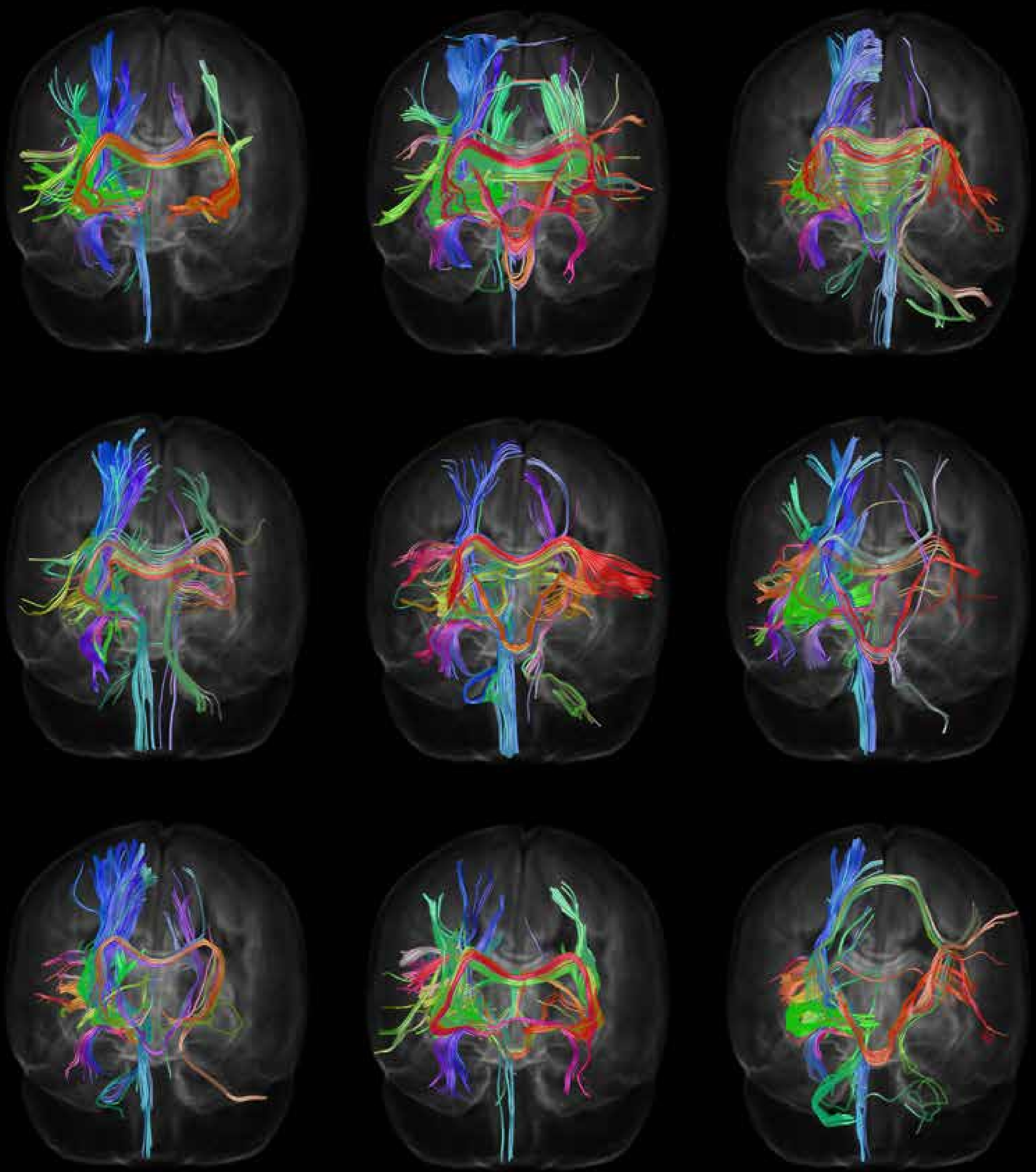
MASSIVE Annual Report 2015—2016



MONASH University CSIRO Australian Synchrotron ansto CIBF CENTRE FOR ADVANCED MOLECULAR IMAGING AN ARC CENTRE OF EXCELLENCE

Partners

Affiliate Partners

Characterisation Funders and NCRIS Project Partners

FRONT COVER Professor Nellie GeorgiouKaristianis and her team are using MASSIVE for the IMAGEHD study based at Monash University.

This project aims to track the onset and progression of Huntington Disease (HD), a devastating neurological disorder. The MASSIVE platform has significantly enhanced the project's capabilities in achieving its deliverables to better characterise how the disease develops and progresses over time. Through this research, the team found that the number of poorly connected neural networks significantly increased in people diagnosed with HD, compared to those without the disease. They also found that as the disease develops, the changes in the brain become more widespread. These findings have important implications for drug development, particularly in terms of treatments geared toward preventing loss of neural connections, strengthening neural connectivity, and/or improving functional outcomes.

Contents

Dr Robert Hobbs
Chair, MASSIVE
Steering Committee

From the Chair

Welcome to the MASSIVE annual report for 2015-16. The past 18 months have been one of continuing growth and achievement.

I'm pleased to report that during 2015 two national ARC Centres of Excellence joined our consortium. Over fifteen new projects are now using MASSIVE through a dedicated Centre of Excellence allocation and this direct relationship with flagship Australian projects is already generating impact.
This report details the development of the Australian mirror of the Human Connectome Project, a collaboration with the ARC Centre of Excellence in Integrative Brain Function, and the way the data generated by the project will be used nationally.

Our growth in projects and users, including new projects through both the Australian Synchrotron and the Ramaciotti Centre for Electron Microscopy, is a direct outcome of our close engagement with these instruments. The usage and the early-stage discoveries, reported in Achievements, provide an exciting glimpse into the future.

In this past year MASSIVE has been laying the groundwork for the future.The M3 computer is a much-needed investment that will continue the project's impact for many years to come. I had great pleasure in participating in the launch of the new system in March 2016 by the Australian Chief Scientist, Dr Alan Finkel, and NVIDIA CTO Steve Oberlin. The highlight of the launch was to hear directly how researchers are going to use M3 and the impact that this computer will have across areas such as neuroscience and biomedical discovery.

The architecture of the M3 computer has been designed to grow significantly over the coming years as the M1 and M2 computers approach their retirement.

These computers have served the Australian research community well: over 1000 scientists across 200+ individual projects have used the systems. They have provided nearly 100 million CPU core hours of time to Australian researchers.

In another important development, I'm very happy to welcome a new MASSIVE partner in mid 2016: the Australian Nuclear Science and Technology Organisation (ANSTO) is both a major operator of flagship scientific instruments and a world-class research facility. ANSTO is an important contributor to Australia's future as a knowledge economy. It both supports a wide range of scientists and provides critical nuclear research capability. ANSTO's partnership in MASSIVE will leverage a large body of work in computational imaging infrastructure that Monash University, CSIRO and the Australian Synchrotron have led, and will extend MASSIVE to a wider cohort of researchers, with a particular focus on material sciences and characterisation.

This report will be my last as the Chair of MASSIVE. In July 2016, I will be handing over to a newly elected chair, Dr Greg Storr, who is a nuclear scientist and a former director at ANSTO.

I am pleased and proud of the progress of MASSIVE since my tenure began in 2012.

In addition to the support provided to the research sector MASSIVE has contributed to the success of several start-up companies. I'd like to single out the article about 4Dx and the way this Australian start-up company has used MASSIVE to develop, demonstrate and commercialize their innovative imaging algorithms. At the M3 launch, Dr Alan Finkel mentioned that high performance computing helps to build bridges between industry and academia and accelerates research translation, and I consider this an outstanding example.

I would like to acknowledge the excellent support that I have had from the members of the Steering Committee and the outstanding work of the talented MASSIVE staff, in particular its Director, Dr Wojtek Goscinski, and our many collaborators and users over the past four years. They are the key contributors that have made MASSIVE such a great success.

I wish all those associated with MASSIVE all the best for the future.

Dr Robert Hobbs
Chair, MASSIVE Steering Committee

Dr Wojtek James Goscinski
MASSIVE Coordinator

Coordinator's Message

Welcome to our 2015-16 annual report. I'm very happy to report on a number of specific highlights, including the onboarding of our new ARC Centre of Excellence Affiliate Partners and our new computer, M3 that was purchased through significant support from Monash University and the Monash University Faculty of Medicine.

We are excited to have been onboarding two new affiliate partners: the ARC Centre of Excellence for Integrative Brain Function, which is focused on understanding how the brain interacts with the world; and the ARC Centre of Excellence for Advanced Molecular Imaging, which is developing and applying innovative microscopy techniques to observe the details of how immune systems function at the molecular level.

Our new M3 system is well timed as we are now approaching the retirement of our existing systems. It also allows us to re-architect our technical services. M3 leverages both our work on the Australian research cloud and our instrument integration projects. We've re-architected the way we deliver clusters – using cloud-based tools over the top of dedicated HPC hardware. This work builds on local and national investment in the Monash University node of the NeCTAR research cloud. We think it will lead to a more scalable system that is easier to manage and will provide easier entry points for researchers to scale from local cloud systems to high performance data processing. I'd like to thank our industry partners, NVIDIA, Dell and Mellanox for their effort in helping us architect and deliver this system.

Further to this, M3 will bring together investment in the Characterization Virtual Laboratory. A portion of the machine will be used to provide desktops for the national CVL community. New NVIDIA Graphics Processing Units (GPUs) will be used to support both the peak high end imaging community and users with more modest requirements. Efficiency is crucial: this past year has seen a huge flow of projects through our instrument work and our systems now support over 1000 user accounts.

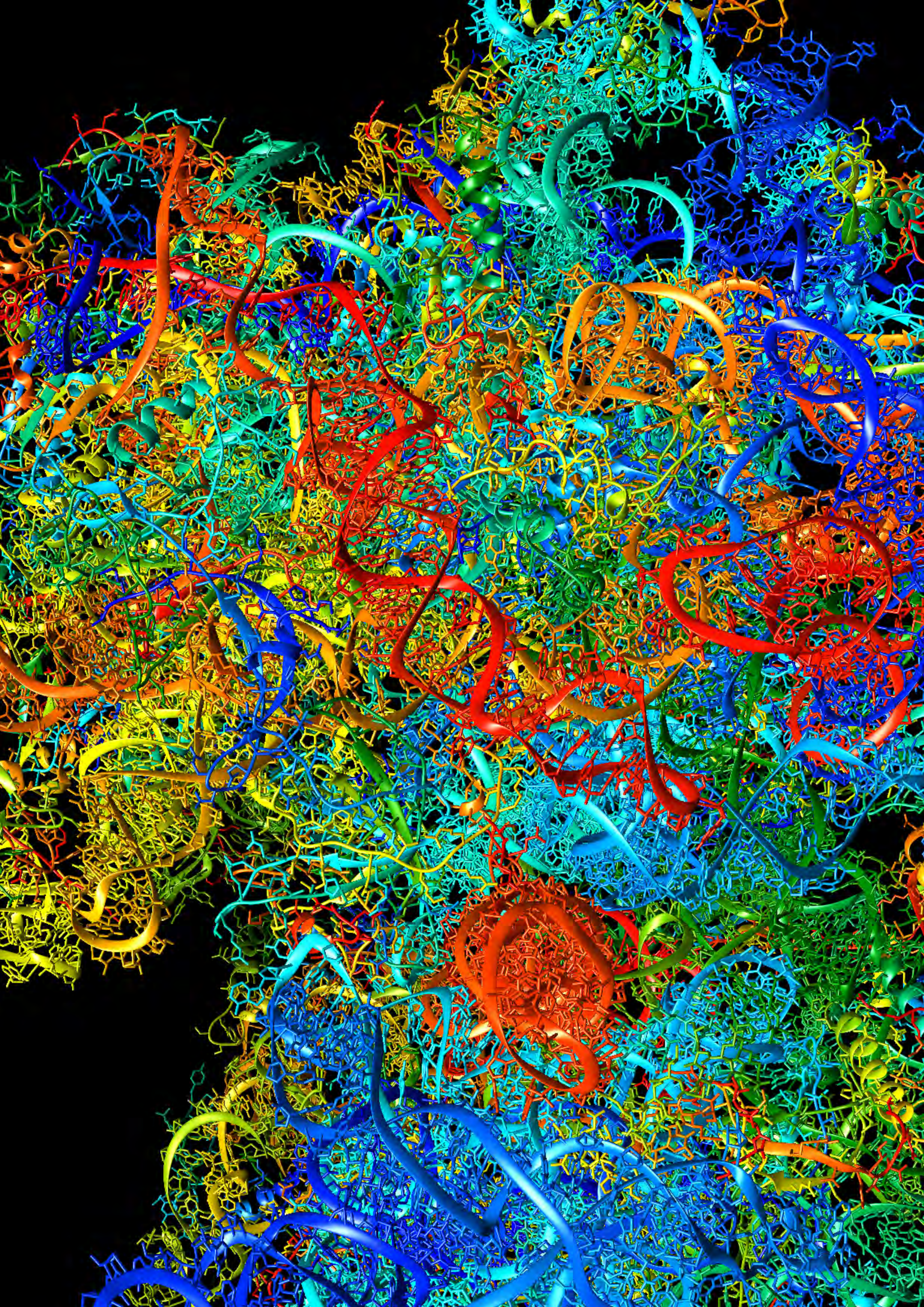
I encourage you to read about the launch of the M3 system – we were honored to have Dr Alan Finkel and Steve Oberlin launch the system.

I'd like to thank our growing research community for their support and their research achievements.

I would also like to thank our team, which has recently grown to six dedicated staff members plus contributions from the core Monash University eSolutions team, and the Monash eResearch Centre, plus significant contributions from Australian Synchrotron and Monash University.

Finally, I would like to thank our outgoing Chair, Dr Robert Hobbs for his dedicated work as our chair for the last four years. I wish him all the best in future projects.

Dr Wojtek James Goscinski
Coordinator, MASSIVE



/01

Achievements in 2015-16

MASSIVE has secured funding for a new computer, M3, which was launched in March 2015 and is to be made available to first users in mid-2016. This increased investment is set to underpin the thousand plus researchers that rely on MASSIVE, as M1 and M2 are retired in 2017.

OPPOSITE: Nanoscale imaging at the Remaciotti Centre for Cryo Electron Microscopy and supercomputing on the new M3 computer is set to produce incredibly detailed images of the nanomachines of life such as this image by Dr Matthew Belousoff, Dr Mazdak Radjainia, and Prof Trevor Lithgow, Monash University

Jan 2015 to June 2016, MASSIVE achievements included:

> Our work with flagship Australian instruments has received strong uptake and has underpinned significant research outcomes.

Researchers visiting both the Imaging and Medical Beamline (IMBL) and the X-ray Fluorescence Microscopy (XFM) beamline are automatically given a beamline visit project, and user accounts. As of 1st March, 247 projects using the Imaging and Medical Beamline (IMBL) and the X-ray Fluorescence Microscopy (XFM) beamline at Australian Synchrotron have been allocated time on the MASSIVE Desktop using this mechanism. Combined these users have logged into over 1000 desktops sessions.

> In July, MASSIVE welcomes a new partner, the Australian Nuclear Science and Technology Organisation (ANSTO), which is both a major operator of flagship scientific instruments and a world-class research facility. ANSTO is an important contributor to Australia's future as a knowledge economy. It both supports a wide range of scientists and provides critical nuclear research capability. ANSTO's partnership in MASSIVE will leverage a large body of work in computational imaging infrastructure that Monash University, CSIRO and the Australian Synchrotron have led, and will extend MASSIVE to a wider cohort of researchers, with a particular focus on material sciences and characterisation.

> MASSIVE has secured funding for a new computer, M3, which was launched in March 2015 and is to be made available to first users in mid-2016. This increased investment is set to underpin the thousand plus researchers that rely on MASSIVE, as M1 and M2 are retired in 2017.

M3 will extend many of the design decisions that were integrated into M1 and M2. The computer will be an efficient data processing engine with a huge capacity and will provide fast interactive access. The first stage of M3 includes 48 NVIDIA Tesla K80 GPU cards, and a fast parallel file system with over 1 petabyte of capacity.

M3 leverages significant national investment in the Monash University node of the NeCTAR research cloud. This high performance computer is designed to sit alongside other cloud services as part of the ecosystem of services for next-generation virtual laboratories.

> The CVL user community continues to grow and has now been used by 590 unique researchers across Australia, with nearly 60% of users returning to continue access. Researchers combined have run over 23,000 individual desktop sessions on CVL on the NeCTAR cloud, and M1 and M2 systems on MASSIVE.

Dr Rajeev Samarage

Prof Andreas Fouras

Research Stories

Understanding How Embryos Form

A collaboration between biologists and engineers at Monash University has led to the development of a new non-invasive image processing technique to visualise embryo formation. Researchers were able to see, for the first time, the movement of all of the cells in living mammalian embryos as they develop under the microscope. This breakthrough has important implications for IVF (in vitro fertilisation) treatments and pre-implantation genetic diagnosis (PGD). In the future, this approach could help with embryo selection before the embryo is implanted back into the uterus to improve IVF success rates.

This latest research, published in Developmental Cell, and titled 'Cortical Tension Allocates the First Inner Cells of the Mammalian Embryo', provides new insights into embryo formation and challenges the prevailing model of cell placement through division. The three joint first authors are: Dr Melanie White, Research Fellow at the Plachta Lab at Australian Regenerative Medicine Institute (ARMI), Dr Yanina Alvarez of University of Buenos Aires and Rajeev Samarage, PhD candidate supervised by Prof Andreas Fouras at the Department of Mechanical and Aerospace Engineering at Monash University.

