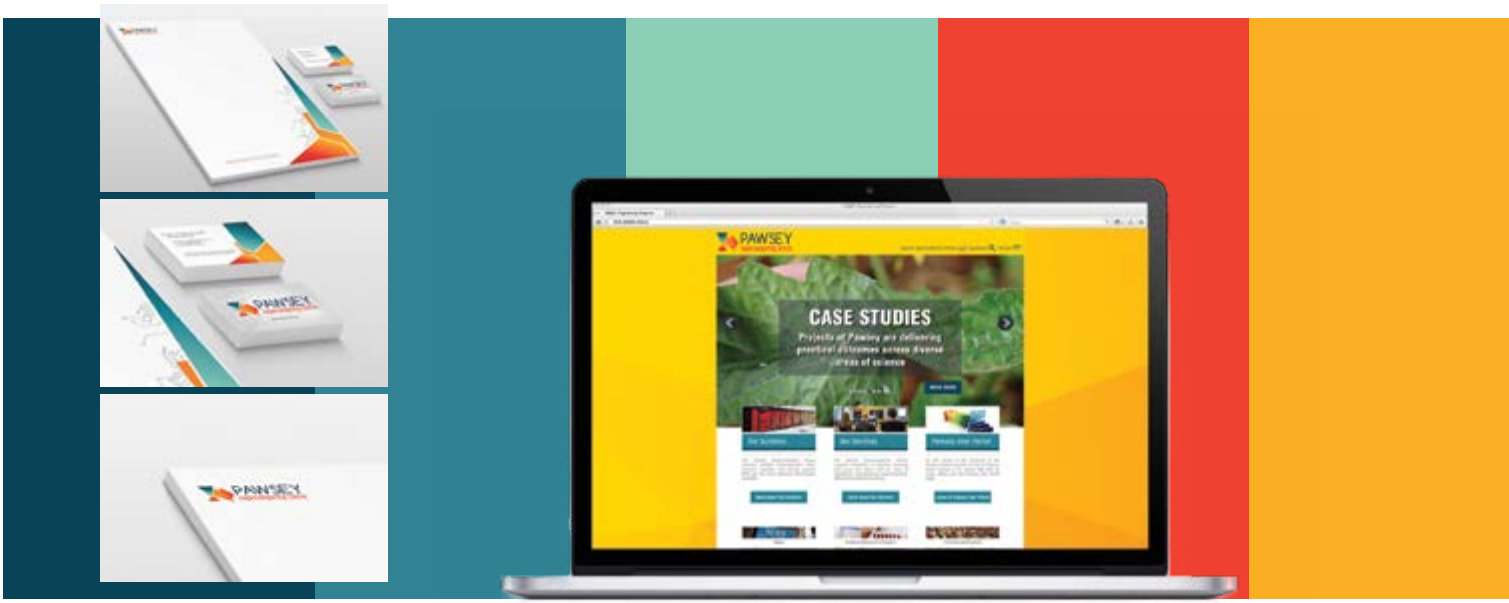
While both positive and negative user comments and observations were recorded, the majority indicated satisfaction. Although not to be considered a 'pattern', there were a few comments about queue time but these were paired with compliments on user support.

When asked to rate Pawsey Supercomputing Centre technical support the majority of respondents were positive but constructive feedback was received that will help improve future processes. Individuals were named and complimented on the service they've provided, along with some general positive comments about the helpdesk.

Overall

Overall satisfaction with Pawsey Supercomputing Services was 84% (good/very good). These ratings are similar to previous years. Over half the respondents said the best features of the Pawsey Supercomputing Centre were the resources available. The results of the user survey show that some areas require investigation and improvement but overall, the indication is that the staff and services provided are more than acceptable.

TRANSFORMATION OF IVEC INTO THE PAWSEY SUPERCOMPUTING CENTRE



2014-15 saw the rebranding of what was formerly iVEC into the Pawsey Supercomputing Centre. This was a significant undertaking and one that is expected to continue into the future as audiences adjust their knowledge based on promotional efforts.

The decision to retire the iVEC brand was not taken lightly, as the iVEC brand had existed for almost fifteen years and had a high local profile for its supply of high performance computing resources and expertise. This was assessed through a number of user surveys and by long term collection of anecdotal evidence. The strength of the brand came from a lack of local competitors, the tight focus of operations within a niche market, from the length of operation, and the efforts of the iVEC marketing team to promote it.

Although there were no negative traits attached to the iVEC brand, an executive decision was made to rebrand to the Pawsey Supercomputing Centre once full operational status was reached. As a world-class facility and one of two leading national supercomputing centres, it was judged that the expansion of operations far beyond the local level reduced the relevance of the iVEC brand.

As an iconic facility that has received considerable national and international promotion, the Pawsey Centre as a physical location already held a strong brand presence prior to and following construction. Rather than manage two brands in tandem, the decision was to incorporate branding in a singular entity, the Pawsey Supercomputing Centre, representing both the location and the organisation.

Rebranding process

An extensive consultation was undertaken prior to final decision making, with Perth rebranding specialists Mindfield employed to aid in the process.

The rebranding was announced internally towards the end of 2014 and officially launched on 5th of December by the Hon. Donna Farragher. The majority of rebranding actions took place in late 2014, such as the alteration of documents, promotional materials and internal signage. The process continued into 2015 with the launch of a new Pawsey-branded website and replacement of external signage on the Pawsey Centre building.

DATA PROJECT LIST

PRINCIPAL DATA CUSTODIAN	PI'S INSTITUTION	DATA COLLECTION NAME	SIZE OF THE COLLECTION IN 12MONTH (TB)
Paul Bourke	Curtin University / The University of Western Australia	Advanced Imaging in Archaeology	From 4 (original) to 10
David Lumley	CSIRO/ Curtin University/ The University of Western Australia	ANLEC passive seismic research project	From 30 to 90
Hayden Walker	The University of Western Australia	ARC Plant Energy Biology NGS Data	From 25 to 75
For Bi-Qing	The University of Western Australia	Arecibo Ultra Deep Survey data	From 20 to 30
Ben Humphreys	CSIRO/ Curtin University	ASKAP Commissioning Archive	From 75 to 600
Ben Humphreys	CSIRO/ Curtin University	ASKAP Commissioning Data	100
Igor Bray	Curtin University	Atomic and molecular collision data	1
Matthew Bellgard	Murdoch University	Barley	From 5 to 11
Matthew Bellgard	Murdoch University	Bioplatforms Australia	From 30 to 40
Luke Edwards	CSIRO/ Curtin University/ Edith Cowan University/ Murdoch University/ The University of Western Australia	CATAMI	From 1 to 2.5
Andreas Wicenec	The University of Western Australia	CHILES Survey	From 50 to 100
Andrew Rohl	Curtin University	Computational Materials Science	From 5 to 7.5
Susan Hill	ECU	Collaborative Research Network Project -Education	From 10 to 90
Robert Bell	CSIRO	ASC Dumps	From 1 to 2
Mollie Hewitt	Curtin University/ Edith Cowan University/ Murdoch University/ The University of Western Australia	Mira Canning Stock Route Project Archive	From 6 to 7
Thomas Poulet	CSIRO/ The University of Western Australia/ UNSW	CT scan data	38
Phill Bland	Curtin University/ The University of Western Australia	Desert Fireball Network (DFN) image database	From 6 to 18
Paolo Raiteri	Curtin University	Computational study of the dissolution and growth of minerals	From 11 to 15
Katherine Zdunic	Department of and Wildlife/ Landgate	DPaW Imagery	From 6 to 12
Dareen Gibson	Edith Cowan University	ECU eResearch	From 3 to 20
Jonathan Anderson	CSIRO/ The University of Western Australia	Genomics on fungal plant pathogens	From 8 to 10
Michael Black	ECU/ Murdoch University	Global Health and Genomics	From 6 to 20
Richard Dodson	The University of Western Australia / Raman Research Institute	GMRT Data for investigation of SKA Methods	40
David Howard	CSIRO/ Curtin University/ The University of Western Australia/ WA Departments of Agriculture; Water; Private exploration and natural resource management companies	GSWA State Geophysical Compilation Grids	From 1 to 2
Phillip Melton	The University of Western Australia	Human Genomic Data for Complex Traits.	From 20 to 50