Mammalian embryos start out as a small group of identical cells. At an early stage, some of the cells take up an internal position within the embryo. These internal cells go on to form all of the cells of the body while the remaining outer cells go on to form other tissues such as the placenta.

For many years, researchers theorised that the internal cells adopt their position through a special process of cell division, but due to technological limitations, this had never actually been shown. Using their newly developed imaging methods, the Monash University researchers were able to demonstrate that this model of embryo formation was incorrect.

The researchers then applied cutting-edge laser techniques to the mammalian embryo (previously used in fly and plant embryos or cultured cells only) to determine what forces were acting on the cells to make them move inside the embryo.

Using these new imaging techniques, researchers were able to see how the cells moved and changed shape over time as they were 'pushed' inside to form the internal mass. They showed that there are differences in the tension of the membranes of the cells and these differences are what determine which cells will move inside to form the body. By altering the tension of the cells using lasers or genetic manipulations, researchers could change which cells move to inside the embryo.

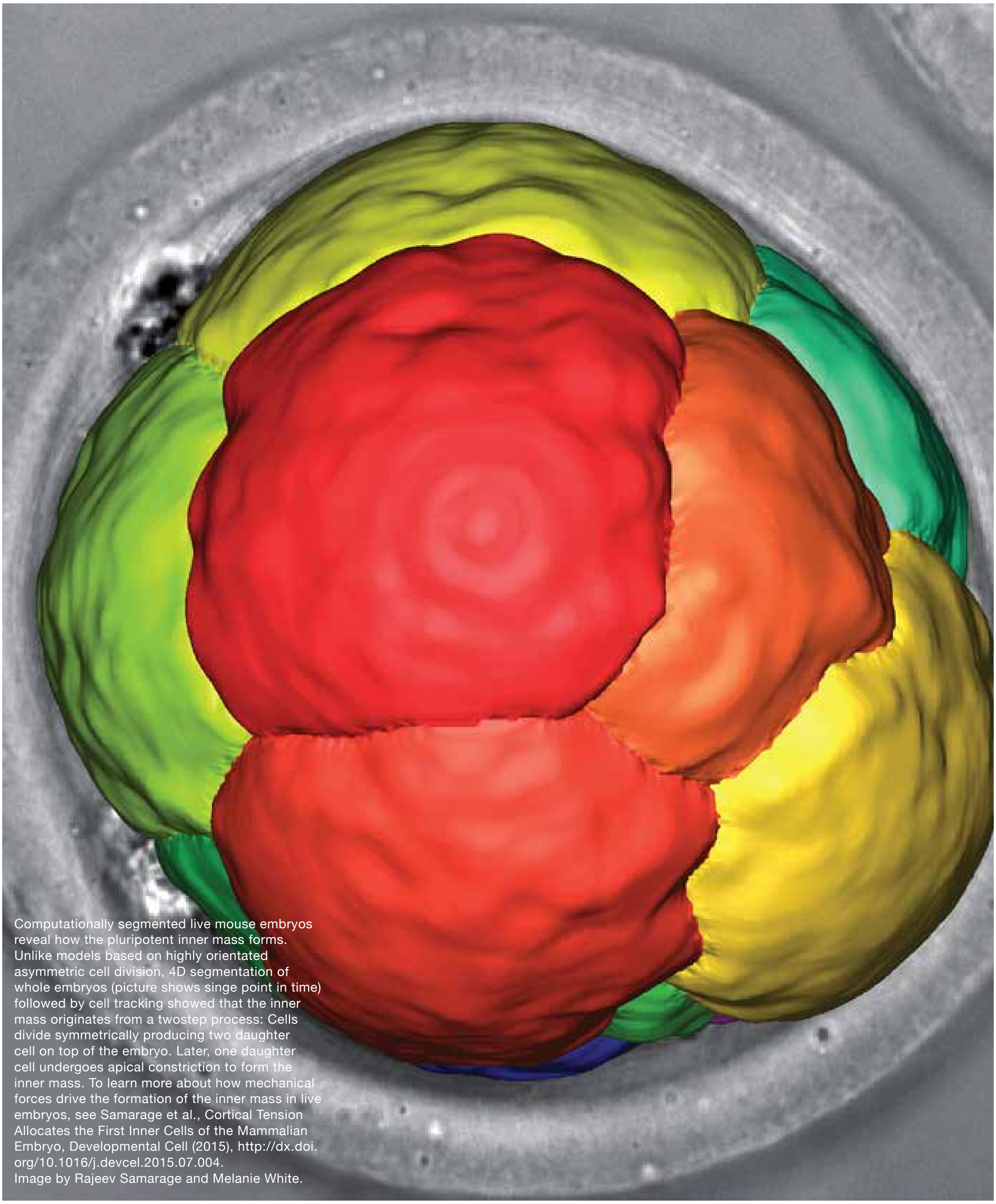
These findings also offer potential to make alterations to improve inter-cellular forces and cell formation.

"Our findings offer an attractive possibility where alterations to the inter-cellular forces could increase embryo viability leading to better IVF outcomes. We can think of this as a 'push in the right direction'," Mr Samarage said.

Work is under way to use this new custom image segmentation technology with non-invasive imaging approaches to see how human embryos used in IVF or PGD first organise their cells.

"If in the future, we can combine our new image processing technique with non-harmful dyes that can label the membranes of human embryos, we may be able to evaluate embryos used in IVF and decide which ones to implant to have the best chance of success," said Dr Melanie White.

Originally published at: http://monash.edu/news/show/new-embryo-image-processing-technology-could-assist-in-ivf-implantation-success-rates%20/t%20_blank



Computationally segmented live mouse embryos reveal how the pluripotent inner mass forms. Unlike models based on highly orientated asymmetric cell division, 4D segmentation of whole embryos (picture shows singe point in time) followed by cell tracking showed that the inner mass originates from a twostep process: Cells divide symmetrically producing two daughter cell on top of the embryo. Later, one daughter cell undergoes apical constriction to form the inner mass. To learn more about how mechanical forces drive the formation of the inner mass in live embryos, see Samarage et al., Cortical Tension Allocates the First Inner Cells of the Mammalian Embryo, Developmental Cell (2015), http://dx.doi.org/10.1016/j.devcel.2015.07.004.
Image by Rajeev Samarage and Melanie White.

/02

Launch of the M3 Computer

Australian research was given a boost on the 29th of February 2016 through a new and major investment in MASSIVE—a five-year collaboration between Monash University, CSIRO and the Australian Synchrotron.

OPPOSITE TOP: Dr Olivier Salvado (CSIRO), AProf Hans Elmlund (Monash University), Prof Trevor Lithgow (Monash University) and Dr Marta Garrido (University of Queensland) discuss how they plan to use M3

OPPOSITE BOTTOM: Dr Alan Finkel, Australian Chief Scientist, Dr Robert Hobbs, Chair MASSIVE Steering Committee, and Ms Leonie Walsh, Victorian Lead Scientist

Australian Chief Scientist turns on the new MASSIVE computer, M3

MASSIVE (Multi-modal Australian ScienceS Imaging and Visualisation Environment) is a high performance computing facility designed specifically to process complex data. Since 2010, MASSIVE has played a key role in driving discoveries across many disciplines including biomedical sciences, materials research, engineering and geosciences.

High performance computing helps to build bridges between industry and academia while accelerating research translation. To support both, Monash University has invested a further $4.1m in this new $5.7m project to fund a new high performance computing capability, M3.

"M3 will be particularly important to the Faculty of Medicine by providing computing capacity that is malleable, connected and can be shaped to support the needs of Monash's strategic research domains," says Professor Christina Mitchell, Dean, Faculty of Medicine, Nursing and Health Sciences.

Alan Finkel AO, Australia's Chief Scientist, joined Professor Mitchell and Professor Ian Smith, Monash University Vice-Provost (Research and Research Infrastructure), to "switch on" M3.

Dr Finkel says our nation needs superb science, and superb science only emerges when our scientists are able to access first-class infrastructure such as MASSIVE.

"You cannot understand what you cannot see," the Chief Scientist says. "MASSIVE provides specialised processing power to build three dimensional X-ray images at micrometre resolution or complex maps to summarise the interconnections between millions of brain cells. At a glance, scientists can now visualise and understand these complex structures."

Over five years, MASSIVE has built a reputation as a leader in coordinating imaging informatics infrastructure across Australia, and as such, works closely with many national initiatives. This new investment will therefore have a significant impact, for example in life sciences research.

MASSIVE welcomes two new contributing affiliate partners, the ARC Centre of Excellence in Advanced Molecular Imaging and the ARC Centre of Excellence for Integrative Brain Function. The CSIRO and the Australian Synchrotron have both committed funds to continue their support.

Dr Marta Garrido is a neuroscientist working at the University of Queensland in the ARC Centre of Excellence for Integrative Brain Function; she is interested in the brain mechanisms and the connectivity underpinning perception.

"The research done in my lab focuses on understanding what we can learn about brain activity patterns to try and understand which brain pathways are engaged when something unexpected happens," Marta explains.


MONASH University
Technology
Research
MONASH University
Medicine,
Nursing
and Health

Guests at the MASSIVE M3 launch view MASSIVE processed data in the Monash Univeristy CAVE2.

OPPOSITE: Dr Alan Finkel, Professor Ian Smith and Professor Christina Mitchell press the big red button to turn on the new M3 system.

"The brain is wired in an extremely complex way. To make sense of the pathways engaged in perception and action we need to use brain imaging techniques that result in vast amounts of data. We then use mathematical modelling to decipher the data — these analyses require a lot of computing power and so access to supercomputers like M1, M2 and now M3 is critical."

Professor Trevor Lithgow, a Monash researcher, is using a range of next generation microscopes to understand how bacteria develop resistance to antibiotics.

"The knowledge gained from the application of ultra-high resolution imaging techniques coupled with a data processing engine like MASSIVE not only enlightens us on how bacteria become antibiotic resistant but also guides the development of the next generation of antibiotics," Trevor says.

"As the Chief Scientist says, 'you cannot understand what you cannot see' and in order to make drugs able to control and kill bacteria we need visual knowledge of how these molecular machines work," Trevor concludes.

M3 is pioneering and building high performance computing upon Monash's specialist Research Cloud fabric. It has been supplied by Dell with a Mellanox low latency network and NVIDIA GPUs.

M3 will be available to early adopter researchers in July 2016 onward.

The M3 Computer

A Data Processing Engine

M3 is an efficient data processing engine with a huge capacity. It has a 1.15 petabyte parallel file system that has been designed for ultra fast reading and writing of data.

Built on top of the Monash Research Cloud

M3 leverages significant national investment in the Monash University node of the NeCTAR research cloud. This high performance computer is designed to sit alongside other cloud services, and is provisioned using cloud tools.

Fast Interactive Access

M3 has been designed for fast interactive access: M3 includes 48 NVIDIA Tesla K80 GPU cards. These cards will be available for interactive access—allowing researchers access to 4992 parallel cores per card for ultra-fast data processing or visualisation.

The M3 system also includes 8 NVIDIA K1 GPU cards that will be sliced up to up to 16 users concurrent users to provide a medium-end remote desktops for users who are not doing high end rendering or those who just want to quickly log in to check their results.

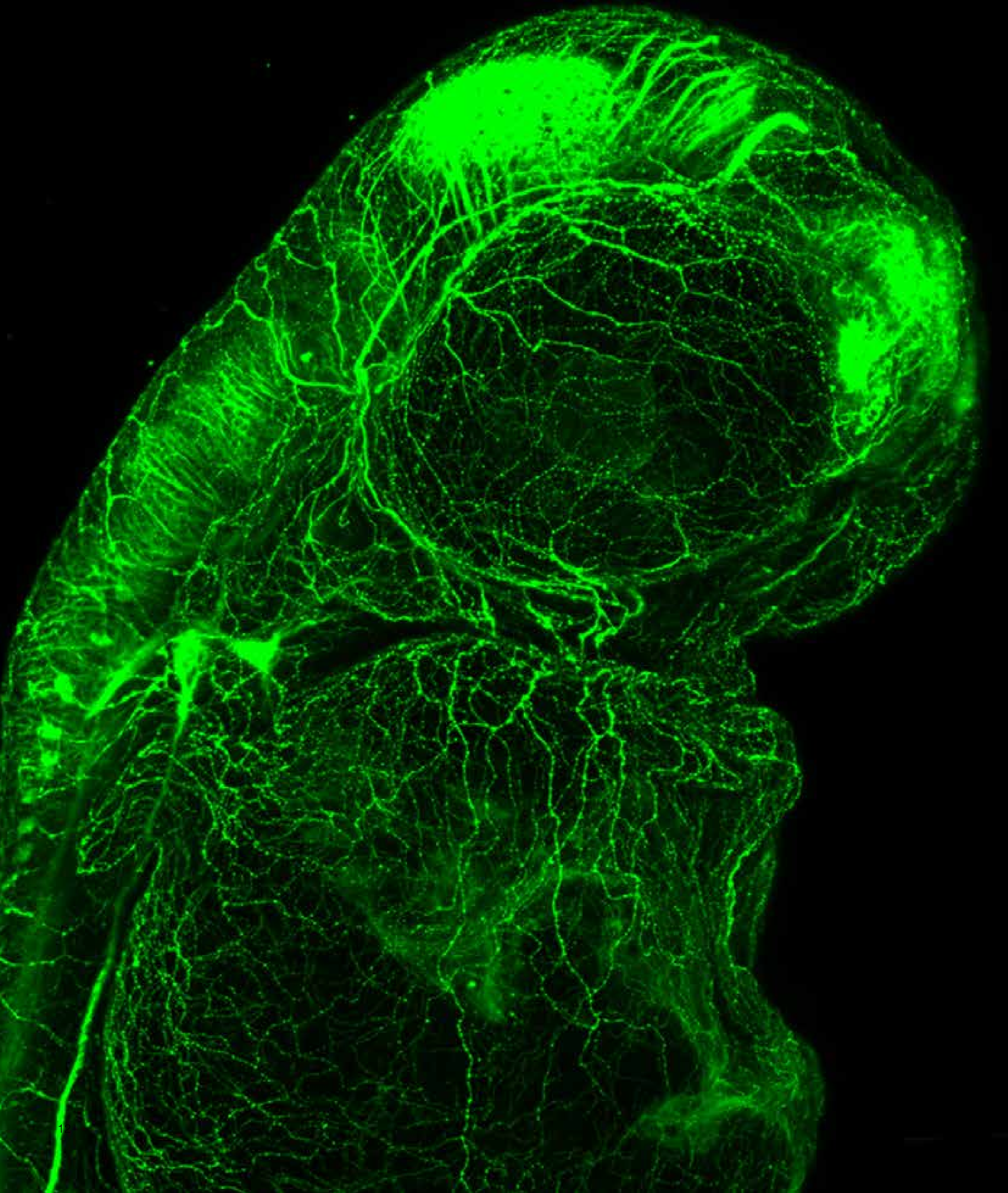
An Ecosystem of Services for Next-Generation Virtual Laboratories

Over the last 5 years, scientific computing has significantly evolved: researchers now need access to a complete landscape of services and technologies, including: data collections, databases, web portals and remote desktop access alongside high performance computing. Placing M3 as part of the Monash research cloud means MASSIVE users will have low-barrier access to this whole range of critical services.

This includes tight integration with the data storage funded by the NCRIS Research Data Storage, desktop environments developed under the NeCTAR funded Characterisation Virtual Laboratory, plus many other services.

Micrograph showing zebrafish axon tracts captured at Monash Micro Imaging. MASSIVE coordinates a program of work to integrate imaging instruments across Australia, funded through NeCTAR and the RDS.

Source: Aminah Giousoh, Department of Biochemistry and Molecular Biology, Monash University



/03

MASSIVE: Integrative High Performance Computing

MASSIVE is an integrative HPC facility that underpins a wide selection of next-generation Australian instruments and their users.

Our capabilities are applied across a range of research disciplines, including biomedical science, materials research, engineering and geosciences. The facility underpins a range of scientific instruments, including synchrotron X-ray and infrared imaging, functional and structural magnetic resonance imaging (MRI), X-ray computer tomography (CT), electron microscopy and optical microscopy.

MASSIVE is unique in a number of ways:

MASSIVE runs a dedicated program to integrate instruments with HPC, thus providing scientists with the ability to perform fast and sophisticated analysis of captured data.

Data processing and analysis is increasingly a core real-time part of scientific experiments. An integrative HPC facility supports large-scale analysis in real-time during an experiment which allows researchers to make real-time decisions about their experiment. In turn, this increases the return-on-investment — in both the experiment, and the underpinning infrastructure — by ensuring that resources are used in the most efficient way possible and that researchers are able to make faster decisions.

MASSIVE provides support and programs to on-board and support new researchers from fields of science that have not traditionally used HPC.

The uptake of advanced instrumentation by scientific communities is driving demand for computing services by fields of science that are new to the problems associated with big data. For example, the uptake of functional MRI techniques is creating significant demand for specialised MRI processing by the psychological sciences, a community that has not traditionally used high-end computing infrastructure.

HPC facilities increasingly need to support easier access – and this must extend beyond the expert command line interfaces – to build usage from amongst the wide cohort of experimental or wet-lab scientists. For example, explicit support for remote desktop and visualisation allows a range of scientists, including a large cohort of inexperienced HPC users, to access important tools and data.

MASSIVE has a focus on applied data science, including applied artificial intelligence, to address the data challenges being faced by a broad spectrum of researchers – including wet and experimental research laboratories.

The confluence of big data, deep neural networks and tightly coupled parallel computing is enabling large commercial multinational companies and innovative start-ups to apply artificial intelligence across a wide range of problems, with increasing sophistication, insight and accuracy. Applied artificial intelligence is of increasing relevance to research as it provides researchers the ability to gain insight from data that might otherwise be unfathomable.

/04

Services and Capabilities

MASSIVE's services and capabilities are delivered through the combination of computing hardware, software and expertise located at the Australian Synchrotron and Monash University.

MASSIVE also provides services to users on the cloud as the lead developer and operator of the CVL.

MASSIVE provides a number of services to the research community:

1. An HPC capability that is used across a wide selection of data processing problems. This includes processing and interactive analysis and visualisation of very large and multidimensional datasets in near real-time. Our computers are regularly updated with a library of specialised data analysis, data processing and scientific software;

2. Specialised user support, training and engagement;

3. An Instrument Integration Program to integrate scientific instruments with HPC capability. This work allows scientists to use complex and computationally demanding data processing workflows within minutes of data capture;

4. A research infrastructure development program for platforms such as the CVL, and research tools.

Hardware

The MASSIVE computers, M1, M2 and most recently M3, were designed specifically with a number of features that fulfil the core data processing and visualisation requirements.

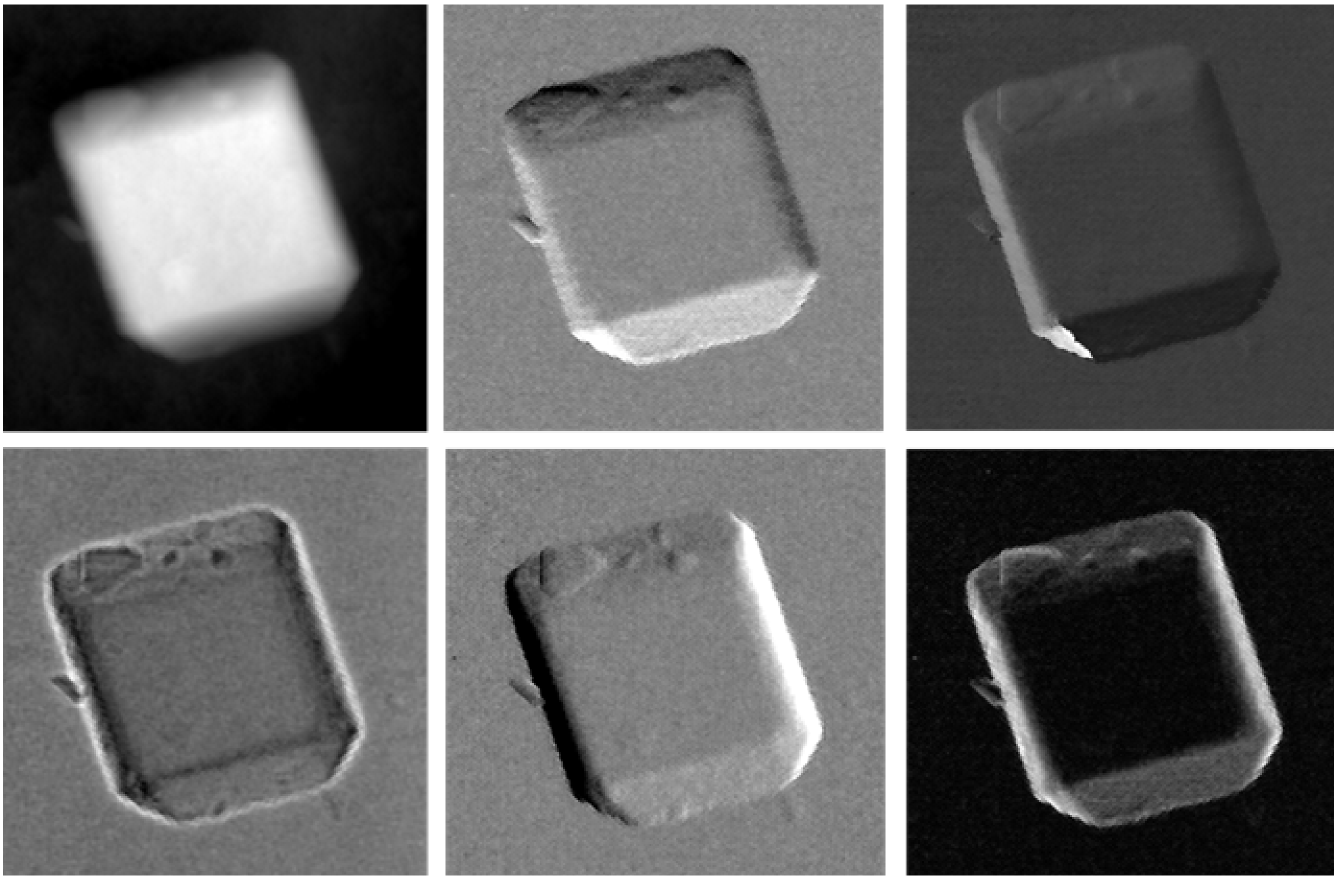
Our computers are underpinned by three high performance parallel file systems with a total of over 1.8 petabytes (PB) of storage. Fast reading and writing of data is essential to enable image processing such as that required at the Imaging and Medical Beamline (IMBL) and Ramaciotti Centre for Structural Cryo Electron Microscopy.

All three computers are equiped with NVIDIA GPUs that are used for fast rendering, remote visualisation and are being applied across a wide range of data processing and simulation problems.

General Support

In 2015 MASSIVE provided significant help and support to users, answering over 1200 help enquiries ranging from software installation requests to challenging computational problems.

OPPOSITE: A sugar crystal is imaged using single-grid phase contrast imaging, as a part of image technique development. This technique allows several imaging modes to be extracted from a single exposure, including edge-enhanced phase contrast, projected phase, differential phase, and the magnitude and direction of the phase gradient. Without the need for multiple exposures, this technique can be used to capture moving or changing samples in a high speed movie. Dr Kaye Morgan (School of Physics, Monash University), Image reconstruction performed on MASSIVE.



The MASSIVE systems have the following hardware specification:

M1 at Australian Synchrotron

42 nodes with 12 cores per node running at 2.66GHz
(504 CPU-cores total), each with:

> 2 NVIDIA M2070 GPUs with 6GB GDDR5 per node

> 58TB + 95TB of fast access parallel file system

> 4x QDR Infiniband Interconnect

M2 at Monash University

118 nodes (1720 CPU-cores total) in four configurations:

1. 32 with 12 cores per node running at 2.66GHz

> 48GB RAM per node

> 2 x NVIDIA M2070 GPUs with 6GB GDDR5 per node (64 GPUs total)

2. 10 with 12 cores per node (visualisation / high memory configuration)

> 192GB RAM per node (1,920 GB RAM total)

> 2 x NVIDIA M2070Q GPUs with 6GB GDDR5 per node (20 GPUs total)

3. 56 nodes with 16 cores per node running at 2.66GHz

> 64GB RAM per node

4. 20 nodes with 16 cores per node running at 2.66GHz

> 128GB RAM per node

> 4x QDR Infiniband Interconnect

> 500TB of fast access parallel file system

M3 stage 1: A Computer for Next-Generation Data Science

> 1,600 Intel Haswell CPU-cores

> 48 NVIDIA Tesla K80 GPU coprocessors for data processing and high end visualisation, with 2 GPU chips per card;

> 8 NVIDIA Grid K1 GPUs for medium end visualisation that will support up to 32 users concurrently;

> A 1.2 petabyte Lustre parallel file system that will be capable of reading data at 24 gigabyte a second peak (approx 4 times faster than our current M2 file system)

> A 100 Gb/s Ethernet Mellanox Spectrum network

Supplied by Dell, Mellanox and NVIDIA

CVL on the Monash University Research Cloud

31 nodes (359 cores) in five configuration, setup for desktop and compute purposes:

1. 4 nodes with 10 cores per node

> NVIDIA K1

> 37GB RAM per node

2. 4 nodes with 20 cores per node

> NVIDIA K2

> 75GB RAM per node

3. 2 nodes with 64 cores per node

> 234GB RAM per node

4. 15 nodes with 1 core per node

> 4GB RAM

5. 6 nodes with 16 cores per node

> 64GB RAM per node

Research Stories

Making Sense of Drug Resistance in Pathogenic Bacteria


Dr Matt Belousoff


Prof. Trevor Lithgow

Around the world researchers are striving to find new ways to treat infections as antibiotics lose their ability to halt the spread of pathogenic bacteria.

Over time, the so-called 'superbugs' have developed resistance to the latest and until now the best antibiotics. Clearly, new approaches are needed to understand the process of antibiotic resistance and to design better drugs and treatments.

Monash researchers are making a major contribution to the push to eliminate superbugs. Among them, Dr Matt Belousoff, working together with Professor Trevor Lithgow, spends much of his time looking very closely at the structure of bacterial ribosomes, the molecular machines that make proteins and enable the bacteria to thrive.

He wants to find out how the structure changes when infectious bacteria undergo mutation that leads to drug resistance.

Most antibiotics target a specific aspect of cellular metabolism. Penicillin for example targets the bacterial cell wall. But under constant exposure to the antibiotic, the occasional bacterial cell can mutate to survive treatment and start a new drug-resistant strain.

To try and answer the question of why antibiotics stop working, Belousoff uses advanced imaging techniques to visualise changes in ribosomes that occur in response to certain antibiotics.

He and his colleagues have their sights set on the design of new drugs that are lethal to bacteria despite structural changes to ribosomes – a 'super drugs for super bugs' scenario.

Even though Belousoff is not even sure where the MASSIVE computers are housed, he affirms that MASSIVE plays a central role in moving his research along.

As he puts it, most of his time is spent "staring at a UNIX terminal in my lab and typing commands". His main interaction with MASSIVE is at the human level.

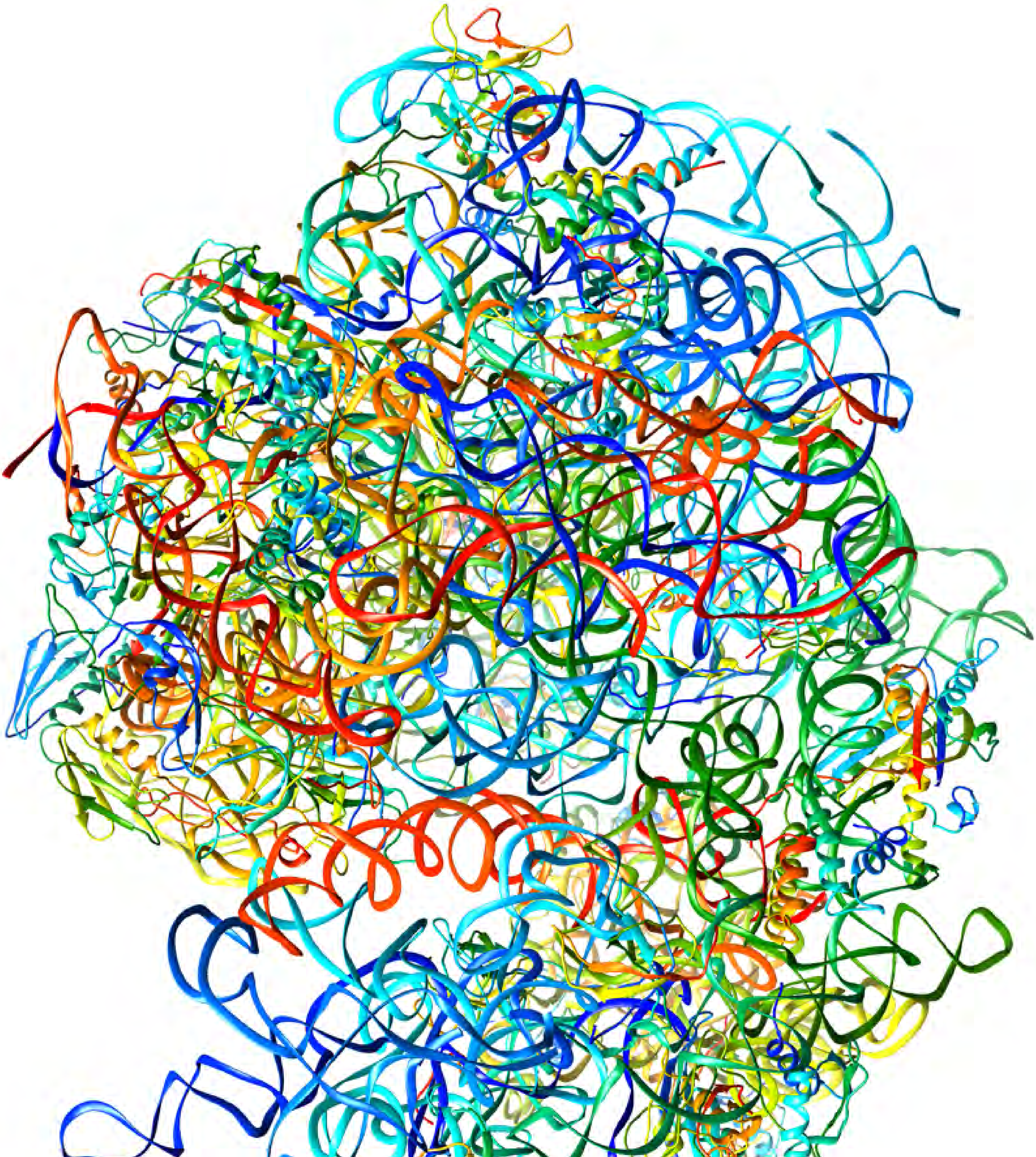
"The software engineers from MASSIVE are really helpful and knowledgeable when I need to get new software up and running," he said.

"The software we use is all open source, which is a plus. But the down side is that nothing works first shot. The published code can need quite a lot of editing before it will do just what I want."

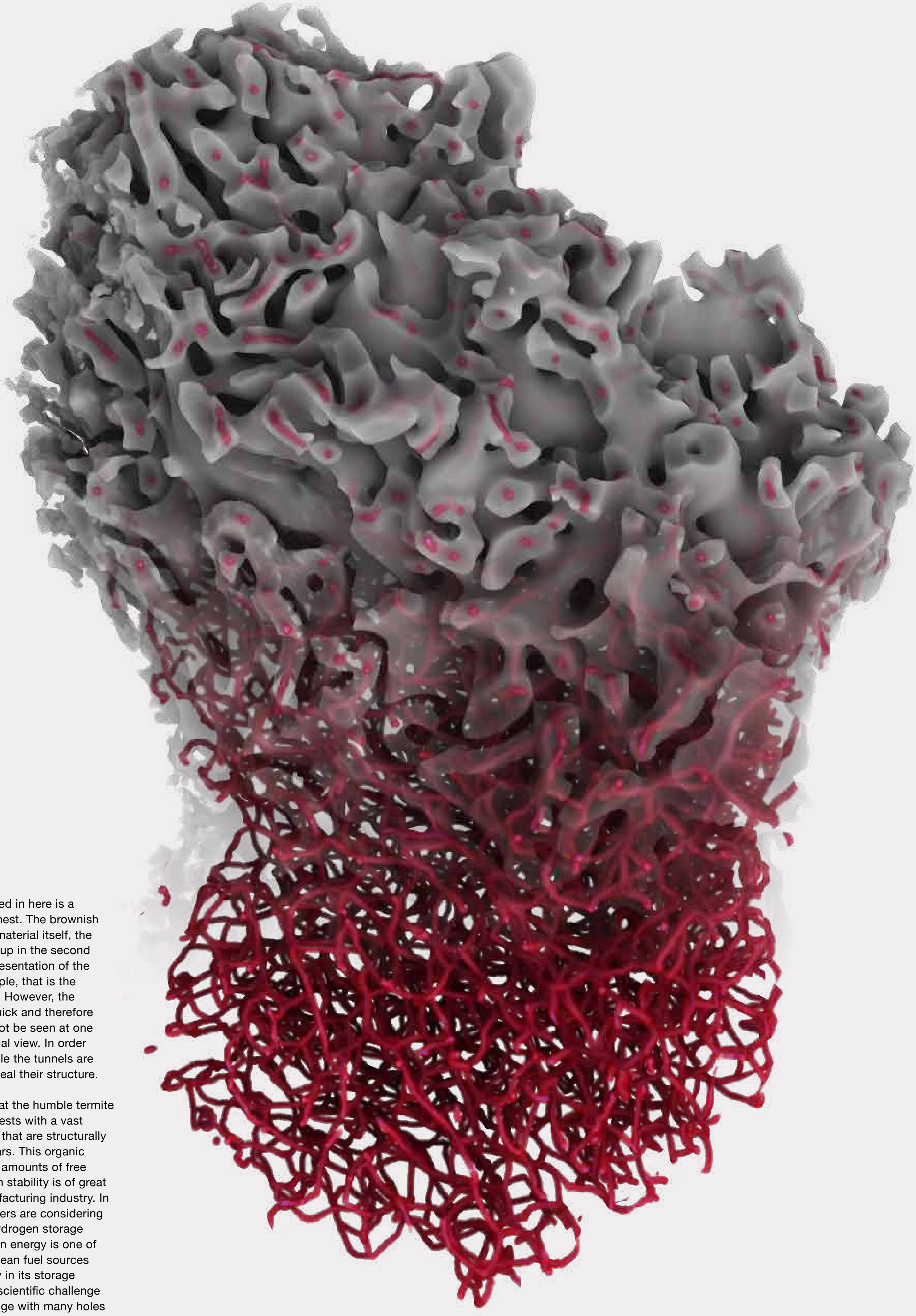
Ready access to MASSIVE's computer cluster is also critical. Matt takes high resolution images (about 500,000 at the movie-frame rate) of pure preparations of ribosomes isolated from hospital-acquired antibiotic-resistant *Staphylococcus aureus*.