PRINCIPAL DATA CUSTODIAN	PI'S INSTITUTION	DATA COLLECTION NAME	SIZE OF THE COLLECTION IN 12MONTH (TB)
Susan Leggate	The University of Western Australia	IRDS Test	1
Yuan Mei	CSIRO	Mei_MD_data	From 3 to 5
Mike Caccetta	CSIRO	Mineral Resources EO Dataset	From 60 to 65
Mark Broomhall	CSIRO/ Curtin University	MODIS L1B Archive	From 86 to 96
Zak Hughes	Curtin University	Molecular Simulations	6.5
Lister Staveley-Smith	CSIRO/ Curtin University/ The University of Western Australia	MWA GLEAM IMAGE ARCHIVE	From 6 to 10
Slava Kitaeff	CSIRO/ Curtin University/ The University of Western Australia	MWA high frequency resolution trial observations of Galactic Centre	From 8 to 15
Steven Tingay	CSIRO/ Curtin University/ The University of Western Australia	Murchison Widefield Array Data Archive	From 1 to 1500
Nick Mortimer	CSIRO/ The University of Western Australia	Nearshore Research Facility Data	From 30 to 54
Dave Edwards	The University of Western Australia/ Bayer CropScience, ICRISAT, UQ, UTS, Institute of Experimental Botany AS CR	NGS anlysis results	From 80 to 90
Laura Boykin	CSIRO/ The University of Western Australia	phylogenetic_trees	From 1 to 10
Dirk Slawinski	CSIRO/ The University of Western Australia	Pilbara Marine Conservation Partnership	From 5 to 20
Parwinder Kaur	Murdoch University/ The University of Western Australia	Subterranean clover (Trifolium subterraneum) GENOMICS Platform	From 8 to 10
Mark Broomhall	Curtin University	Surface Reflectance Data	From 43 to 45
Tom Lyons	Murdoch University/ Coordinated Regional Climate Downscaling Experiment [http://cordex- australasia. wikidot.com/groups],	SWWA Climate Simulations	From 274 to 415
Tom Lyons	Murdoch University	SWWA - downscaled climate	From 150 to 150
Cormac Reynolds	CSIRO / Curtin University	VLBI	From 64 to 120
Luke Edwards	CSIRO/ Curtin University/ Edith Cowan University/ Murdoch University/ The University of Western Australia/ State Gov. Agencies	WAAODN	From 40 to 65
Gabriel Keeble-Gagnere	CSIRO/ Murdoch University/ University of Melbourne	Australia-China Centre for Wheat Improvement (ACCWI) Data Storage	From 10 to 15
Fiona Mcrobie	The University of Western Australia	WRF sensitivity simulations regarding	From 1 to 20

SUPERCOMPUTING PROJECT LIST

Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Aaron Davis	CSIRO	Electromagnetic modelling for geophysical earth structure	180170	epic	Geosciences	2014
Aaron Thorn	Landgate	Advanced Remote Sensing Methods for 3D Vegetation Mapping from Digital Aerial Photography	100000	magnus	Directors	2015
Abishek Sridhar	Curtin University	Sustainable thermal solutions using phase change cooling and microchannels	100000	magnus	Directors	2015
Aibing Yu	University of New South Wales	Simulation and Modelling of Particulate Systems	200000	epic	National Merit	2014
Alan Aitken	The University of Western Australia	Methodologies of large-scale multi-method geophysical inversion	240227	epic	Geosciences	2014
Alan Duffy	Swinburne University of Technology	Smaug - The First Galaxies Simulation Series	3650000	galaxy	Astronomy	2014
		Simulating the Epoch of Reionisation (SMAUG)		magnus	Directors	2014
	University of Queensland	From molecules to cells		epic	National Merit	2014
Alexander Gofton	Murdoch University	Uncovering the microbiome of Australian ticks	150000	magnus	Partners	2015
Ali Karrech	The University of Western Australia	Computational Multi-physics for Fault Reactivation in Resource Reservoirs	55000	magnus	Geosciences	2014
Alpeshkumar Malde	University of Queensland	From molecules to cells Understanding the structural and dynamic properties of cellular components	2000000	magnus	National Merit	2015
Amanda Barnard	CSIRO	Virtual Nanoscience	8100000	magnus	Directors	2014
				magnus	Partners	2015
Amir Karton	The University of Western Australia	Mimicking nature: computational design of better antioxidants	595800	fornax	Partners	2015
				zythos	Directors	2014
				fornax	Directors	2014
				magnus	Partners	2014
Andreas Wicenec	ICRAR	Radio Astronomy Data Intensive and HPC Research Projects from ICRAR ICT Team	320000	fornax	Partners	2014
				magnus	Partners	2014
Andrew King	CSIRO	Modelling of induced seismicity	357000	magnus	Directors	2015
	Curtin University	Data Center Cooling By Using CFD		magnus	Directors	2015
		Flow Induced vibrations		epic	Directors	2014
		Wave Energy Characterisation		magnus	Directors	2014
		Mechanical Engineering Final Year Projects		epic	Directors	2014
		Hydrodynamic Response of an Underwater Membrane for Wave Energy Conversion		magnus	Partners	2015
Andrew Ooi	University of Melbourne	Computational Fluid Dynamics Studies of Bluff Body and Heat Transfer in a Buoyant Channel	2000000	magnus	National Merit	2015
		Direct numerical simulation of turbulent mixed turbulent convection in a vertical plane channel		galaxy	Directors	2015

Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Andrew Rohl	Curtin University	Curtin - Chemical Research Methods 362	1510000	epic	Directors	2014
		Realistic Modelling of the Effects of Solvent and Additives on Crystal Growth		epic	National Merit	2014
Andrew Squelch	Curtin University	Seismic imaging and modelling for mineral and hydrocarbon exploration and production monitoring	1324568	magnus	Geosciences	2014
				epic	Geosciences	2014
		Finite Difference/Finite Element modeling of elastic waves		fornax	Geosciences	2014
				fornax	Partners	2015
Andrew Turner	EPCC	Petascale benchmarking of CP2K on Intel Haswell/Cray XC30	200000	magnus	Directors	2014
Andrew Wilkins	CSIRO	Coal mining and groundwater in the Hunter valley	250000	magnus	Partners	2015
Andy Fourie	The University of Western Australia	Paste tailings beach slope prediction with CFD simulation(This is for my PhD project)	227648	epic	Partners	2014
		Beach slope prediction of thickened tailings using the CFD method (For my PhD project)		magnus	Partners	2015
Anirudh Rao	Monash University	Advanced Modelling of Biological Fluid Flows	10000	magnus	Directors	2014
Bansikumar Kathrotiya	Curtin University	Simulation of 1hexanol using Gromacs	17500	magnus	Directors	2015
Ben Corry	Australian National University	Simulation studies of biological and synthetic channels	2600000	magnus	National Merit	2015
				epic	National Merit	2014
Ben Mullins	Curtin University	Modelling of particle deposition in the upper airways and lungs	400001	magnus	Partners	2014
		Simulation of air flow and particle deposition in the lungs		magnus	Partners	2015
		Zythos - CFD mesh generation		zythos	Directors	2014
Ben Thornber	University of Sydney	Mix in high-acceleration implosions driven by multiple shocks	400000	magnus	National Merit	2015
Berwin Turlach	The University of Western Australia	Alternative Spatiotemporal Imputation Methods for Catch Rate Standardisation.	417	fornax	Directors	2014
Biao Sun	Curtin University	Modeling and optimization of LNG regasification technologies	500000	epic	Partners	2014
Brian Skjerven	Pawsey Supercomputing Centre	Pawsey Student Cluster Competition	10000	magnus	Directors	2015
Carlo Pacioni	Murdoch University	Applying coalescent-based genetic simulations to the conservation of endangered species	130000	epic	Partners	2014
				magnus	Partners	2015
Carol Wang	The University of Western Australia	Western Australian Pregnancy (Raine) Cohort and the Preterm Birth Genome Project - Magnus	300000	magnus	Partners	2015
Casper Boon		Modelling estuary health	10000	zythos	Directors	2014
Cathryn M Trott	ICRAR	Detection of the Epoch of Reionisation using the Murchison Widefield Array	530000	galaxy	Astronomy	2015
	Curtin University	Detection and Estimation of the Epoch of Reionisation with the Murchison Widefield Array		fornax	Partners	2015