His images take a huge amount of storage and processing, which, without MASSIVE, would be prohibitively expensive. And supercomputing through MASSIVE makes sense of all the images by transforming a 3-D electron density map into a meaningful molecular model that he can work with.

"The knowledge gained about the effects of mutations that lead to drug-resistance on the ribosome binding site will help us to re-engineer the binding site in the future. It's an exciting idea from the perspective of drug-development, and could lead to one drug for the treatment of all antibiotic-resistant strains," Belousoff said.



One of Dr Matt Belousoff and Professor Trevor Lithgow ribosome structures illustrating the complicated details that can be determined using the Titan Krios at the Ramaciotti Centre for Cryo Electron Microscopy and MASSIVE



The object visualised in here is a piece of a termite nest. The brownish component is the material itself, the grey filling coming up in the second episode is the representation of the cavities in the sample, that is the tunnels in the nest. However, the tunnels are quite thick and therefore their network cannot be seen at one glance in the original view. In order to make them visible the tunnels are skeletonised to reveal their structure.

It is no accident that the humble termite can build porous nests with a vast network of tunnels that are structurally stable up to 50 years. This organic structure with vast amounts of free space coupled with stability is of great value for the manufacturing industry. In this case, researchers are considering how to redesign hydrogen storage materials. Hydrogen energy is one of the world's most clean fuel sources but lacks efficiency in its storage performance. The scientific challenge is to design a sponge with many holes that absorb and store enough hydrogen while remaining stable under industrial conditions.

Source: Aaron Thornton, CSIRO, Anton Maksimenko, Australian Synchrotron

/05

National Cloud and Data Projects

The Characterisation Virtual Laboratory

The Characterisation Virtual Laboratory (CVL) is a NeCTAR-funded project to develop online environments for researchers using advanced imaging techniques, and demonstrate the impact of connecting national instruments with computing and data storage infrastructure.

Under MASSIVE's leadership, with NeCTAR funding, and with the exceptional support of project partners, the CVL user base grew to 590 unique researchers. Plus we continued new deployments at new sites. Some key highlights include:

> Researchers combined have run over 23,000 desktop sessions on CVL on the NeCTAR cloud, M1 and M2 systems on MASSIVE.

> CVL has underpinned workflow deployment at two Australian Synchrotron beamlines for access to the MASSIVE Desktop. Researchers visiting both the Imaging and Medical Beamline (IMBL) and the X-ray Fluorescence Microscopy (XFM) beamline are automatically created a beamline visit project, and user accounts. Authentication is integrated with Australian Synchrotron so that users can use their AS credentials to log into the system. A set of beamline change over scripts, developed in collaboration with Australian Synchrotron, control the flow of data.

The impact of this work is significant. Researchers are provided with access to a remote desktop environment for the duration of their beamline visit that provides access to the data captured, and tools for data processing and visualisation. The same desktop environment can be used after their visit for ongoing processing. **As of 1st March, 247 projects, and 246 Australian Synchrotron users have been allocated time on the MASSIVE Desktop using this mechanism. Combined these users have notched up over 1000 desktops sessions.**

> MASSIVE is working with the Terrestrial Ecosystem Research Network (TERN) at the University of Queensland to deploy a new CVL-like service for the use of TERN researchers.

> The CVL project has developed a set of Ansible scripts that orchestrate the launch of a desktop cloud service, including: VM instances running VNC servers; identity sources (username/password and group membership), persistent storage accessible to all Instances (i.e. a networked file system), automatic mounting file systems, scheduling to allocate instances between CVL users, and login node(s) to request access to an instance. These scripts have significantly increased our ability to deploy new instances of the CVL.

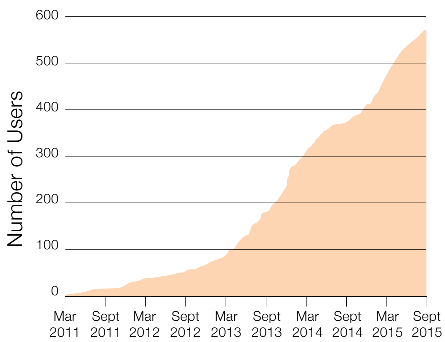
> The CVL is now more easily accessible through Strudel Web, a web based desktop access portal that is now deployed across 2 sites (TERN and MASSIVE) and being used to access resources from MASSIVE, CVL, MonARCH, and TERN.

> Additionally, CVL software is now being adopted by two major international supercomputing centres:

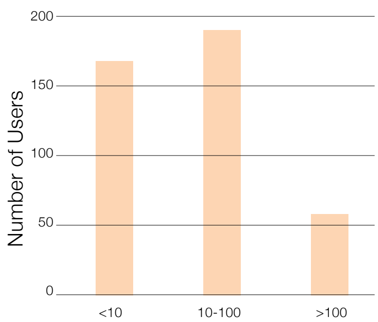
> Julich Supercomputing Centre, is in the process of deploying Strudel to support visualisation users and high-end commercial engineering applications;

> Edinburgh Parallel Computing Centre for industry access to HPC systems under the EU FP7 project, Fortissimo.

CVL Usage



Growth of users



Total sessions launched per user illustrating that researchers continue to use the CVL after their first trial

Strudel Making Visualisation of Data More Accessible

MASSIVE's Strudel tool is gaining traction in national research institutions and making a difference to how research involving high-powered computing and visualisation is undertaken.

Strudel, originally called the ScienTific DEsktop Launcher, makes it easy for scientists to click through a few dialog boxes and gain access on their office computer to a remote desktop running in a high-powered computing environment or cloud.

Dr Will Ryder, NIF Facility Fellow at the University of Sydney/ANSTO node of the National Imaging Facility located at the Brain and Mind Centre, has been involved in a pilot of Strudel for University of Sydney medical imaging researchers.

Medical imaging modalities, such as MRI, PET and CT, generate huge amounts of data. Computer-based visualisation of such data involves high-powered computing, which is very technical and often beyond the expertise of newcomer researchers, including graduate students.

But Strudel is already making visualisation of data more accessible to such 'inexpert' users. MASSIVE assisted the Brain and Mind Centre to set up a test cluster at the University of Sydney that has enabled students to collaborate across the campus. For example, thanks to the capability provided by Strudel an Honours student was remotely trained in the use of software for visualisation of CT scans acquired at the Sydney Node of the Australian Microscopy & Microanalysis Research Facility.

"It would have been virtually impossible to share software in this way without this software, let alone to do it efficiently," says Ryder.

"Strudel opens the door to students and researchers who are less technical in the area of high-powered computing to allow access to state-of-the-art tools for image processing," he said.

The roll-out of Strudel is making similar changes to the accessibility of visualisation technology at the Pawsey Supercomputing Centre in Western Australia. Jonathan Knispel, a member of Pawsey's visualisation team, has been working with MASSIVE to make it easier for researchers to access remote visualisation.

Like Ryder, he works in large data sets that have to be processed into 3-D images to allow researchers to interact with and make sense of them.

Researchers familiar with command-line access to Pawsey's supercomputing facilities are already using Strudel for a more convenient start to their remote visualisation sessions.

Pawsey's team also supports non-supercomputing researchers from a diverse range of disciplines, including humanities, the life sciences and business. Those users typically bring their data to a Pawsey partner facility where they can use powerful, 3D workstations to visualise them.

"Strudel's new ability to reserve remote sessions in advance will help researchers with no supercomputing experience to access visualisation facilities from the convenience of their own office," Knispel says.

MASSIVE and Pawsey have worked together to extend STRUDEL to support the way Pawsey allocates and manages visualisation sessions. The new capability allows scientists to book visualisation computing nodes so that they can use the capabilities at a pre-arranged, convenient time.

Strudel was developed by the MASSIVE team as part of the NeCTAR Characterisation Virtual Laboratory to access remote scientific desktops. It is now being extended to foster re-use at other HPC and cloud facilities.

Characterisation Virtual Laboratory Partners and Collaborators

Monash University

Australian Synchrotron

Australian Microscopy and Micro Analysis Facility

National Imaging Facility

ANSTO

Centre for Advanced Imaging, University of Queensland

Queensland Brain Institute, University of Queensland

Research Computing Centre, University of Queensland

Brain and Mind Research Institute, University of Sydney

University of Melbourne

Central Queensland University

RMIT University

Deakin University

School of Physics, Australian National University

Intersect

QCIF

National Computational Infrastructure

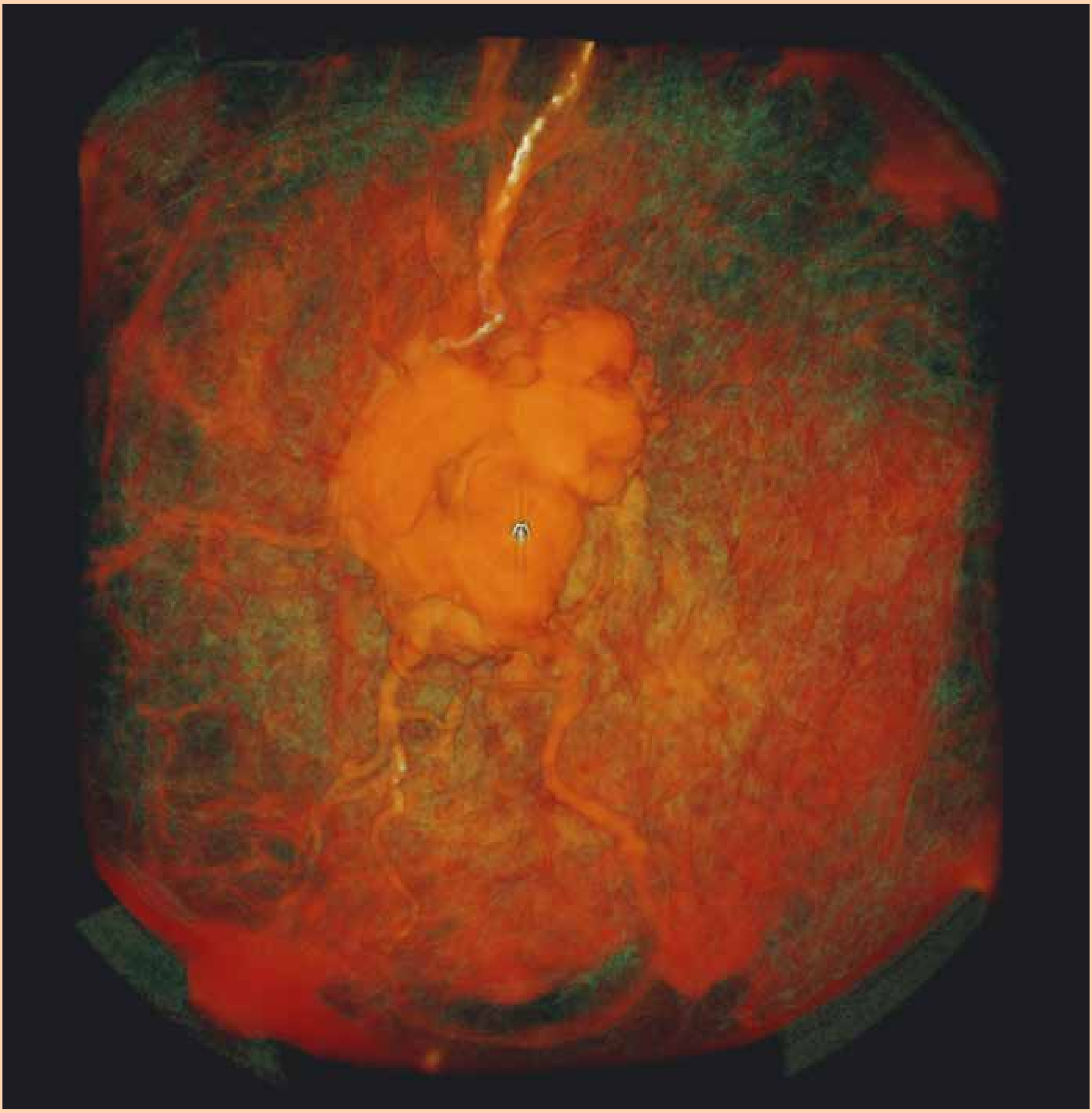
VicNode University of Melbourne, Monash University

The Pawsey Centre

University of Western Australia

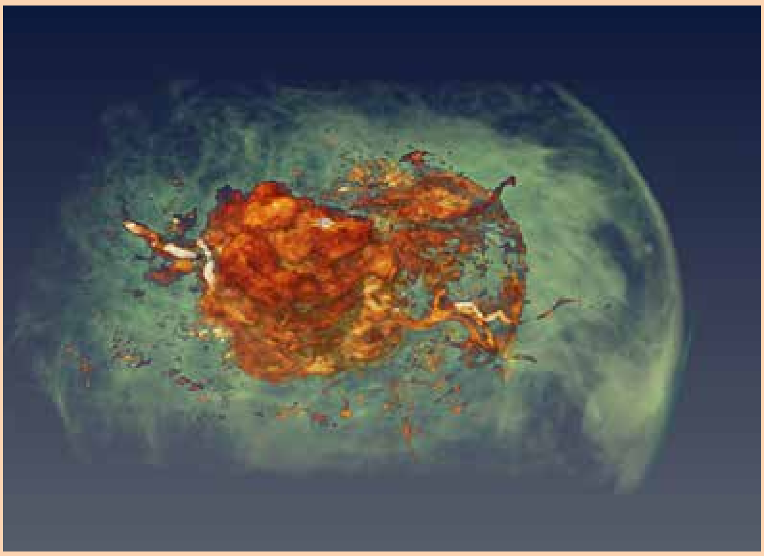
CSIRO

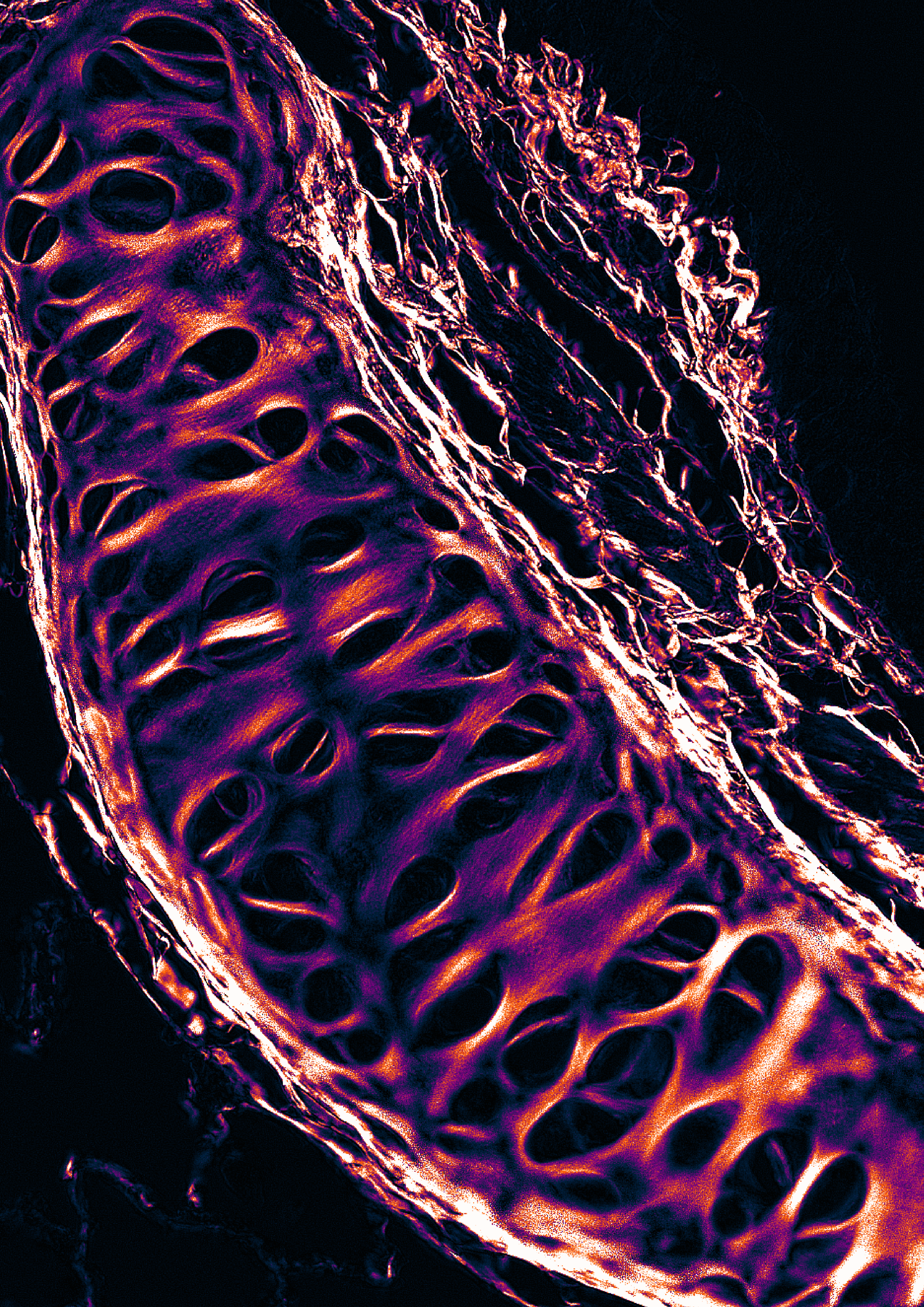
Funding: NeCTAR and partners



ABOVE and RIGHT: Dr Sherry Mayo and Darren Thompson and colleagues are helping develop techniques for breast tumour imaging a project that is partially funded by the National Breast Cancer Foundation. The aim is to develop improved diagnostic methods using phase-contrast imaging and tomography. The project is a collaboration between CSIRO, Monash, University of Melbourne University and Univeristy of Sydney and includes imaging scientists, radiologists and clinicians.

Timur Gureyev (The University of Melbourne), Yakov Nesterets, Sheridan Mayo, Frank de Hoog, Darren Thompson (CSIRO) Giuliana Tromba, Serena Pacile, Fulvia Arfelli, Francesco Brun, Diego Dreossi, Sara Mohammadi (Elettra Synchrotron, Trieste) Chris Hall, Andrew Stevenson (Australian Synchrotron) Patrick Brennan (Sydney University) Christian Dullin (University Hospital Goettingen) Matthew Dimmock, David Paganin, Jeremy Brown, Marcus Kitchen (Monash University) Konstantin Pavlov (University of New England) Benedicta Arhatari (La Trobe University) Zdenka Prodanovic, Beena Kumar, Manish Jain, Jane Fox (Monash Health) Darren Lockie (Maroondah BreastScreen) Maura Tonutti, Fabrizio Zanconati (Trieste Hospital) Patrycja Baran (University of Rzeszow) Carolyn Nickson (The University of Melbourne)





Instrument Integration Across Australia

Under the Research Data Services (RDS) Image Publication initiative, three partners — VicNode, QCIF and Intersect — have integrated over 60 instruments with cloud-based data management software to ensure that all data generated by these instruments is automatically captured, managed and delivered to the cloud for processing, analysis and visualisation. The figure below charts the number of instruments that are integrated under this coordinated program and the various organisations involved.

RDS Image Publication leverages investment in community-developed data management tools, including MyTardis, DaRIS, OMERO and XNAT, to capture data, help researchers manage the research data lifecycle and to move data to centrally-hosted analysis environments. These tools are now deployed across a large range of instruments and institutions and are used by hundreds of researchers, including those at University of Queensland, University of Sydney, University of Melbourne, Monash University, ANSTO, and Australian Synchrotron.

This initiative impacts a large and broad range of Australian researchers by helping researchers move data automatically to the cloud and to MASSIVE.

RDS Image Publication extends a major effort under the CVL to prototype integration in specific fields: neuroimaging, structural biology and atom probe microscopy. Key to this effort and the outcomes in Image Publication has been the development of the MyData app that makes instrument integration and data capture at the instrument simpler, therefore allowing instrument facility managers to integrate instruments themselves and make the process less reliant on specialist IT or eResearch support. MyData allows instrument integration to scale: a large cohort of instruments can be supported centrally across a modest number of data storage nodes, and with minimal local technical support.

Instruments Integrated Under this Initiative Include:

> Advanced light microscopy, including widefield, confocal, multi-photon and super resolution microscopes,

> A range of electron microscopes including scanning electron and transmission electron microscopes,

> Magnetic resonance imaging (MRI) and Positron Emission Tomography (PET) instruments,

> Cell sorters and analyzers, and

> Atom probe microscope.

In addition, this project underpins existing efforts at Australian Synchrotron MX1 and MX2, plus beamlines at ANSTO.

MyData for Instrument Facilities

With CVL NeCTAR funding, Monash University is developing an instrument integration app, called MyData to make integration quicker, simpler and less reliant on specialist IT support. As a result of this project MyData is now used at 35 instruments, across 10 facilities, at 4 institutions, in addition 17 further instruments are planned at 4 institutions.

MyData provides instrument facilities a self service mechanism to integrate their instruments with the MyTardis data management platform (and other platforms in the future). Facility administrators can download the application and easily install and configure it themselves on an instrument PC. It is being used for several types of instruments including advanced light microscopy, fluorescence and confocal microscopy, multiphoton microscopy, cryoelectron microscopy, scanning electron microscopy, transmission electron microscopy, and flow cytometry cell sorters and analysers.

MyData monitors a watched folder for new instrument data and automatically ingests data from this folder into MyTardis and assigns the data to the appropriate owner. It supports http uploads as well as SCP; with optimised performance for a range of use cases like large image files (more than 60GB per file), large datasets (datasets containing more than 12,000 small files) and typical imaging datasets that have file sizes ranging from several kilobytes to tens of gigabytes. The integrity of these files is also verified using checksums.

In addition, this project has made MyTardis easier to use for Facility Managers. The Facility Overview feature in MyTardis allows a facility admin to log into MyTardis to answer questions like:

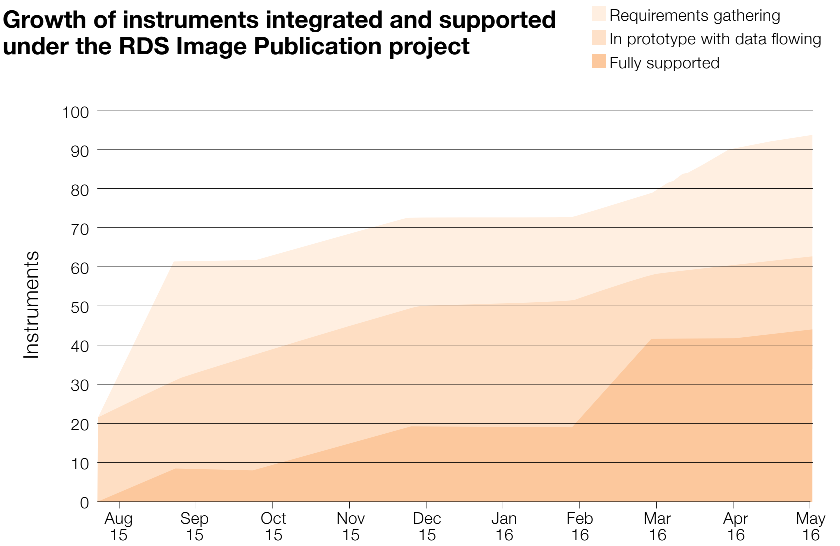
> Is data flowing from my microscope?

> Who owns this orphaned dataset?

> Has all the data been ingested? Can I clear the hard drive?

> How are my instruments pushing data?

Growth of instruments integrated and supported under the RDS Image Publication project



OPPOSITE: Jade Barbuto, Hudson Institute of Medical Research Description: Polarised light microscopy image from a section of a cartilage plate in lung tissue captured at Monash Micro Imaging on microscopes integrated through MASSIVE.

Prof Andreas Fouras

Industry Initiatives

4Dx: Four-dimensional Diagnostics

MASSIVE is helping to underpin 4Dx, an enterprising new international company that aims to revolutionise healthcare by providing doctors with detailed images of the functioning human lung.

Professor Andreas Fouras recently moved to Los Angeles to grow the medical start-up he founded based on technology he developed at Monash University over the past 10 years.

The company, called '4Dx' for 'four-dimensional diagnostics', is developing and commercialising patented inventions designed to scan and envisage lungs to a level of detail not previously possible.

Development of the software and the ongoing research associated with supplying 4Dx's product is highly computer intensive.

MASSIVE has played a key role in the successful research and development behind 4Dx and the transition of its technology to hospitals and the patients.

"MASSIVE offers more than just a significant piece of equipment. The great team at MASSIVE has always been responsive and helpful, particularly in ensuring the availability, and accessibility of any new software that we need.

"MASSIVE provided the critical link between high-powered computing and storage and processing of lots of data. We needed that link to progress." Professor Fouras said.

Andreas was researching aeronautics when he had the idea of mixing wind tunnel technology with X-ray imaging to create something that measures how the air flows in a person's lungs rather than how air flows around an aeroplane.

The potential scale of Andreas's operation to improve human health is impressive. In Australia alone, there are about 1 million lung scans performed annually to diagnose asthma, cystic fibrosis and other diseases of the lung and airways.

The number jumps to more than 70 million in the United States – a good starting point for taking 4Dx technology to hospitals around the world.

Traditional technology for the diagnosis of lung disease relies on a picture from a CT scan or X-ray, and a separate function test of how much air is exhaled from the lungs. 4Dx technology combines results of the two tests to create a picture of how the air moves through the lungs over time.

Instead of the doctor having to piece together two independent sets of information, 4Dx provides a single output of the best possible information on which to base a clinical decision.

"A major part of our product pipeline involves software that can effectively tap into a video of a lung X-ray taken using a fluoroscope and do its magic to give a picture of air flow in the moving tissue," Fouras said.

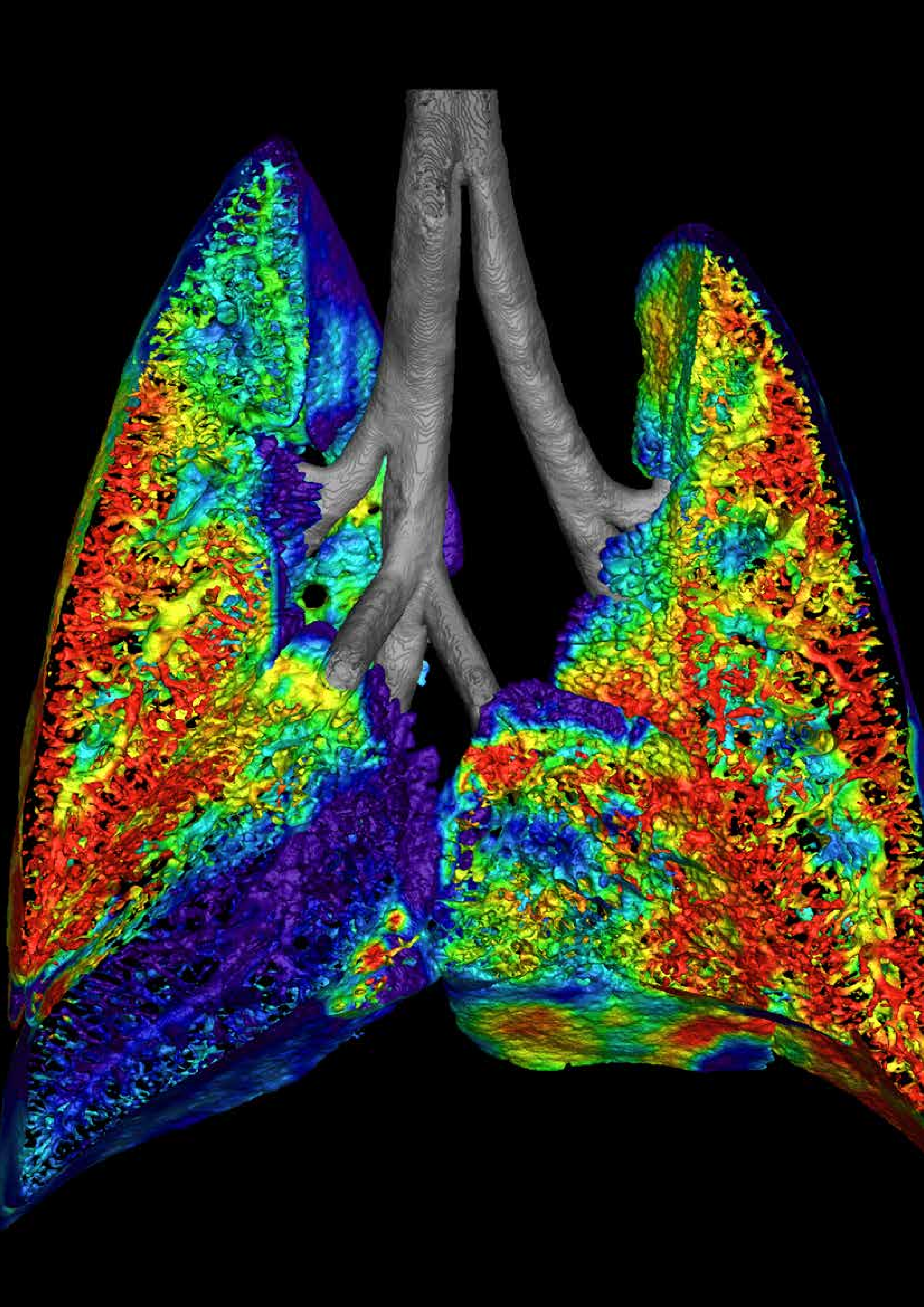
Fluoroscopes are common hospital equipment and provide low-cost, safely acquired images through the use of low-dose radiation. 4Dx software extracts from the images the maximum useful diagnostic information about how a patient is faring.

To fit the business model of a 'cloud-based software-as-a-service' company, 4Dx will continue to need access to the latest and best computing technology to develop its products, for which MASSIVE will continue to play its crucial role.

As Adjunct Professor of Mechanical & Aerospace Engineering and head of the Laboratory of Dynamic Imaging, Andreas maintains his close links with Monash University.

4Dx is a commercial user of MASSIVE

RIGHT: Lung coloured by expansion including transparent airways. Regions of diseased lung tissue in a mouse model exhibiting lung disease similar to cystic fibrosis (CF) was visualised here using phase contrast X-ray imaging in conjunction with 4-dimensional computed tomography.



Industry Initiatives

NVIDIA-Monash Collaboration

After years of successful collaboration with NVIDIA, the relationship has been formalised with Monash University becoming the first spoke of the NVIDIA Technology Centre Asia Pacific—whose hub is in Singapore.

OPPOSITE: Steve Oberlin, NVIDIA, Chief Technology Officer of Accelerated Computing and Prof Ian Smith, Vice Provost (Research and Research Infrastructure) sign the Monash-NVIDIA Collaboration Agreement

The NVIDIA Southeast Asia Technology Centre is based at Singapore's Nanyang Technological University and has a core focus on deep learning research and development.

"Collaboration with multinationals is a step towards the Australian Government's current agenda on the commercialisation of publicly funded research and provides broad benefits to the community at large," Professor Ian Smith said.

Australia's Chief Scientist Dr Alan Finkel AO recently said that innovation is a continuum starting with research and invention, which continues through to translation for economic and societal benefits. He also acknowledged that it is not up to government and chief scientists to make it happen, saying all they can do is advise and encourage.

"Collaboration is essential if Australia is to transition to a knowledge economy," Dr Finkel said.

"Universities and industry with the determination to connect and encourage the development of science is where the real work will be done."

A brilliant imagination and a brilliant piece of code lay behind most new computationally driven developments in science and technology. Monash University researchers have for years developed code to leverage ultra fast processing using the NVIDIA GPU accelerated computing platform, some of which will transform how robots see the world while others help us to understand, for example, protein function.

"To 'teach' robots how to see and understand our world we need to write algorithms that can process huge numbers of parameters at the same time. By parameters we mean that the robots need to understand structure, so they can 'see' the world in three dimensions, but they also need to 'know' what it is they are seeing and where they are in relation to these things," said Professor Tom Drummond, Chief Investigator at the ARC Centre of Excellence for Robotic Vision.

Associate Professor Hans Elmlund, Chief Investigator in the ARC Centre of Excellence in Advanced Molecular Imaging, processes data from Australia's most powerful electron microscope for biological applications.

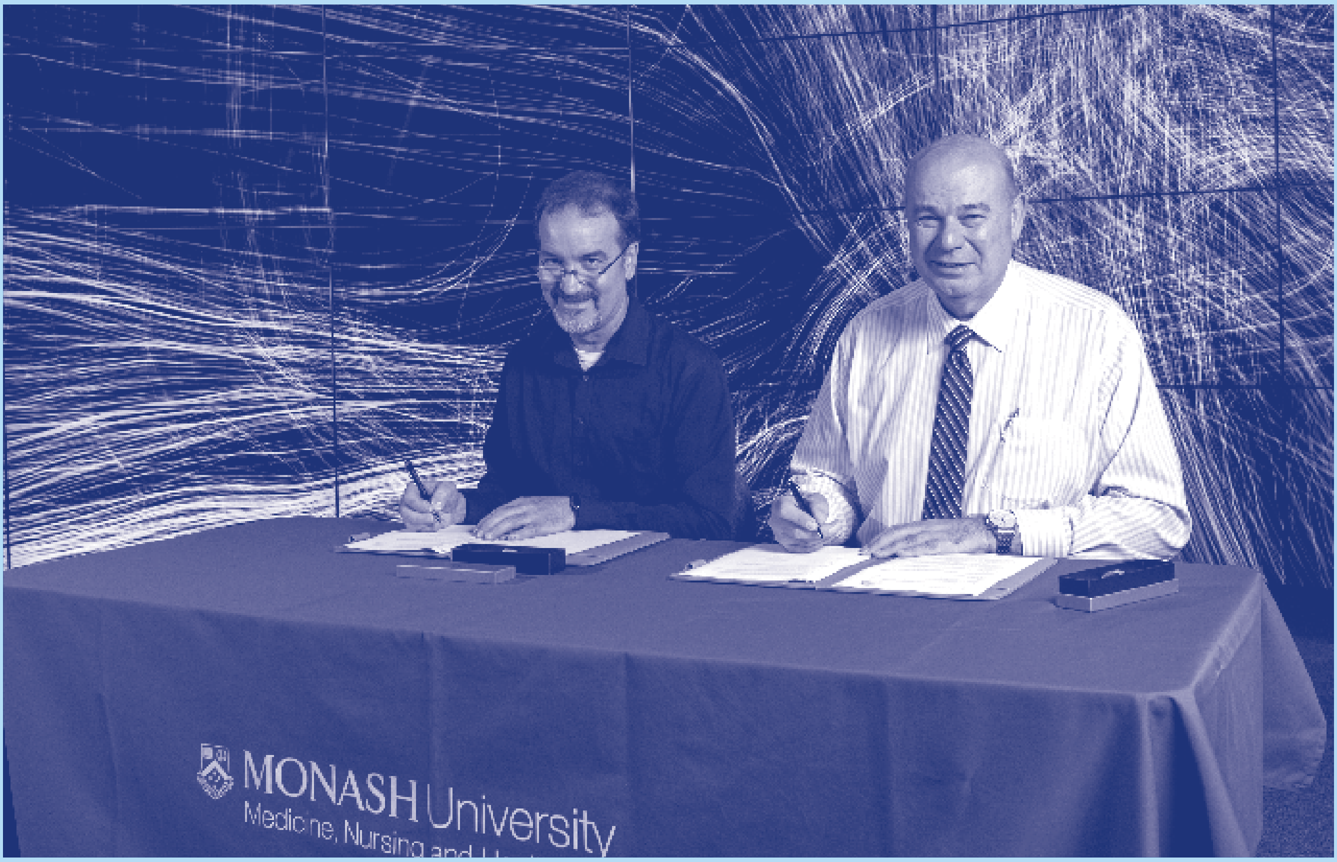
"We develop code to understand the 3D structure and function of proteins. Using NVIDIA technology accelerates our code and we are moving closer and closer to the goal of real time image processing," Professor Elmlund said.