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Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Chandana Jayasundara	CSIRO	Simulation of Underground Coal Mines	2742498	magnus	Directors	2015
		Simulation of Underground Coal Mines and Mineral processing		epic	Geosciences	2014
Charitha Pattiaratchi	The University of Western Australia	Surface gravity waves and circulation on the Rottnest continental shelf, Western Australia	2300000	magnus	Directors	2014
		Developing better predictions for extreme water levels and waves around Australia		magnus	Partners	2015
Charlotte Oskam	Murdoch University	Troublesome Ticks	200000	galaxy	Directors	2015
Chenghua Sun	Monash University	Computer-aided Design of Dye/TiO2 Interface for High Performance Solar Cells	400000	epic	National Merit	2014
Chi Minh Phan	Curtin University	Adsorption Layer Properties of CnTAB at the oil-water Interface	16500	epic	Directors	2014
		Adsorption layer structure of gemini surfactant at the air/water interface		magnus	Partners	2015
Chris Bording	The University of Western Australia	Moose train course	1	epic	Directors	2014
Chris Green	CSIRO	High resolution density-driven convection in 3D porous media using MOOSE	10000	epic	Directors	2014
Chris Power	ICRAR	SSimPL-ACS The Survey Simulation PipeLine - Alternative Cosmologies Study	14900000	magnus	National Merit	2015
		Galaxy Formation in the Cosmic Web		magnus	Directors	2014
		Lurking in the Darkness: Intermediate Mass Black Holes in Low-Mass Galaxies		magnus	Partners	2015
		DRAGONS Dark-ages Reionization and Galaxy Formation Simulation		epic	Partners	2014
		Detecting Missing Baryons in the Cosmic Web		epic	Partners	2014
		Developing & incorporating models of AGN feedback in cosmological simulations		epic	Partners	2014
		Testing Dark Matter Models with the Milky Ways Satellites		magnus	National Merit	2015
		The Genetics of the Magellanic Clouds		galaxy	Astronomy	2015
Christoph Arns	The University of New South Wales	Integration of Conventional and Digital Core Analysis	1000000	galaxy	Directors	2015
Christopher Fluke	Swinburne University of Technology	Performance testing of the national network when transferring very large astronomical datasets	10000	galaxy	Directors	2014
Christopher Harris	The University of Western Australia	African and Australian whiteflies: outbreak causes and sustainable solutions (Fornax)	340000	fornax	Partners	2015
				magnus	Partners	2015
Chunsheng Lu	Curtin University	Molecular dynamics simulations of the novel mechanical behaviour of nano-structured ceramics	1750000	epic	Partners	2014
				magnus	Partners	2015
Chunyan Fan	Curtin University	Fundamental Study of Adsorption Processes in Novel Nanoporous Materials and Characterization	70000	epic	Partners	2014
		Mechanisms of Adsorption in Novel Nanoporous Materials and the Characterization		magnus	Partners	2015

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Cihan Altinay	University of Western Australia	Methodologies of large-scale multi-method geophysical inversion	2900000	magnus	Geosciences	2015
		Finite Element Inversion of Lithospheric Density Structure (FEILDS)		magnus	Directors	2014
Cormac Reynolds	ICRAR	High Angular Resolution Radio Astronomy with the Long Baseline Array.	315000	galaxy	Directors	2014
		High Angular Resolution Radio Astronomy with the LBA and AuScope		magnus	Partners	2015
Craig O'Neill	Macquarie University	Tracking mantle slab dewatering using ASPECT	500000	magnus	Directors	2015
				magnus	Geosciences	2015
Craig Pennell	The University of Western Australia	Western Australian Pregnancy (Raine) Cohort and the Preterm Birth Genome Project	500000	epic	Partners	2014
		Preterm Birth Genome Project and Raine Study		galaxy	Directors	2015
Cuong Van Nguyen	Curtin University	Adsorption Layer Properties of CnTAB at the oil-water Interface	10000	magnus	Directors	2014
Damien Carter	Curtin University	Realistic Modelling of the Effects of Solvent and Additives on Crystallisation	25000000	magnus	National Merit	2015
Daniel Grimwood	Pawsey Supercomputing Centre	SKA Science Data Processor Workpackage	21000	epic	Directors	2014
Daniel Mitchell	Curtin University	Estimation of the Epoch of Reionisation with the Murchison Widefield Array	30000	fornax	Partners	2014
Darren Rowland	Murdoch University	Fundamental characterisation of multicomponent aqueous electrolyte solution thermodynamics	25000	magnus	Directors	2014
Dave Morrison	CSIRO	CASDA (CSIRO Australian Square Kilometre Array Science Data Archive)	1	galaxy	Astronomy	2015
David Annetts	CSIRO	Probabilistic inversions for lithological units	445927	epic	Geosciences	2014
		Bayesian Lithological Inversion		magnus	Geosciences	2015
David Antoine	Curtin University	Australian Regional Environmental Remote Sensing	230000	magnus	Partners	2015
				epic	Partners	2014
David Henry	Murdoch University	Nanoscale materials and Nanoscale Interactions - From Catalysts through to Hydrophobic Soils	62000	fornax	National Merit	2015
		Theoretical Design of Nanocatalysts and Materials		epic	National Merit	2014
David Huang	The University of Western Australia	Design of Turbo Massive MIMO Communication Systems	400000	magnus	Partners	2015
David Lumley	The University of Western Australia	HPC simulation, imaging and inversion of passive seismology data	2555362	fornax	Geosciences	2014
		GPU-based imaging/inversion of complex 3D/4D seismic wavefields		fornax	Geosciences	2014
		Computational modelling, imaging and inversion of 3D/4D seismic wavefields		epic	Geosciences	2014
		Full Waveform Inversion of 3D seismic data on GPU arrays		fornax	Geosciences	2014
		Full Waveform Inversion of 3D seismic data on HPC x86 clusters		magnus	Geosciences	2015
David Poger	The University of Queensland	Selective targeting of membranes by antimicrobial peptides	1500000	galaxy	Directors	2015
David Schibeci	Pawsey Supercomputing Centre	Remote Visualisation Users	100000	zythos. pawsey	Directors	2015

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Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
David Wilson	La Trobe University	Quantum Chemical Molecular Properties	40000	epic	National Merit	2014
Defeng (David) Huang	The University of Western Australia	Design of High-Speed Underwater Acoustic Communication Systems Using Block-by-Block Turbo Processing	500000	epic	Partners	2014
				magnus	Partners	2014
Derek Leinweber	University of Adelaide	Electromagnetic Structure of Matter	500000	epic	National Merit	2014
Dermot Kennedy	CRAY	Cray Support Staff (internal application)	1	magnus	Directors	2015
Dietmar Mueller	University of Sydney	Towards dynamic tectonic reconstructions	7060000	epic	National Merit	2014
		Quantifying resource requirements for mantle convection models on Magnus		magnus	Directors	2014
		Towards dynamic tectonic reconstructions		magnus	National Merit	2015
Dilusha Silva	The University of Western Australia	Optical characteristics of a MEMS infra-red spectrometer	10000	epic	Directors	2014
Dino Spagnoli	The University of Western Australia	Molecular dynamics simulations of the aggregation of polyaromatic hydrocarbons	458000	epic	Partners	2014
		Density Functional Theory Study of Semiconductors and their Surfaces		epic	Partners	2014
Dion Weatherley	University of Queensland	Petascale simulation of granular flow in underground mass-mining	1100000	magnus	Directors	2014
Dipanjan Mukherjee	Australian National University	Astrophysical Accretion Disks, Jets and Winds and Interactions with the Surrounding Medium	1000000	magnus	National Merit	2015
Ekaterina Pas	Monash University	Development and Application of Quantum Chemistry Methods for the prediction of physicochemical prope	400000	magnus	National Merit	2015
Emanuelle frery	CSIRO	Great Australian Bight Chevron	100000	magnus	Directors	2015
Erdinc Saygin	Australian National University	3D Seismic Imaging of South East Asia	1900000	magnus	Geosciences	2015
Evatt Hawkes	University of New South Wales	Direct Numerical Simulations and Large Eddy Simulations of Turbulent Combustion	13500000	magnus	National Merit	2014
		Direct Numerical Simulations of Turbulent Combustion		magnus	National Merit	2015
		Massively parallel combustion modelling to enable breakthroughs in low-carbon gas-turbines		magnus	Directors	2014
Evelyne Deplazes	University of Queensland	Developing computational methods to improve the accuracy of structural data obtained from DEER	80000	epic	National Merit	2014
Feifei Tong	The University of Western Australia	CFD modelling of flow/structure/seabed interactions	6810000	magnus	Partners	2015
		Estimation of extreme loads on wave energy devices		magnus	Partners	2015
		Classification of wake flow patterns around four cylinders in square arrangement in steady flow		epic	Directors	2014
		The effects of wave breaking on cylindrical structures		magnus	Partners	2014
Florian Wellmann	CSIRO	Efficient estimation of information correlation in 3-D	75860	fornax	Geosciences	2014
		Uncertainty quantification in subsurface flow fields		magnus	Geosciences	2014
Gabriel Keeble-Gagnere	Murdoch University	BPA wheat activities - Assembly of chromosome 7A and SNP analysis for 16 varieties	150000	magnus	Partners	2014
		Wheat Chromosome 7A assembly, diversity and post-genomics analysis		magnus	Partners	2015