"Running our algorithms on new generation microchips allow us to solve structures faster and with more precision. This gives medical researchers increased knowledge of fundamental biological phenomena and action. These insights are extremely useful in driving new drug development programs."

Steve Oberlin, Chief Technology Officer of NVIDIA's Accelerated Computing, says that the collaboration of this type is the only one in the world outside the Technology Centre Asia Pacific.

"We view this collaboration as an ideal opportunity to make big impacts," Mr Oberlin said.

"By continuing to leverage GPU processing we hope to revolutionise the world by providing scientists with tools to develop insightful algorithms that will be used in fields as disparate as robotics and medicine. Imaging the dynamics of complex proteins supports the development of personalised medicines and enhancing computing power will allow robots to understand and navigate our four dimensional world."


MONASH University

/06

Training and Outreach

MASSIVE staff organised or presented at over 20 events in 2015. This includes National Young Leaders Day which is an annual event created in 1997 by the Halogen Foundation to develop strong leadership values amongst young Australians. February this year Dr Paul McIntosh, Technical Lead for the MASSIVE project, was invited to take part in a panel discussion for 4,500 upper primary students at the Melbourne Convention Centre. Paul, along with Dr Alan Duffy (Astronomer, Swinburne), Anita Lougrah (Co-Owner, Cat Café Melbourne) and Elliot Costello (Co-Founder & CEO, YGAP) pitched why their jobs were the coolest in the world and then discussed life lessons to inspire young leaders. Paul compared his job to hunting for Bluestone in the computer game Minecraft but way cooler because, MASSIVE was hundreds of times more powerful than any game console, and that he got “to help scientists hunt for things that are so rare that we don’t even know what they look like”.

Training Events

Title		Location	Date/s
Slurm Workshop	MASSIVE team	Meeting Room, Monash Biomedical Imaging (MBI), 770 Blackburn Road, Monash University, Clayton Campus VIC	23/01/15
Introduction to Linux	Monash eResearch Centre	G15, 23 College Walk, Monash University, Clayton Campus VIC	09/04/15
NCI Training at Monash	National Computational Infrastructure (NCI)	G15, 23 College Walk, Monash University, Clayton Campus VIC	10/04/15
GeoPIXE at X-ray Fluorescence Microscopy Beamline Workshop	Australian Synchrotron & CSIRO, with support from MASSIVE team	Conference Rooms 1, 2 & 3, Australian Synchrotron, 800 Blackburn Rd, Clayton VIC	25/08/15 — 26/08/15

Outreach Events

Launch of The Clive and Vera Ramaciotti Centre for Structural Cryo-Electron Microscopy	MASSIVE team	Foyer, 15 Innovation Walk, Monash University, Clayton Campus VIC	02/02/15
Australian Microscopy & Microanalysis Research Facility (AMMRF) Informatics Workshop	MASSIVE team (Presentation)	The Rydges, Southbank, Brisbane, QLD	24/03/15
Human Brain Project —ARC Centre of Excellence for Integrative Brain Function Collaboration Workshop	MASSIVE team (Presentation)	Monash University, Prato Centre, Prato, Italy	28/05/15
VicNode Workshop	MASSIVE team (Presentation)	Monash University City Offices, Melbourne, VIC	10/07/15
ARC Centre of Excellence for Integrative Brain Function Science Meeting	MASSIVE team (Presentation)	Pullman Cairns International, 17 Abbott St, Cairns QLD	19/08/15

National Young Leaders Day

Title		Location	Date/s
Neuroinformatics 2015	MASSIVE team (Presentation)	Pullman Cairns International, 17 Abbott St, Cairns QLD	20/08/15 — 22/08/15
GPU Technology Conference Asia South 2015	MASSIVE team (Presentation)	Suntec Singapore Convention & Exhibition Centre, Singapore	27/08/15
European Molecular Biology Laboratory Australia—Monash University Workshop	MASSIVE team (Presentation)	European Molecular Biology Laboratory, Heidelberg, Germany	01/09/15 — 02/09/15
International Conference on Accelerator & Large Experimental Physics Control Systems (ICALEPCS) 2015	MASSIVE team, partners and collaborators (Paper and presentation)	Melbourne Convention& Exhibition Centre, Melbourne VIC	19/10/15 — 23/10/15
eResearch Australasia 2015	MASSIVE team (Presentation)	Brisbane Convention & Exhibition Centre, Merivale Street, South Brisbane, Brisbane QLD	20/10/15 — 22/10/15
European Grid Infrastructure (EGI) Community Forum 2015	MASSIVE team (Presentation)	Villa Romanazzi, Carducci, Bari, Italy	10/11/15 — 13/11/15
9th Asia Oceania Forum for Synchrotron Radiation Research (AOFSRR 2015), in conjunction with User Meeting 2015	Sponsored, including booth demonstration by MASSIVE team	National Centre for Synchrotron Science, Australian Synchrotron, 800 Blackburn Rd, Clayton VIC	25/11/15 — 27/11/15
OzViz 2015	MASSIVE team (Presentation)	UTS Data Arena, Room 405, Building 11, University of Technology Sydney, City Campus NSW	01/12/15 — 02/12/15

/07

Usage and Users

Dr Sherry Mayo, CSIRO, addresses attendees at the Imaging and Medical Beamline Workshop

Since its inception, MASSIVE has steadily grown the number of institutional users from 11 in 2011 to over 100 in 2015.

The organisations involved cover research institutes, hospitals, universities, private industry and government departments across Australia and internationally.

In 2015, this equated to supporting over 498 active projects and more than 1,300 individual user accounts – a sharp increase that reflects the increased number of projects being automatically generated at the IMBL and XFM beamlines at Australian Synchrotron, and data processing at the Ramaciotti Centre for Cryo Electron Microscopy.

Facility Access

Access to MASSIVE is open and free of charge to all users who secure an allocation of system units (SU) through a partner or investor Merit Allocation Scheme (MAS). Priority access to the system is given to researchers in the MASSIVE area of specialisation based on:

1. Their use of imaging and visualisation, or their use of, or alignment to, characterisation capabilities.

2. Their intended use of the unique MASSIVE capabilities — including GPUs and the MASSIVE Desktop.

MASSIVE Usage Data for 2015 (in system units)

			Projects	Jan-Jun 2015	Jul-Dec 2015	Total 2015
Total Available				**9,741,120**	**9,741,120**	**19,482,240**
Dynamically Scheduled	Monash		87	611,124	816,118	1,427,242
	NCMAS		18	417,362	296,617	713,979
	Synchroton-ANSTO					
		Direct	28	810,802	867,081	1,677,883
		Beamline Allocations	292	402	94,387	94,789
	CSIRO		11	22,924	33,587	56,511
	Discretionary		23	710,244	260,856	971,100
	ARC CoE for Integrative Brain Function		13	93,327	497,484	590,811
	ARC CoE for Advanced Molecular Imaging		10	1,044	819,480	820,524
	Total		**498**	**2,667,229**	**3,685,610**	**6,352,839**
On-Demand Processing and Visualisation	Instruments					
		CT processing at IMBL beamline	10 nodes	518,400	518,400	1,036,800
		GeoPIXE processing at XFM beamline	2 nodes	103,680	103,680	207,360
		AutoRickshaw at MX beamline	1 node	51,840	-	51,840
		Ramaciotti CryoEM	13 nodes	898,560	898,560	1,797,120
	MASSIVE Interactive Desktop		20 nodes	1,382,400	1,382,400	2,764,800
	System Testing and Maintenance		~2 nodes	103,680	103,680	207,360
Total Used				**5,725,789**	**6,692,330**	**12,418,119**
Unused				4,015,331	3,048,790	7,064,121
Percentage Unused				41.22%	31.30%	36.26%

MASSIVE supports a large proportion of near realtime use (interactive desktop and instrument processing) and therefore aims for usage of approximately 60-80% of CPU time available – allowing space on the system for near realtime projects to access CPU time when needed.

Assoc. Prof Hans Elmlund

Research Stories

Caught on Camera: The First Glimpse of Powerful Nanoparticles

Researchers have developed a new method to capture the 3D structures of nanocrystals. Scientists believe these tiny particles could be used to fight cancer, collect renewable energy and mitigate pollution.

Metallic nanoparticles are some of the smallest particles. Their dimensions are measured in nanometres, with each nanometre being one millionth of a milimetre. Until now, it has been difficult to know how they work, because they are so small their structure is impossible to see.

The novel imaging method, developed by an international team from the US, Korea and Australia will allow researchers to investigate the 3D structure of these miniscule particles for the first time.

The research, published in Science in July 2015, was co-led by Associate Professor Hans Elmlund from the ARC Centre of Excellence in Advanced Molecular Imaging based at Monash University. The work, performed in collaboration with researchers from Princeton, Boston and Harvard Universities, reveals the details of the method and shows how it can be used to characterise the 3D structures of these miniscule particles for the first time.

The method is called “3D Structure Identification of Nanoparticles by Graphene Liquid Cell EM (SINGLE)” and it exceeds previous techniques by combining three recently developed components.

The first is a graphene liquid cell, a bag one molecule thick that can hold liquid inside it while being exposed to the ultra high vacuum of the electron microscope column. The second is a direct electron detector, which is even more sensitive than traditional camera film and can be used to capture movies of the nanoparticles as they spin around in solution. Finally, a 3D modeling approach known as PRIME allows use of the movies to create three-dimensional computer models of individual nanoparticles.

Movie clips that accompany the publication capture the structure of two platinum nanoparticles, which have never been seen in such detail before. Elmlund and his colleagues were able to draw new conclusions about how these highly useful particles grow at the level of individual atoms.

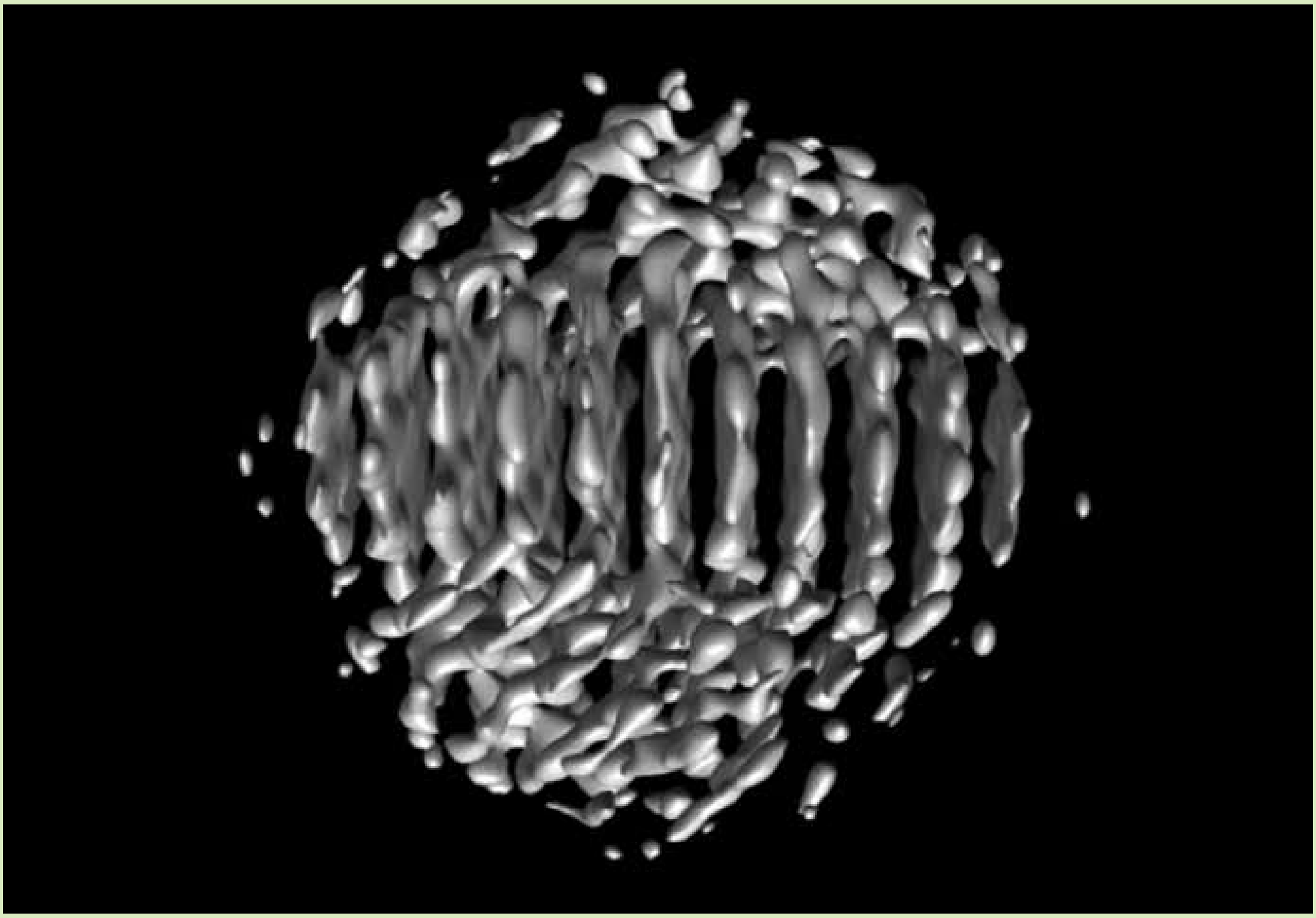
The field had anticipated cubical or at least highly symmetrical platinum nanocrystals. “It was surprising to learn that they form asymmetrical multi-domain structures,” Elmlund said.

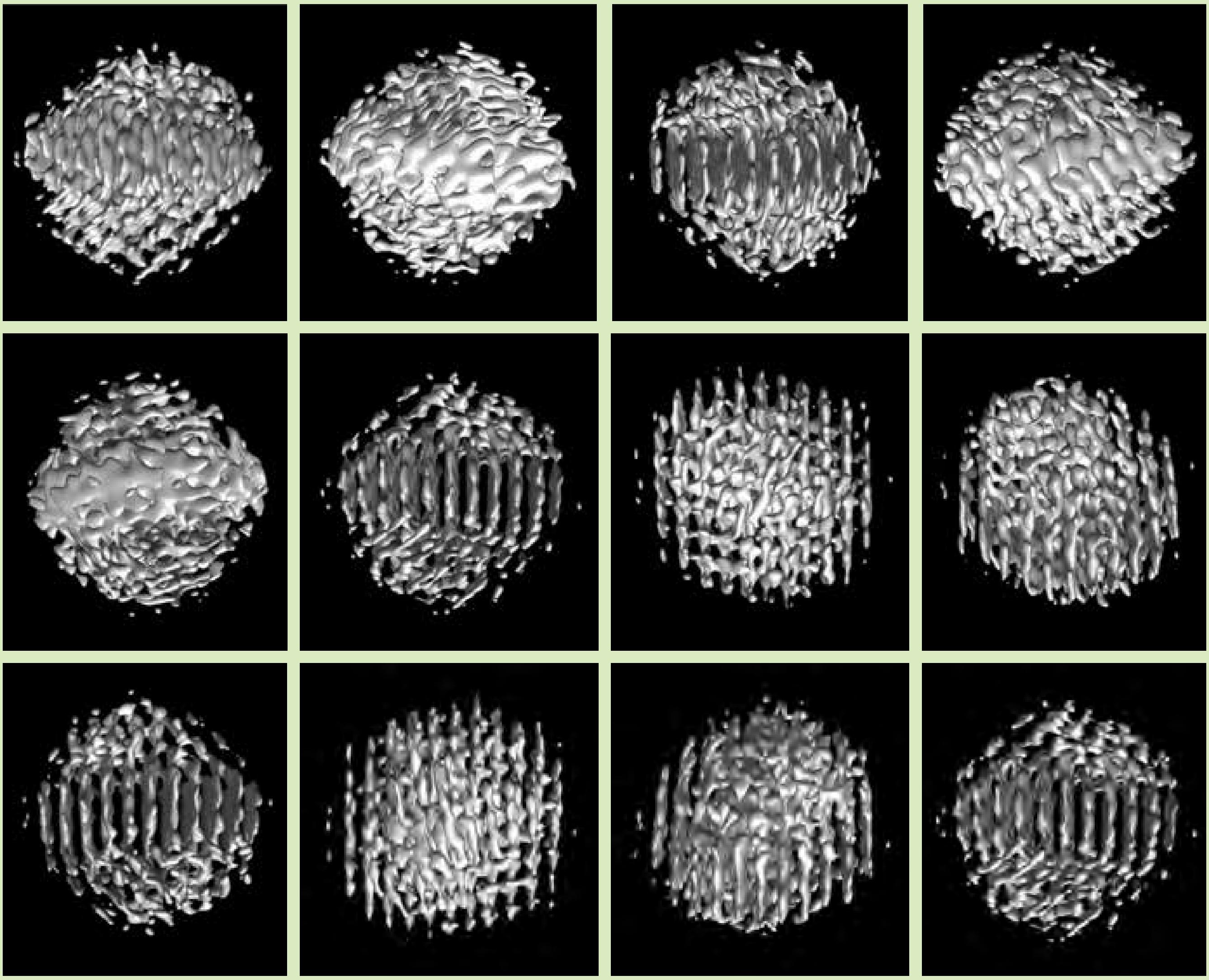
The next steps in the project will include investigating the formation and evolution of nanoparticles and characterising the transitions they go through to reach their final form. “It is important for us to understand this, so that we can design new materials, for example, to build better or more efficient solar cells, or make better and more economical use of fossil fuels,” Elmlund said.