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Gavan McGrath	The University of Western Australia	Quantifying tropical cyclone impacts to Australian vegetation and water resources	10000	magnus	Directors	2015
Grant Morahan	The University of Western Australia	Enabling Personalized Medicine by Predicting Genetic Signatures of Disease	1864400	galaxy	Directors	2015
		Genetic Signatures in Complex Human Diseases		magnus	Partners	2015
		Cane Toad Genome Sequencing		magnus	Partners	2015
				magnus	Partners	2014
Greg Poole	University of Melbourne	Tiamat and DRAGONS - the Dark-ages Reionisation and Galaxy Formation Simulation Program	400000	epic	National Merit	2014
Guangyao Li	Australian National University	Dynamics of Open-Dissipative Exciton-Polariton Condensates	60000	fornax	National Merit	2015
Heather Sheldon	CSIRO	Geothermal multiphysics simulations	50000	magnus	Geosciences	2015
Henning Prommer	CSIRO	NCGRT Worlking Group - Reactive Transport Modelling of Groundwater Systems	384000	magnus	Partners	2015
Hong Hao	The University of Western Australia	Development of Fuel Storage Tank with Frangible Roof to Resist Accidental Explosion Load	301440	epic	Partners	2014
Hongwei An	The University of Western Australia	numerical simulations of wave boundary layer effect on the stability of small diameter pipeline	1788000	epic	Partners	2014
		Effect of natural seabed on hydrodynamics around cylindrical structures		magnus	Partners	2015
Hongwei Wu	Curtin University	1-Modelling of LNG dispersion 2-Modelling of bio-oil/char slurry in a fluidized bed reactor	520000	epic	Partners	2014
				magnus	Partners	2015
Hongyi Jiang	The University of Western Australia	Numerical modeling of scour below an offshore pipeline	100000	magnus	Directors	2014
Huaiyu Yuan	The University of Western Australia	Full waveform inversion for the seismic anisotropy in the global and regional upper mantle	1173104	magnus	Geosciences	2014
	Macquarie University	Multiple scale seismic structural inversion in Australia and other continents globally		magnus	Geosciences	2015
Hugh Blackburn	Monash University	High-Order Methods for Transitional and Turbulent Flows	2600000	magnus	National Merit	2015
Ian Small	The University of Western Australia	Constraint-based approach for simulating plant heterosis	410000	galaxy	Directors	2015
		Evolution of the pentatricopeptide repeat (PPR) protein family in plants		magnus	Partners	2015
Igor Bray	Curtin University	Atomic Collision Theory	4904000	magnus	National Merit	2015
				epic	National Merit	2014
		Computational collision physics		fornax	Directors	2014
Ingo Jahn	University of Queensland	Performance Enhancement in Access-to-space Scramjets	1000000	magnus	National Merit	2015
Irene Suarez-Martinez	Curtin University	Atomistic Modelling of Carbon Nanostructures	1600000	magnus	National Merit	2015
Irene Yarovsky	RMIT	Theoretical Investigation of novel materials for industrial and biomedical applications	2200000	magnus	National Merit	2015
				epic	National Merit	2014

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Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
James Haile	Environment and Agriculture	Analysis of Trace and Environmental DNA	833	fornax	Directors	2014
James Hane	CSIRO	Genome analysis of plants, pathogen and pests relevant to wheat, lupin and other legumes	780000	fornax	National Merit	2014
	Curtin University	Bioinformatic analysis of agriculturally important plants, pathogen and pests		magnus	Partners	2015
		Computational Anaylsis of whole-genome sequences of fungal pathogens		galaxy	Directors	2015
James Jewkes	Curtin University	The Phenomenology of Unsteady Impinging Jets: Fluid Dynamics and Heat Transfer	1738000	epic	Partners	2014
		OpenFOAM 4th year mechanical engineering student projects		epic	Directors	2014
		The Phenomenology of Unsteady Impinging Jets: Fluid Dynamics and Heat Transfer		magnus	Partners	2014
Jan Dettmer	Australian National University	Bayesian Approaches to Earthquake and Tsunami Source Estimation	2185000	magnus	Geosciences	2015
Jason Holmberg	Murdoch University	ECOCEAN Whale Shark Photo-identification Library	6000	epic	Partners	2014
Jason Kennington	The University of Western Australia	Population genomic analysis of a tuskfish endemic to Western Australia	100000	magnus	Directors	2015
Jason Park	Curtin University	Valuation of Collateralized Debt Obligations: An equilibrium model	20000	epic	Directors	2014
Jason Wang	ICRAR	Investigation of Adaptive IO System (ADIOS) as SKA Storage backend	1440000	galaxy	Directors	2015
		Radio Astronomy Data Intensive and HPC Research Projects from ICRAR ICT Team		epic	Partners	2014
		A combination of ICRAR Data Intensive Astronomy and SKA Science Data Processor projects		fornax	Partners	2015
				magnus	Partners	2015
Jeffrey Dick	Curtin University	Gold-organic sulfur interactions at high temperature	120114	epic	Geosciences	2014
Jeffrey Shragge	The University of Western Australia	Large-scale Computational Modelling of 3D Passive Elastic Seismic Wavefields	15862500	magnus	Directors	2014
		GPU-based modelling, imaging and inversion of complex 3D/4D seismic wavefields		Zeus	Directors	2015
		Computational modelling, imaging and inversion of 3D/4D seismic wavefields		magnus	Geosciences	2015
		GPU-based modelling, imaging and inversion of complex 3D/4D seismic wavefields		fornax	Geosciences	2015
		Computational modelling, imaging and inversion of 3D/4D seismic wavefields		magnus	Geosciences	2014
Jess Robertson	CSIRO	Scale-sensitive algorithms for data-driven resource discovery	110057	magnus	Geosciences	2014
		Sloshing silicates and sulfides - the fluid dynamics of magmatic sulfide deposits		epic	Geosciences	2014
Jie Liu	The University of Western Australia	Quantitative analysis of microtomography and pore-scale hydrodynamic simulations	35000	fornax	Geosciences	2014
Jim Falter	The University of Western Australia	Geophysical and Environmental Computational Fluid Dynamics Research	5000000	magnus	Partners	2015

Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Jim Gunson	CSIRO	Littoral-zone modelling of morphodynamic changes on bathymetry and shorelines	144136	epic	Geosciences	2014
Jimmy Philip	The University of Melbourne	A numerical investigation of entrainment in turbulent buoyant jets	250000	magnus	National Merit	2015
Jingbo Wang	The University of Western Australia	Quantum walk based simulation of electron trasport	157500	fornax	Partners	2014
				magnus	Partners	2014
		Magnus access for students in SHPC4001 at UWA		magnus	Directors	2015
Joel Brugger	University of Adelaide	Mobility of platinum group elements in hydrothermal system: insights from molecular dynamics	750000	magnus	Geosciences	2014
John Lattanzio	Monash University	Convective nuclear burning in 3D - Fixing the weak link in stellar models	1200000	magnus	National Merit	2015
Jonathan Kirby	Curtin University	3D Christmas Trees: Anisotropic Rheology of the Lithosphere	24263	epic	Geosciences	2014
Joseph Awange	Curtin University	Projecting Future Climate of Bhutan and its Impact on Stored Water using RCMs and GRACE satellites	850000	magnus	Directors	2014
		Future Climate Projections over Bhutan		magnus	National Merit	2015
Joshua Izaac	The University of Western Australia	Quantum computation of molecular dynamics	50000	magnus	Partners	2015
Judith Lichtenzveig	Curtin University	Genomics of fungal pathogens and grain legume crops	20000	magnus	Partners	2015
Julian Gale	Curtin University	Atomistic simulation of minerals and geochemistry	60104622	epic	Geosciences	2014
				magnus	Geosciences	2014
				magnus	Geosciences	2015
		Biomineralisation		magnus	Directors	2014
		Can we trust force field simulations of biomineralisation?		galaxy	Directors	2015
Julien Cisonni	Curtin University	Mechanical Engineering Honours Projects	1130000	magnus	Directors	2015
		Modelling and prediction for tailored treatment of sleep-related breathing disorders		magnus	Partners	2015
				epic	Partners	2014
Julio Soria	Monash University	Direct Numerical Simulation of Equilibrium Adverse Pressure Gradient Turbulent Boundary Layers	15000000	magnus	Directors	2014
		Investigations of transitional and turbulent shear flows		epic	National Merit	2014
Junfang Zhang	CSIRO	Molecular Study of Gas Adsorption on Coal	197097	magnus	Geosciences	2014
		Molecular Dynamic Study of Gas Adsorption on Coal		fornax	Partners	2014
				epic	Geosciences	2014
		Molecular Dynamics Study of Gas Storage and Transport in Coals		fornax	National Merit	2015
				magnus	Partners	2015
Justin Leontini (	Monash University	Transition in Fluid Flows	800000	magnus	National Merit	2015
Kane O'Donnell	Curtin University	Computational x-ray absorption spectroscopy for materials science	1300000	magnus	Partners	2015
				magnus	Directors	2015

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Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Karl-Heinz Wyrwoll	The University of Western Australia	Modelling of the climatology of the northwest Australian summer monsoon over the last 22,000 years	180170	epic	Geosciences	2014
Katarina Miljkovic	Curtin University	Modelling of impact cratering mechanics with applications to terrestrial and planetary geophysics	100000	magnus	Directors	2015
Kenji Bekki	ICRAR	Simulating dust and molecular cloud formation in dwarf galaxies	41400	epic	Partners	2014
		Simulating the two-stage formation process of the Galactic globular clusters		fornax	Partners	2014
		Galactic star formation regulated by interstellar dust		fornax	Partners	2015
Kenneth Chan	The University of Western Australia	crop genome informatics	225000	zythos	Directors	2014
	UQ	Analysis of complex genomes		magnus	National Merit	2015
Kerensa McElroy	CSIRO	Predicting evolutionary potential under climate change from phylogenomic data	200000	galaxy	Directors	2015
Kerry Hourigan	Monash University	Advanced Modelling of Biological Fluid Flows	1100000	magnus	National Merit	2015
				epic	National Merit	2014
Kym Ottewell	Department of Parks and Wildlife	Developing optimised workflows for phylogenomic and population genomic analyses of Aust species	200000	galaxy	Directors	2015
Laura Boykin	The University of Western Australia	MrBayes and BEAST analyses of agriculturally important organisms (Epic)	550000	epic	Partners	2014
		MrBayes and BEAST analyses of agriculturally important organisms (Magnus)		magnus	Partners	2014
		MrBayes and BEAST analyses of agriculturally important organisms (Fornax)		fornax	Partners	2014
		ExaBayes on Magnus		magnus	Directors	2014
Lauren Schmied	DHI	DHI compatibility pilot project	1000	epic	Directors	2014
Laurent Chardon	Environment Canada	GEM Benchmark	50000	magnus	Directors	2014
Liam Menaglio	The University of Western Australia	Numerical Simulation of Turbulence Generated Noise Sources around Submarine Sonar Arrays	500000	magnus	Partners	2015
Lihong Wu	The University of Western Australia	Numerical simulations of folating bodies in waves	5000	magnus	Partners	2015
Linqing Wen	The University of Western Australia	GPU Accelerated Gravitational Wave Signal Processing	240000	fornax	Partners	2015
Louis Moresi	University of Melbourne	Instabilities in the convecting mantle and lithosphere - Underworld	1400000	magnus	National Merit	2015
Lutz Gross	University of Queensland	Numerical Simulation of Seismo-electric Coupling in Non-homogenous Porous Media	500000	magnus	Geosciences	2015
Mahmudul Raz	Edith Cowan University	Rendering project	417	fornax	Directors	2014
Mahreen Arooj	Curtin University	Probing Features that Modulate Catalytic Mechanism and Redox Biochemistry of Cholesterol Oxidase	530000	magnus	Partners	2015
				fornax	Partners	2015
Mahyar Madadi	Curtin University	Geophysical subsurface modelling and imaging	10800000	magnus	Geosciences	2015

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Manolo Per	CSIRO	Predicting properties of nanoclusters using High Throughput and High Accuracy computation	500000	magnus	Partners	2015
Marcela Bilek	University of Sydney	Harnessing the bioactivity of protein fragements and peptides	400000	magnus	National Merit	2015
Marco Ghisalberti	The University of Western Australia	Geophysical and Environmental Computational Fluid Dynamics Research	3120000	fornax	Partners	2015
		Numerical study of particle capture in aquatic ecosystems		epic	Partners	2014
		Influence of turbulence in particle capture in aquatic systems		magnus	Partners	2014
Marco Marinelli	Landgate	Statistical modelling of relationship between winter storms and storm surge.	10100	magnus	Directors	2015
	Curtin University			epic	Directors	2014
Marcus Thatcher	CSIRO	Exploring new techniques for simulating the global climate	15000000	magnus	Directors	2014
Maria Albertsen	Edith Cowan University	Epigenetic regulation of alternative splicing	21000	fornax	Directors	2014
	The University of Western Australia	Disease-related epigenetic variation in twins		zythos	Directors	2014
Mark Randolph	The University of Western Australia	Dynamic simulation of impacts on pipeline by submarine landslide with material point method	100000	magnus	Directors	2015
Martin Ebert	The University of Western Australia	Monte Carlo Simulations in Medical Physics	311000	fornax	Directors	2014
		Development and Modelling of Advanced Radiation Guided Technologies in Medical Physics		fornax	Partners	2015
		Development and Characterisation of Online Detector for Advanced Radiotherapy Treatment Verification		magnus	Partners	2015
Matthew Bellgard	Murdoch University	Barley genome assembly	1050000	zythos	Directors	2014
		High performance computing for bioinformatics analysis across 'omics platforms		epic	Partners	2014
		Large genome activities		magnus	Partners	2014
Matthew Hipsey	The University of Western Australia	Pathways to Production : Biogeochemical Processes in the Kimberley Region	100000	magnus	Directors	2015
Matthew Tuson	The University of Western Australia	Statistical analysis and research conducted by the Centre for Applied Statistics (CAS), UWA	30000	magnus	Partners	2015
Mehdi Khiadani	Edith Cowan University	ECU - CFD Concrete Mattress, Jet in Cross Flow, Flash Evaporation, Spatially Valid Flow	10000	epic	Directors	2014
Mehrdad Kimiaei	The University of Western Australia	Probabilistic models for dynamic collapse of offshore platforms under extreme waves	50000	magnus	Directors	2014
Mervyn Lynch	Curtin University	Developing modeling-related tools for energy prediction and wind resource assessment	809200	magnus	Directors	2014
		Simulations using WRF, OpenFOAM, SEGMENT-Landslide packages		magnus	Partners	2015
Michael Black	Murdoch University	Establishing a standard analysis protocol for genomic analysis of rare diseases	250000	magnus	Directors	2015
		Pain-OMICS: Omic risk factors of chronic pain		magnus	Partners	2015
	Edith Cowan University	Genomic and glycomic risk factors of chronic disease in Australia and PR China		epic	Partners	2014