Elmlund and his laboratory use MASSIVE to provide the data processing to undertake this work and other projects as part of the ARC Centre of Excellence in Advanced Molecular Imaging.

SOURCE: www.monash.edu/news/show/caught-on-camera-the-first-glimpse-of-powerful-nanoparticles

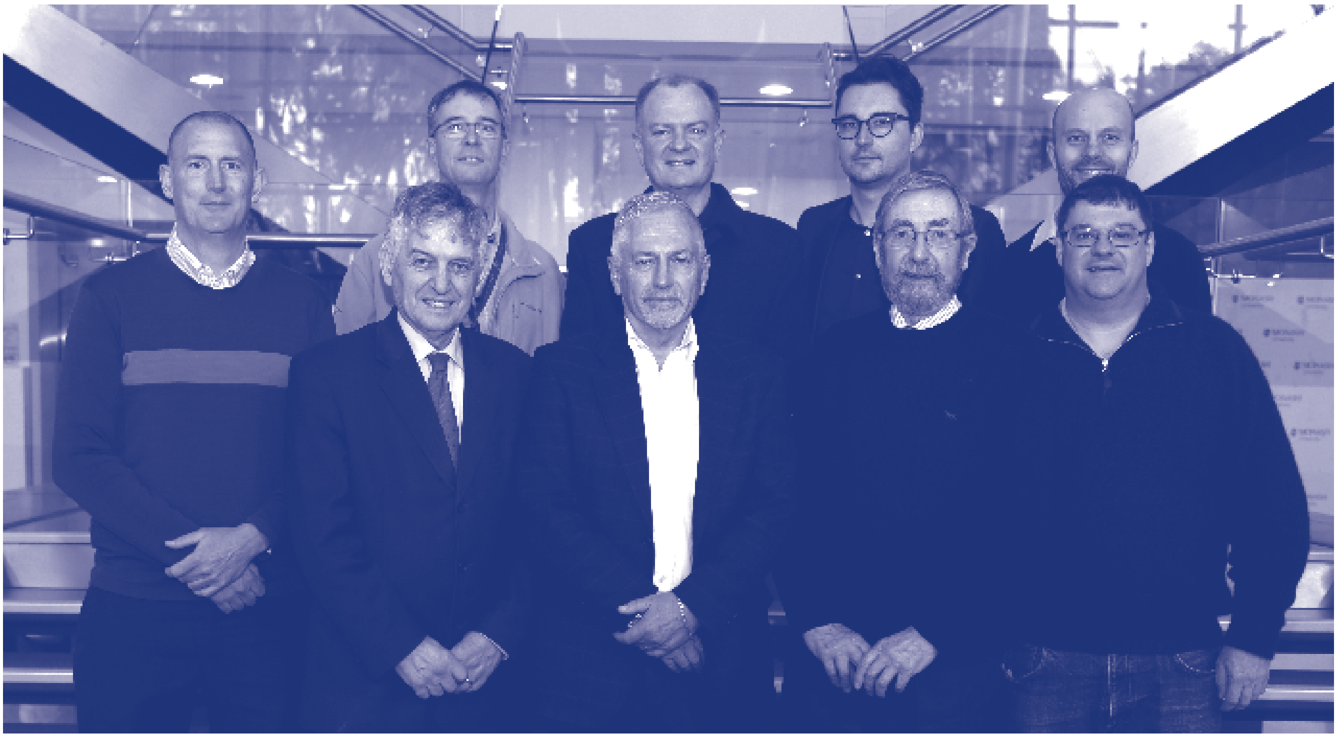
OPPOSITE: 3D structures of platinum nanocrystals.





/08

Governance



Steering Committee

The Steering Committee is composed of the MASSIVE Partners and Affiliated Partners. Since 2012, it has been chaired by Dr Robert Hobbs. From July 2016, Dr Greg Storr is the new chair.

MASSIVE Steering Committee meeting on the 14th July 2016.

Members and observers along top row, left to right:

Andrew Peele
Australian Synchrotron member

Michael James
Australian Synchrotron observer

Paul Bonnington
Monash University member

Wojtek James Goscinski
Coordinator, MASSIVE

Alf Uhlherr
CSIRO member

Members and observers along bottom row, left to right:

George Borg
Australian Synchrotron member

Greg Storr
Chair, 2012 - June 2016

Robert Hobbs
Chair, July 2016 onward

James Whisstock
ARC CoE for Advanced Molecular Imaging

Absent:
Gary Egan
ARC CoE for Integrative Brain Function

/09

Team and Operations

The MASSIVE team

The MASSIVE team is the most vital part of the project. Members of the team possess a wide range of expertise, including skills in high performance computing, software development, systems administration and project management. A number of staff members possess higher graduate degrees in visualisation, physics, geoscience and computing.

The MASSIVE is listed here and is underpinned by significant contributions from the Monash HPC and Research Cloud teams at the Monash eResearch Centre and Monash eSolutions.

From left to right:

Kai Xi PhD
HPC Consultant

Chris Hines PhD
Senior HPC Consultant

Damien Leong
Senior HPC Consultant

Wendy Mason PhD
eResearch Engagement Specialist

Paul McIntosh PhD
Technical Manager and Senior HPC Consultant

Jupiter Hu
Software Specialist (CVL)

Wojtek James Goscinski PhD
MASSIVE Coordinator

Absent (commenced in early 2016):

Kerri Wait
Software Specialist

Lance Wilson PhD
Senior HPC Consultant

Research Stories

An Australian Mirror of the Human Connectome Project

Assoc. Prof Alex Fornito

The ARC Centre for Integrative Brain Function and MASSIVE are together playing an active part in Australia's involvement in an ambitious program to understand the nerve connections in the human brain, the so-called 'connectome'.

The scale of the Human Connectome Project is grand from various perspectives. Operating across a number of major universities in the US, the HCP aims to publish for use by the scientific community data from high resolution MRI scans of about 1,200 individuals comprising four or more brothers and sisters — including twin pairs — from 300 families.

Nothing as big has been done in relation to charting the brain before, but the project has a parallel in the Human Genome Project, completed more than a decade ago.

To help Australian neuroscience researchers, MASSIVE is both hosting a mirror of the HCP data and providing critical large-scale storage space and the many hours of computing time needed to make sense of the data.

Associate Professor Alex Fornito is receiving first-hand the benefits of a local mirror of HCP data. His key research interests lie in identifying the genes that determine how networks of nerves are connected in the brain and piecing together how the connectome influences different behaviours, cognitive abilities and the personalities of individuals.

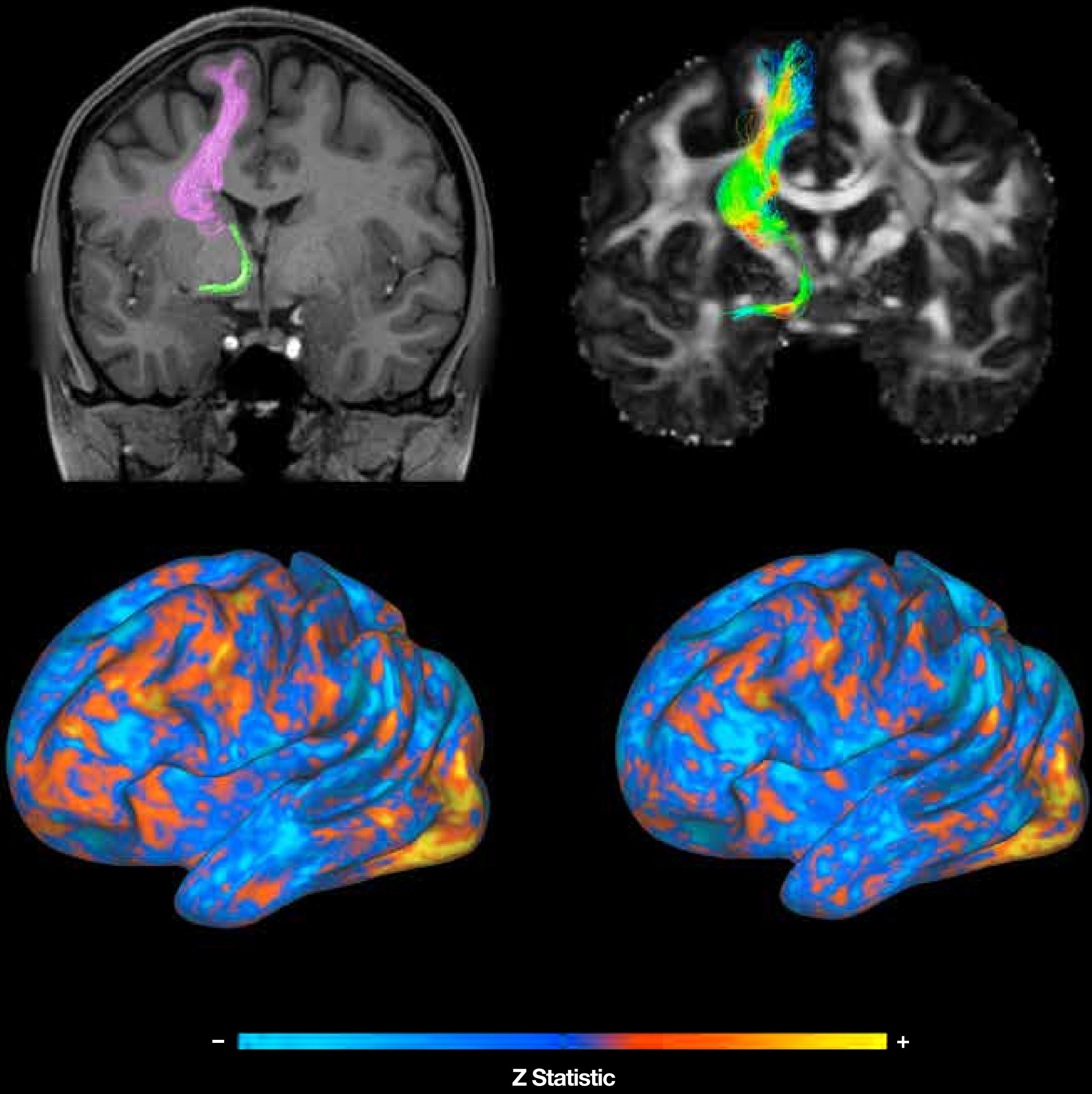
"We simply could not do our studies if the Australian mirror of the HCP did not exist," says Alex. "Thanks to its availability through MASSIVE, members of my lab require only a notebook computer to log in and gain full access to the storage, computing power and time we need."

The MASSIVE mirror site receives HCP data in the form of brain images. Alex and other researchers then subject the image to various processing algorithms to extract the measures they need. The software required to run the analysis is installed and maintained by MASSIVE staff.

Alex will use the resources to understand the connectivity of 'hub' regions of the brain – regions with a larger number of connections than other areas. Rather like the role of Heathrow or Dubai International airports in distributing passengers around the world, these hubs play an important role in routing information traffic in the brain.

Alex has a good starting point for his HCP-related research. His work in mice has revealed hubs of brain network activity that are enriched for the expression of certain classes of genes, in particular those involved in regulating the synthesis and breakdown of ATP. He now aims to extend these findings to humans.

Since the HCP data became available to researchers in October 2015 six Australian research groups have tapped into the wealth of information it contains.



Understanding Reward and Punishment

There exist drastic individual differences in how humans respond to reward and punishment, with these differences directly influencing behavior and character traits such as risk-taking and impulsivity. Modern neuroscience has begun to elucidate the neural bases for these differences showing that both activation within and connectivity among a complex network of cortical and subcortical areas underlie these individual differences. However, most of these studies have been performed with relatively small sample sizes. Dr Alexander Puckett from the University of Queensland is using the recently released Human Connectome Project (HCP) 500 dataset and the high-performance computing resources made available on MASSIVE to examine these differences in a much larger population.

The figure above illustrates the different types of neuroimaging data being analyzed for each individual subject from the HCP dataset. Diffusion Tensor Imaging (DTI) is used to track white matter connecting regions of interest and to examine the integrity of these fibers. Functional magnetic resonance imaging (fMRI) is used to investigate differences in the neural processing of reward and punishment. The relationships between these neuroimaging data and an extensive set of behavioral measures are being investigated to gain a better understanding of how connectivity among and processing within cortical and subcortical areas are related to impulsive behavior.

This work is being performed by Alexander Puckett, Georg Kerbler, and Ross Cunnington at the Queensland Brain Institute, The University of Queensland.

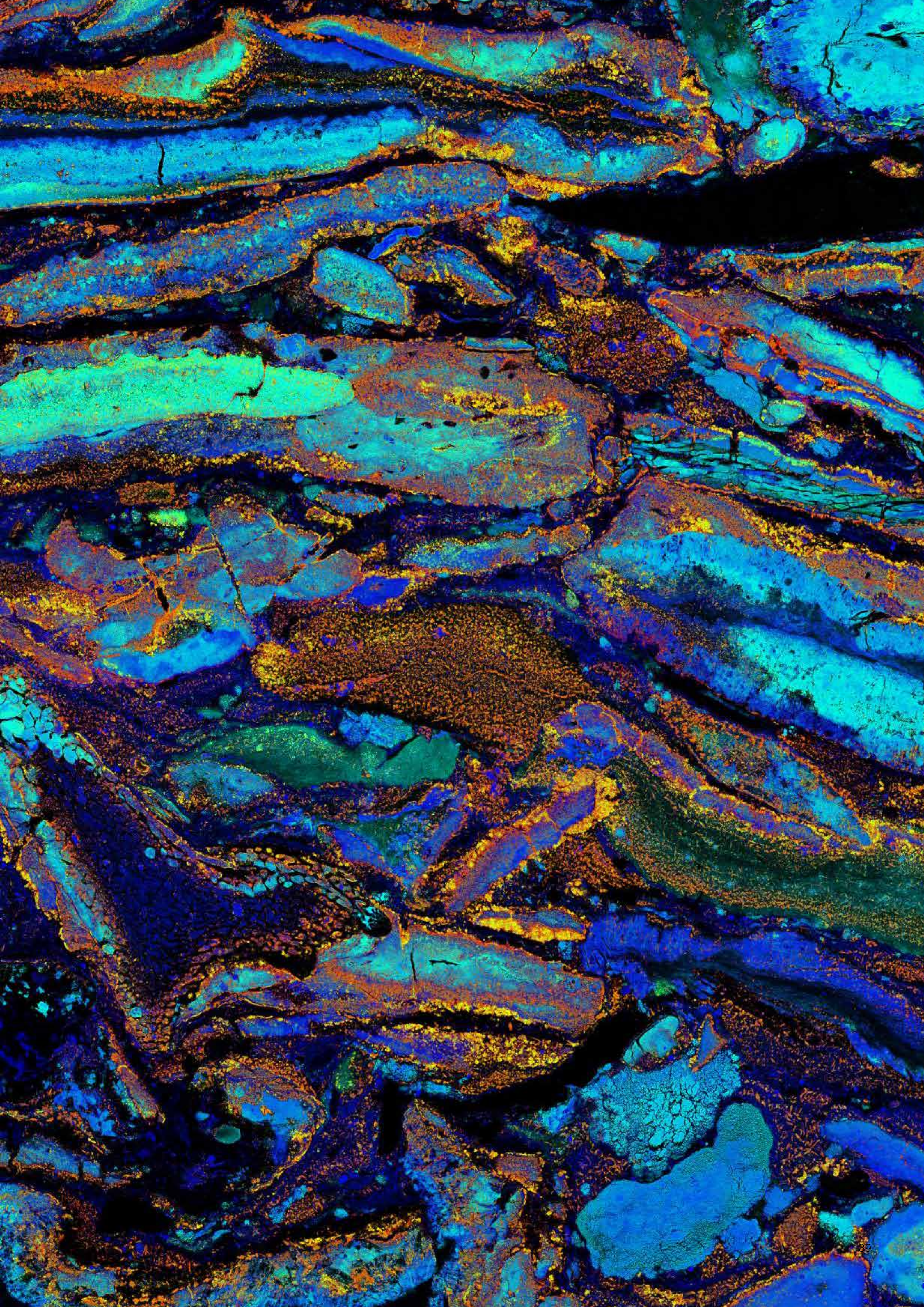
/10

Projects

The following is a list of projects that have used MASSIVE in 2015, including merit allocated projects through the National Computational Merit Allocation Scheme and beamline access at Australian Synchrotron.