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Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Michael Cortie	University of Technology - Sydney	Investigation of High Entropy Alloys for advanced nuclear applications	20000	epic	National Merit	2014
Michael Dentith	The University of Western Australia	3D Inversion of Magnetotelluric Data Applied to Exploration for Natural Resources	250000	magnus	Geosciences	2015
Michael Kuhn	Curtin University	100 m-resolution model of Earth's global gravity field	158102	epic	Geosciences	2014
				magnus	Partners	2015
Michael Meuleners	The University of Western Australia	Hydrodynamic modelling of ocean currents for use in operational forecasting and oil spill response.	320000	magnus	Partners	2015
				epic	Partners	2014
Michael Stat	Curtin University	TrEnD lab bioinformatics; from ancient DNA to traditional medicines	100000	magnus	Directors	2015
Michal Zawierta	The University of Western Australia	Integrated on-chip force and displacement sensors for high-speed AFM of ultimate sensitivity	105000	epic	Directors	2014
				magnus	Directors	2014
Michelle Spencer	RMIT	Modelling Nanoscale Materials for Sensing and Device Applications	400000	magnus	National Merit	2015
				epic	National Merit	2014
Mike Ford	University of Technology - Sydney	Electron beam induced etching and deposition	400000	epic	National Merit	2014
				magnus	National Merit	2015
Milinkumar T. Shah	Curtin University	Multiphase interactions in riser and bubble column	2500000	magnus	Partners	2015
Mohamed Ismail	Edith Cowan University	Flume Open Channel	2000	epic	Directors	2014
Mohammednoor Altarawneh	Murdoch University	Fundamental Understanding of the Role of Singlet Molecular Oxygen in Spontaneous fires	425667	magnus	Partners	2015
				fornax	Directors	2014
				fornax	Partners	2015
		A First-Principle Investigation into Combustion Chemistry of Novel Brominated Flame Retardants.		magnus	Partners	2015
Monica Gumuliya	Curtin University	Simulations of Dilute Gas-Solid Flow in Risers	100000	magnus	Directors	2014
Munish Mehta	The University of Western Australia	Cane Toad Genome Sequencing	614400	epic	Partners	2014
Nader Issa	The University of Western Australia	HPC simulation, imaging and inversion of passive seismology data	7880000	magnus	Geosciences	2014
				magnus	Geosciences	2015
Natasha Hurley-Walker	Curtin University	New Calibration and Imaging Algorithms for the Murchison Widefield Array	100000	zythos	Directors	2014
		MWA GLEAM: The GaLactic/Extragalactic All-sky MWA survey		fornax	Partners	2014

Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Neha Gandhi	Curtin University	Large scale molecular dynamics simulations of macrobiomolecular complexes	8151000	fornax	Directors	2014
				magnus	Partners	2014
				magnus	Partners	2015
		Molecular dynamics simulations of tau protein aggregation		epic	Partners	2014
		Molecular dynamics simulations of tau protein folding and aggregation		fornax	Partners	2014
		Molecular dynamics simulations of folding of IDPs		fornax	Partners	2015
		Molecular dynamics simulations of tau protein aggregation		magnus	Partners	2015
Neil Francis	CSIRO	Molecular Modelling of Hydrometallurgical Reagents	100000	epic	Partners	2014
Nicolas Flament	The University of Sydney	Towards dynamic tectonic reconstructions	3603406	epic	Geosciences	2014
Nigel Marks	Curtin University	Modelling of Nuclear Materials and Carbon Nanostructures	1100000	epic	National Merit	2014
Nikhil Medhekar	Monash University	Atomistic simulations for electronic, chemical amd mechanical properties of nanoscale materials	1000000	epic	National Merit	2014
				magnus	National Merit	2015
Nilimesh Halder	The University of Western Australia	UWA Dengue Spread Model	100833	fornax	Directors	2014
				magnus	Directors	2015
Nima Nadim	Curtin University	Development of Lattice Boltzmann Method for Multi-phase flow	100000	magnus	Directors	2015
Omid Amili	Monash University	Investigations of transitional and turbulent shear flows using direct numerical simulations and larg	3600000	magnus	National Merit	2015
Ondrej Hlinka	CSIRO	CSIRO genome-assembly project	1	zythos	Directors	2014
Parwinder Kaur	The University of Western Australia	Subterranean clover GENOMICS platform	150000	magnus	Partners	2015
Patrice Rey	The University of Sydney	Modelling the formation of sedimentary basins and continental margins	2000000	magnus	National Merit	2015
Paula Moolhuijzen	Murdoch University	Large complex genome assembly and annotation	500001	magnus	Partners	2015
		CCG Bioinformatics		zythos	Directors	2014
Peter Edwards	CSIRO	Applications Support, Management of allocations; monitoring	10000	magnus	Directors	2014
Peter Jones	University of Technology - Sydney	Plasmodium falciparum neutral aminopeptidases structure-function analysis	300000	fornax	National Merit	2014
		Structure-function analysis of PfL-M17 for the discovery of anti-malarial drugs		fornax	National Merit	2015
Peter Metaxas	The University of Western Australia	Strongly coupled nanomagnets: applications to reconfigurable spintronic devices	11000	fornax	Partners	2014
		Dynamic nanodetectors for magnetic nanoparticles		Zeus	Directors	2015
Peter Munro	The University of Western Australia	Evaluation of three widely used biomedical optical imaging techniques	10000000	magnus	National Merit	2015
Phil Cummins	Australian National University	Development of a better physics behind the tsunami modelling and coastal infrastructure behaviour.	180170	epic	Geosciences	2014

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Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Piotr Kowalczyk	Curtin University	Thermodynamics and Kinetics of Multi-Component Greenhouse Gas Mixtures in Nanoconfinement	330000	epic	Partners	2014
	Murdoch University	Quantum-mediated Freezing and Melting of Hydrogen Isotopes in Nanopores		magnus	Partners	2015
Rachel Binks	Department of Parks and Wildlife	Genomics of West Australian flora	6000	zythos	Directors	2014
Ramesh Narayanaswamy	Curtin University	The Phenomenology of Unsteady Impinging Jets: Fluid Dynamics and Heat Transfer	1000000	magnus	Partners	2015
Ramin Rahmani	Curtin University	Hydrogen storage	20000	epic	Directors	2014
Randall Wayth	Curtin University	MWA GLEAM: The GaLactic/Extragalactic All-sky MWA survey	573536	fornax	Partners	2015
		MWA data preprocessing: flags and compression		zythos	Directors	2014
		MWA Operations		galaxy	Astronomy	2015
		MWA survey data processing		epic	Astronomy	2014
Ranjeet P. Utikar	Curtin University	Gas-Solid Flow Modelling in FCC Riser	1500000	epic	Partners	2014
Ravichandar Babarao	CSIRO	Understanding how to make porous materials robust for energy applications	1500000	magnus	Partners	2015
		Enhancing storage and delivery of small molecules in porous materials from molecular perspective		epic	Partners	2014
Rebecca Hartman-Baker	Pawsey Supercomputing Centre	Student Cluster Competition Team Training 2014	210000	zythos	Directors	2014
		Benchmarking for Early Access to Petascale Magnus		magnus	Directors	2014
		Student Cluster Competition Team Training 2014		magnus	Directors	2014
Ricardo L Mancera	Curtin University	Molecular simulation of the self-assembly lipoproteins and protein aggregation complexes	170000	fornax	Partners	2015
		Large-scale molecular dynamics simulations of macrobiomolecular complexes		magnus	Directors	2014
Richard Sandberg	The University of Western Australia	High-fidelity simulations of low-pressure turbine stages	100000	magnus	Directors	2015
Robert Wittenmyer	University of New South Wales	Studying the Dynamics of Multiple Planetary Systems	150000	epic	National Merit	2014
Robin Pearce	CSIRO	Modelling microstructures of composite materials	1	zythos	Directors	2014
Roman Pevzner	Curtin University	Seismic monitoring of CO2 geosequstration: optimising data acquisition and processing	4927830	magnus	Geosciences	2015
Ronald Monson	Edith Cowan University	Knowing thyself or knowing thy hive mind - MOOCs big-data conundrum.	5000	zythos	Directors	2014
Rudi Appels	Murdoch University	BPA wheat activities - Assembly of chromosome 7A and SNP analysis for 16 varieties	550000	epic	Partners	2014
		Collaborative project for wheat gene annotation and analysis		magnus	Directors	2014
Ruslan Puscasu	The University of Queensland	Large scale flow dynamics simulations for block caving research	9595000	magnus	Geosciences	2015
Ryan Lowe	The University of Western Australia	Highly-resolved ocean simulations of the northwest Australian coast	3022056	epic	Geosciences	2014

Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Ryan Mead-Hunter	Curtin University	Simulation and characterisation of oil-mist filtration	100000	magnus	Partners	2015
Salman H. Khan	The University of Western Australia	Large scale feature extraction using Convolutional Neural Networks (CNNs)	10000	epic	Directors	2014
Samuel Tan	Monash University	Fragment molecular orbital approach for liquid electrolytes	100000	magnus	Directors	2014
Sanjib Sharma	University of Sydney	Understanding Galaxy Formation	400	fornax	National Merit	2014
Scott G Wilson	The University of Western Australia	Understanding complex human genetic diseases through whole genome sequencing	65000	epic	Partners	2014
		Relative importance of genetic and epigenetic factors in the aetiology of common complex disease		magnus	Partners	2015
Sean Smith	University of New South Wales	Computational Nanomaterials Science and Engineering	1000000	magnus	National Merit	2015
Sebastien Allgeyer	Australian National University	Development of a better physics behind the tsunami modelling and coastal infrastructure behaviour.	300000	magnus	Geosciences	2015
Sergiy Shelyag	Monash University	Radiative magneto-hyrdrodynamic modelling of interconnected solar interior and atmosphere	1800000	magnus	National Merit	2015
Shane Evans	Moombarriga Geoscience	3D Inverse Modelling of Magnetotelluric Data:A Useful Regional Mineral Exploration Targeting Tool?	300284	epic	Geosciences	2014
Shane Henderson	Edith Cowan University	ECU 3D Animation renderfarm 2014	18000	fornax	Partners	2014
		ECU Renderfarm		Zeus	Directors	2015
		ECU Renderfarm 2015		fornax	Partners	2015
Shin Kee Chung	The University of Western Australia	Gravitational Wave Search with Application of GPUs	438200	fornax	Partners	2014
		GPU Accelerated Gravitational Wave Signal Processing		Zeus	Directors	2015
		Australian Collaboration of Gravitational Wave Signal Processing		magnus	Partners	2015
Simon Campbell	Monash University	Three-dimensional Simulations of Stars	10500000	magnus	Directors	2014
Simon Grabowsky	The University of Western Australia	Quantum crystallography on vitamin B12 coenzyme	901000	fornax	Directors	2014
		Quantum crystallography on large systems		epic	Partners	2014
Slava Kitaeff	ICRAR	Detection of Spectral Lines with MWA	50000	magnus	Partners	2015
Stefan Iglauer	Curtin University	Molecular dynamics predictions of fluid-fluid-rock interfacial properties	30000	magnus	Partners	2015
Stuart Walsh	CSIRO	GEOS software demonstration	100000	magnus	Directors	2015
Taka Miyoshi	The University of Western Australia	HPC simulation, imaging and inversion of passive seismology data	120000	fornax	Geosciences	2015
Tara Murphy	The University of Sydney	MWA Science pre-processing	276000	galaxy	Astronomy	2015
Thomas Poulet	CSIRO	Multiphysics simulations using MOOSE	340227	epic	Geosciences	2014
		Tackling the unconventional resources challenge with multiphysics simulations		magnus	National Merit	2015
Tiffany Walsh	Deakin University	Development and application of bio/nano interfacial simulations	1000000	magnus	National Merit	2015
Toby Allen	Royal Melbourne Institute of Technology	Mechanisms of charge-membrane interactions and transport	2000000	magnus	National Merit	2015
				epic	National Merit	2014

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Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Tom Lyons	Murdoch University	Past and Future Temperature Extremes and Vegetation in Western Australia	3650000	magnus	National Merit	2015
				epic	National Merit	2014
Tongming Zhou	The University of Western Australia	Vortex and force characteristics of inclined offshore cylindrical structures in oscillatory flows	250000	epic	Partners	2014
Tony Ambaum	CSIRO	ASKAP	1000000	galaxy	Astronomy	2015
Tony Chiffings	The University of Western Australia/Sohar University	Developing a water quality forecast system for the Sohar industrial port, oman	70000	epic	Partners	2014
Tony Rafter	CSIRO	High-res simulation of regional climate to capture extreme rainfall events over SE Queensland	4000000	magnus	Directors	2014
		Continuous 2km regional climate simulations to analyse future changes in climate extremes		magnus	Partners	2015
Travis Endersby	The University of Western Australia	Statistical Genetic and Epidemiological Analyses for Complex Diseases	450000	epic	Partners	2014
				magnus	Partners	2015
Tristan Salles	CSIRO	Stratigraphic & Geomorphic Forward Modelling Infrastructure (SGFM)	3600000	epic	Partners	2014
		Continental rifting - Surface processing : Coupling Framework		magnus	Partners	2015
	University of Sydney	Continental rifting & Surface processing		magnus	Directors	2014
U Geun Jang	The University of Western Australia	Full Waveform Inversion of 3D seismic data on HPC x86 clusters	750000	magnus	Geosciences	2014
Ute Mueller	Edith Cowan University	Geostatistical simulation and estimation of material types	50000	epic	Partners	2014
Vahid Etminan	The University of Western Australia	Geophysical and Environmental Computational Fluid Dynamics Research	100000	magnus	Directors	2015
Valerie Maxville	Pawsey Supercomputing Centre	Interns 2013 - 2014	100001	epic	Directors	2014
		Interns 2014-2015		magnus	Directors	2015
Waseem Kamleh	University of Adelaide	Dynamical Fermions and Chiral Symmetry in Lattice QCD	12500000	magnus	Directors	2014
		Form Factors, Chiral Symmetry and Dynamical Fermions in Lattice QCD		galaxy	Directors	2015
		Electromagnetic Structure of Matter		magnus	National Merit	2015
Wei Hu	Curtin University	Reload option pricing	300	fornax	Directors	2014
Weiguang Cui	The University of Western Australia	SimPL (Survey Simulation PipeLine) - The Universes under various cosmological models	4000000	magnus	National Merit	2015
Weihua Liu	CSIRO	Molecular dynamics simulations of gold speciation in ore fluids	1188600	magnus	Geosciences	2015
Weronika Gorczyk	The University of Western Australia	Multiscale Dynamics of Orebody Formation	580454	epic	Geosciences	2014
		Multi-scale four-dimensional large scale tectonics and genesis, transfer and focus of fluids		magnus	Partners	2015
Willy Susilo	University of Wollongong	Quantum Simulator	200000	fornax	National Merit	2014
Wisam Al-saadi	Monash University	Rotating horizontal convection at high Rayleigh number	100000	magnus	National Merit	2015
Wouter Schellart	Monash University	Role of subduction zone interface mechanical coupling on subduction dynamics	400000	magnus	National Merit	2015

Principal Investigator	Institution	Project name	Total Allocation/ cores hours	System	Allocation	year
Xiaoliang Wu	CSIRO	Urban Monitor	550000	epic	Partners	2014
				magnus	Directors	2014
				magnus	Partners	2015
Xihong Zhang	The University of Western Australia	Development of Design and Analysis Methods for Blast Resistant Window Structures	90000	fornax	Partners	2015
Yanhua Zhang	The University of Western Australia	Coupled geologic simulations using MOOSE: understanding ore deposits and aiding mineral exploration	100000	magnus	Partners	2015
Youkou Dong	The University of Western Australia	GPU parallelisation of Material Point Method oriented to submarine landslide	1000	fornax	Directors	2014
Yuan Mei	CSIRO	Gold transport in geofluids during phase separation: insights from molecular dynamics simulation	1891090	epic	Geosciences	2014
		Modeling Metal Transport During Phase Separation Using Molecular Dynamics Simulation		fornax	Geosciences	2015
Yucang Wang	CSIRO	Simulation of bore hole breakouts and particle breakage in ball mills	100000	magnus	National Merit	2015
Yuqing Feng	CSIRO	discrete particle simulation of particulate multiphase flow	20000	epic	Partners	2014
Zak Hughes	Curtin University	Large scale molecular dynamics simulations of macrobiomolecular complexes	500000	epic	Partners	2014
Zheng-Xiang Li	Curtin University	4D Global Geodynamic Modelling	50000	magnus	Directors	2015
Zhenlin Zhang	The University of Western Australia	Geophysical and Environmental Computational Fluid Dynamics Research	1000000	magnus	Partners	2015
	Pawsey Supercomputing Centre	Quarterly allocations test	100000	magnus	Directors	2015

2014 PUBLICATIONS LIST

1. A. Levy and A.B. Yu (guest editors), Special issue on conveying and handling of particulate solids - Challenges of discrete element simulation, application and calibration, Particuology, 12 (1) (2014) 1-122.

2. X.H. Yang, H.T. Fu, X.C. Jiang and A.B. Yu. Silver Nanoparticles: Synthesis, Growth Mechanisms and Bioapplications (Chapter 19 in the book "Silver Nanoparticles: Synthesis, Uses and Health Concerns"), pp. 395-460. 2014, Nova Science Publishers, ISBN: 978-1-60741-028-7.

3. K. Li, S.B. Kuang, R.H. Pan and A.B. Yu, Powder Technology, 51 (2014) 15–24.

4. S.D. Liu, Z.Y. Zhou, R.P. Zou, D. Pinson and A.B. Yu, Powder Technology, 253 (2014) 70-79.

5. K.W. Chu, S.B. Kuang, A.B. Yu, A. Vince, G.D. Barnett, P.J. Barnett, Minerals Engineering, 56 (2014) 91-101.

6. S.B. Kuang, Z. Qi, A.B. Yu, A. Vince, G.D. Barnett and P.J. Barnett, Minerals Engineering, 62 (2014) 43-54.

7. J. Chen, K.W. Chu, R.P. Zou, A.B. Yu, A. Vince, G.D. Barnett and P.J. Barnett, Minerals Engineering, 62 (2014) 55-65.

8. S.B. Kuang, Z.Y. Li, D.L. Yan, Y.H. Qi, and A.B. Yu, Minerals Engineering, 62 (2014) 43-54.

9. K.W. Chu, S.B. Kuang, A.B. Yu, A. Vince, G.D. Barnett and P.J. Barnett, Minerals Engineering, 56 (2014) 91-101.

10. M. Ghodrat, S.B. Kuang, A.B. Yu, A. Vince, G.D. Barnett and P.J. Barnett, Minerals Engineering, 62 (2014) 74-84.

11. Q.F. Hou, K.J. Dong and A.B. Yu, Powder Technology, 256 (2014) 529-539.

12. Q.F. Hou, M. Samman, J. Li and A.B. Yu, ISIJ International, 54 (2014) 1772-1780.

13. K.W. Chu and A.B. Yu, Powder Technology, 254 (2014) 460-469.

14. B. Wang, K.W. Chu, A.B. Yu and A. Vince, 62 (2014) 111-119.

15. Y.S. Shen, T. Shiozawa, P. Austin and A.B. Yu, Minerals Engineering, 63 (2014) 91-99.

16. M. Ghodrat, S.B. Kuang, A.B. Yu, A. Vince, G.D. Barnett and P.J. Barnett, Minerals Engineering, 63 (2014) 125-138.

17. D. Yan, H. Zhang, S. Li, G. Zhu, Z. Wang, H. Xu and A.B. Yu, Journal of Alloys and Compounds, 607 (2014) 245-250.

18. X. Zhang, H. Xu, Y. Zhao, G. Zhu and A.B. Yu, Materials Letters, 129 (2014)101-103.

19. C.J. Gil, A. Pham, A.B. Yu and S. Li, Journal of Physics Condensed Matter, 26 (30) (2014), art. no.306004.

20. A. Pham, M.H.N. Assadi, A.B. Yu and S. Li, Physical Review B - Condensed Matter and Materials Physics, 89 (15) (2014), art. no.155110.

21. D. Rangarajan, T. Shiozawa, Y.S. Shen, J.S. Curtis and A.B. Yu, Industrial and Engineering Chemistry Research, 53 (13) (2014) 4983-4990.

22. M. Capece, Z. Huang, D. To, M. Aloia, C. Muchira, R.N. Davé and A.B. Yu, Powder Technology, 254 (2014) 103-113.

23. C. Cao, A.B. Yu and Q.H. Qin, WIT Transactions on Modelling and Simulation, 56 (2014) 61-72.

24. D. Yan, H. Zhang, L. Chen, G. Zhu, Z. Wang, H. Xu and A.B. Yu, RSC Advances, 4 (45) (2014) 23649-23652.

25. A. Levy and A.B. Yu, Particuology, 12 (1) (2014)1.

26. B.Y. Guo, J. Guo and A.B. Yu, J. Electrostatics, 72 (2014) 301-310.

27. Y. Kaneti, Z.J. Zhang, J. Yue, Q.M.D. Zakaria, C.Y. Chen, X.C. Jiang, and A.B. Yu, Phys. Chem. Chem. Phys. 16 (2014) 11471-11480.

28. Z.J. Zhang, Y.V. Kaneti, X.C. Jiang and A.B. Yu, Sensor & Actuators B: Chemical, 202 (2014) 803-809.

29. H.T. Fu, X.H. Yang, X. C. Jiang and A. B. Yu, Sensors & Actuators: B. Chemical, 203 (2014) 705-711.

30. Y. V. Kaneti, Q.M.D. Zakaria, Z.J. Zhang, C.Y. Chen, J. Yue, X.C. Jiang, and A.B. Yu, J. Mater. Chem. A, 2 (2014) 13283-13292.

31. X.H. Yang, H.T. Fu, X.C. Wang, J.L. Yang, X.C. Jiang and A.B. Yu, J. Nanopart. Res, 16 (2014) 2526.

32. R. Wen, J. Yue, Z.F. Ma, W.M. Chen, X.C. Jiang and A.B. Yu, Chinese Science Bulletin, 59(18) (2014) 2162. (Invitation)

33. Z.A. Tian, K.J. Dong and A.B. Yu, Physical Review E, 89 (3) (2014) 032202.

34. R. Chandratilleke, A.B. Yu, J. Bridgwater and K. Shinohara, Industrial & Engineering Chemistry Research, 53 (10) (2014) 4119-4130.

35. Q.J. Zheng and A.B. Yu, Physical Review Letters, 113 (2014) 068001.

36. S. Shahbazi, X.C. Jiang, J.L. Yang and A.B. Yu, World Journal of Cancer Research, in press (accepted in Feb 2014, MS No. 14-38-R).

37. W.J. Yang, Z.Y. Zhou, D. Pinson and A.B. Yu, Industrial & Engineering Chemistry Research, 53 (2014) 8245-8256.

38. K.M. Komiyama, B.Y. Guo, H. Zughbi, P. Zulli and A.B. Yu, Metallurgical Transaction B (Process Metallurgy), 45 (5) (2014) 1895-1914.

39. L.W. Rong, K.J. Dong and A.B. Yu, Chemical Engineering Science, 116 (2014) 508-523.

40. W.F. Sun, Q.H. Zeng and A.B. Yu, Chemical Engineering Science, in press (accepted in June 2014).

41. B.Y. Guo, A.B. Yu and J. Guo, Journal of Aerosol Science, 77 (2014) 102-115.

42. Z.Y. Zhou, R.P. Zou, D. Pinson and A.B. Yu, Granular Matter, 16 (2014) 695-709.

43. W.J. Yang, Z.Y. Zhou, D. Pinson and A.B. Yu, Metallurgical Transaction B (Process Metallurgy), in press (accepted in Sept 2014).

44. W.F. Sun, Q.H Zeng and A.B. Yu, RSC Advances, 4 (2014) 38505-38516.

45. M. Halidan, R. Chandratilleke, S. Chan, J. Bridgwater and A.B. Yu, Chemical Engineering Science, 120 (2014) 37-48.

46. Entry in the AuScope Newsletter: FEILDS:Australia - Construction of the Lithospheric Density Structure of Australia with Auscope Infrastructure http://www.vision6.com.au/em/message/email/view?a=36413&id=1116273

47. Talk presented at the Geological Survey of Western Australia: Interim results of 3D joint magnetic/gravity inversions of the Kimberley Region.

48. An Applied Mathematics/Physics student Honours Thesis: Generating Layered-Earth Models for 3D Gravity Inversion in Escript

49. A.R. Duffy, J.S.B. Wyithe, S.J. Mutch, G.B. Poole, "Low-mass galaxy formation and the ionizing photon budget during reionization", Monthly Notices of the Royal Astronomical Society, Volume 443, Issue 4, p.3435-3443 (2014).

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57. A. Karrech, C. Schrank and K. Regenauer-Lieb, "A parallel computing tool for large-scale simulation of massive fluid injection in thermo-poro-mechanical systems", Submitted for publication in the Philosophical Magazine.

58. A. Karrech, C. Schrank, K. Regenauer-Lieb, "Damage propagation due to massive fluid injection", Symposium of Instabilities across the scales - IAS 2014.

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