Title	Organisations	Users	Allocation
3D EM reconstruction of plasma-derived proteins	Monash University	Andrew Ellisdon, Bradley Spicer, Charles Bayly-Jones, Christinace Lucato, Christopher Lupton, James Wettenhall, Kai Xi, Lance Wilson, Mazdak Radjainia, Michelle Dunstone, Natalya Dudkina, Natasha Lukoyanova, Siew Siew Pang	Partner Share
3D modelling of small scale geological structures	Monash University	Alexander Cruden, Mathias Egglseder	Partner Share
3D reconstruction of genome-wide gene expression and regulation in mouse hearts	Monash University	Mirana Ramialison, Nathalia Tan	Partner Share
3D structural analysis of muscle fibre architecture in diseased human hearts	University of Otago, Australian Synchrotron	Daryl Schwenke, James Pearson	Beamline Project
A bacterial sensor	Monash University	Mazdak Radjainia, Richard Berry	Partner Share
Analysis of 3-D CT data of biosurfactant-based foams	Monash University	Huazhen Li, Lizhong He, Sarah Irvine	Partner Share
Applying 4DxCT to idrug delivery and lung function change of inhaled therapies	Monash University	Isaac Pinar, Jian Li, Jiping Wang, Rhiannon Murrie, Richard Carnibella, Yu-Wei Lin	Partner Share
ARC Amber Project	Monash University	Pedro Viegas	Partner Share

OPPOSITE: Image of polymetallic (Ni-Mo-Zn-PGE) black shale from the Nick deposit in the Devonian Selwyn Basin, Yukon, Canada. Image (Ni As Fe in RGB, 9126 x 5126 pixels, 36.5 x 20.5 mm^2, 0.8 ms/pixel) collected by Anais Pages and Margaux Le Vaillant, CSIRO, using the Maia detector on the XFM beamline.



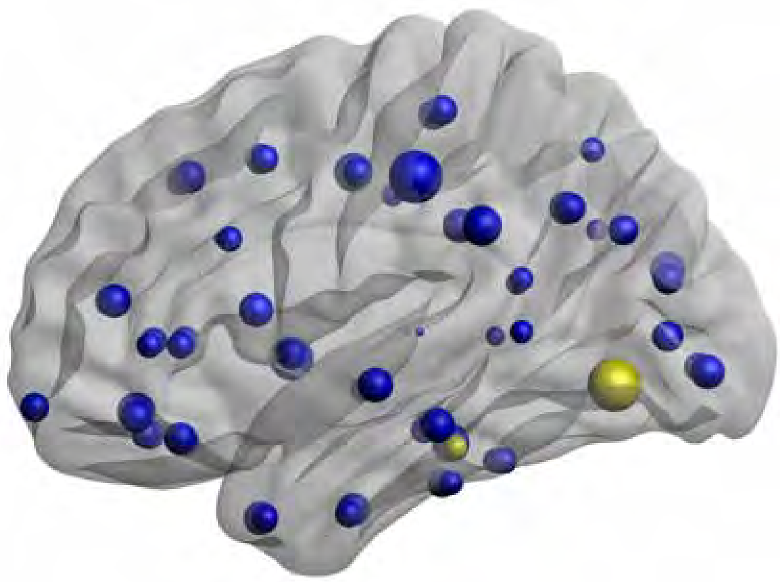
Title	Organisations	Users	Allocation
Assessment of the size-dependence of particle mucociliary clearance in ferret trachea	Women's & Children's Hospital, Monash University	Martin Donnelley, Kaye Morgan, David Parsons, Maged Awadalla	Beamline Project
Australian Synchrotron commercial client #1	Confidential		Beamline Project
Australian Synchrotron commercial client #2	Confidential		Beamline Project
Australian Synchrotron commercial client #3	Confidential		Beamline Project
Australian Synchrotron commercial client #4	Confidential		Beamline Project
Australian Synchrotron commercial client #5	Confidential		Beamline Project
Australian Synchrotron commercial client #6	Confidential		Beamline Project
Australian Synchrotron commercial client #7	Confidential		Beamline Project
Australian Synchrotron commercial client #8	Confidential		Beamline Project
Australian Synchrotron commercial client #9	Confidential		Beamline Project
Australian Synchrotron commercial client #10	Confidential		Beamline Project
Australian Synchrotron commercial client #11	Confidential		Beamline Project
Characterisation of the Imaging and Medical Beamline for Dual Energy X-ray Analysis using Synchrotron Computed Tomography at 30100 keV	RMIT, University of Otago	Nanette Schleich, Stewart Midgley	Beamline Project
Coke strength and reactivity links to coal components	Newcastle University, CSIRO	David Jenkins, Gareth Penny, Hannah Lomas, Karren Warren, Lukas Koval, Merrick Mahoney, Sheridan Mayo	Beamline Project
Computer-aided design of new catalysts for better fuel cells	Monash University	Chenghua Sun	Partner Share
Continuation of : Bubble collapse in experimental samples representative of volcanic plugs	University of Canterbury, CSIRO	Ben Kennedy, C Ian Schipper, Christopher Hall, Darren Thompson, Emma Rhodes, James Cowlyn, Matt Edwards	Beamline Project
Density waves in dipolar gases	Monash University	Chris Billington, Meera Parish	Partner Share
Development of large animal airway surface imaging techniques at the IMBL	Women's & Children's Hospital, Monash Uni	Martin Donnelley, Kaye Morgan, David Parsons, Maged Awadalla	Beamline Project
Dual Energy X-ray Analysis Using Synchrotron Computed Tomography at 30-80 keV	University of Otago	Nanette Schleich, Stewart Midgley	Beamline Project
Dynamo setup	Monash University	Alex De Marco	Partner Share
Epigenetic Regulation Struture & Function	Monash University	Chen Davidovich, Paul McIntosh, Philip Chan	Partner Share

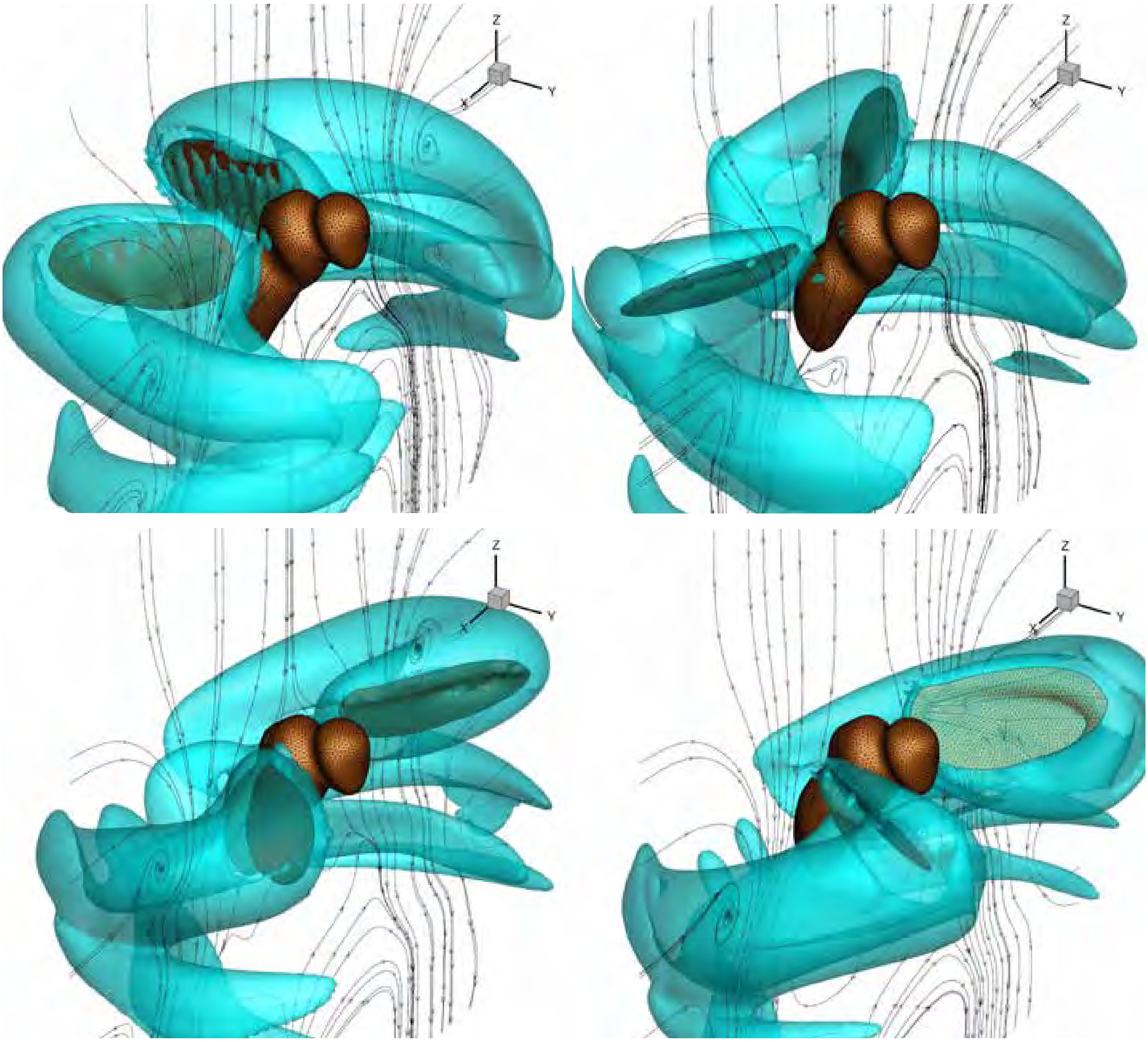
Title	Organisations	Users	Allocation
Evolution of the Australian flora: visualisations of the internal anatomy of permineralised fossil fruits and cones using the Imaging and Medical Beamline (IMBL) at the Australian Synchrotron, Melbourne	Queensland Museum, University of Queensland, Central Queensland University, Australian Synchrotron	Andrew Rozefelds, Anita Milroy, Gary Pattemore, Anton Maksimenko	Beamline Project
Exploring National Treasure: Automatic Photo Search for the Large Collection of National Archives of Australia	University of Woollongong	Ian Comor, Lei Wang, Yan Zhao	National Merit Allocation
Exploring unique aspects of Australian Dinosaurs: (a) post-cranial structure of Leaellynasaura amicagraphica, and (b) locomotion of Triassic dinosauromorphs	Museum Victoria, Uppsala University, CSIRO, Australian Synchrotron	Benjamin Kear, David Pickering, Karen Siu, Karen Siu, Karen Siu, Karen Siu, Martin Kundrat, Robert Acres, Thomas Rich	Beamline Project
Geopixe Training Project	Australian Synchrotron, CSIRO	David Paterson, Alessandro Zucchelli, Heidi Berkenbosch, Jessica Hamilton, Patricia Durance, Weihua Liu	Partner Share
Habitability of meteorites on the martian surface	Monash University	Sasha Wilson	Partner Share
High speed train aerodynamics	Monash University	Mark Thompson, Shibo Wang	Partner Share
How to make a planet: Investigation of early solar system dynamics through meteorites	Macquarie University, Australian Synchrotron	Andrew Tomkins, Daria Czaplinska, Jeremy Wykes, Sandra Piazolo, Tracy Rushmer	Beamline Project
Image processing intensive application in big data	ADFA, University of New South Wales	Andrew Asfaganov, Jiankun Hu, Quang Tran, Xuefei Yin, Yanming Zhu	National Merit Allocation

Children with autism spectrum disorders (ASD) often exhibit motor clumsiness (Developmental Coordination Disorder, DCD), i.e. they struggle with everyday tasks that require motor coordination like dressing, self-care, and participating in sport and leisure activities.

Dr Karen Caeyenberghs, Australian Catholic University, is examining whether motor deficits represent similar impairments in the brain networks of DCD and comorbid DCD-autism. Although small-world properties were present for all networks, the topological architecture of the morphological networks was significantly altered in children with ASD. Moreover, paralimbic regions exhibited nodal clustering coefficient alterations in singular disorders, which were disorder-specific for ASD and DCD children.

Children meeting criteria for both DCD and ASD exhibited topological changes that were more widespread than those seen in children with only DCD or ASD. These results will aid in providing better definitions for comorbid neurodevelopmental disorders.





Free hovering flight of the fruit fly

Insects fly by flapping their wings to generate high aerodynamic forces to keep them aloft and to achieve remarkable maneuvers, which has attracted many researchers' interests in recent years. Because of the inherent flexibility of insect wings, the aerodynamic and inertial forces acting on insect wings can consequently induce considerable elastic deformations during flapping flight. This leads to a strongly coupled fluid-structure interaction (FSI) problem associated with the aerodynamics and structural dynamics of flapping wings, which essentially gives rise to a computational fluid dynamics-computational structural dynamics (CFD-CSD) coupled problem. It is very difficult to tackle this aero-elastic problem experimentally because it usually requires simultaneous direct measurements of the wing kinematics, the wing deformation, the flow fields and the aerodynamic forces. Thus numerical simulations can provide an alternative way to study the physics of insect flight as long as the model has enough accuracy.

Wu Di, John Young, Wendy Kurniawan and Fang-Bao Tian, all of the School of Engineering and Information Technology at University of New South Wales Canberra, are integrating a computational model of insect flapping flight with flexible wings, which is based on a three-dimensional and unsteady FSI analysis. The model extends an existing rigid simulation used to solve the free-flight motion of an insect, and examine the effect of control strategies of the wing kinematics on the insect trajectory. The fluid solver requires significantly more computational power compared to the structural solver. We apply the fluid solver on a GPU card and the structural solver remains on the CPU, giving us a 4-5X speedup on MASSIVE cluster compared to CPU-only implementation.

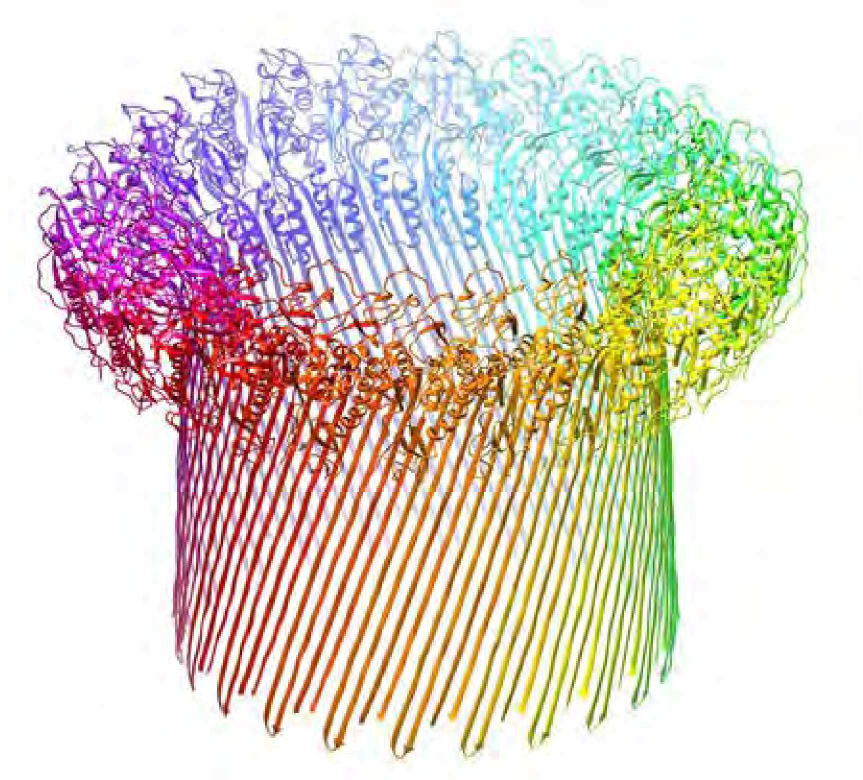
This sequence of images shows the ISO-vorticity of surfaces around the model insect at four consecutive time instances of a wing cycle during hovering. Streamlines of velocity field in X-Z plane are given as well. The bulk of vortical flow is shed via wing tip vortex (WTV) and trailing edge vortex (TEV) from each wing in a continuous fashion during a stroke in an arc around the body.

These voritices generated are roughly symmetric and of equal magnitude in the upstroke and downstroke during hovering. One may also observe the strong jets of flow passing between the WTV and the TEV.

A sequence of these vortices under each wing drives the flow below the wing to support the weight of the model insect.

Title	Organisations	Users	Allocation
Imaging ceramic matrix composites under in-situ loading at 15keV	Australian Synchrotron, DSTO	Matthew Zonneveldt, Andreas Moll, Benedicta Arhatari, John Thornton, Yung Kim, Ulrich Felzmann	Partner Share
Imaging the deformation and fracture onset in human femurs	Flinders University	Egon Perilli, Saulo Martelli	Beamline Project
Improving flood forecast skill using remote sensing data	Monash University	Ashley Wright, Valentijn Pauwels	Partner Share
Investigating brain blood flow regulation in lambs	Australian Synchrotron	James Pearson	Beamline Project
Investigating oxygen shunting in the rabbit renal circulation with microCT	Monash University, Australian Synchrotron	Bianca Le, James Pearson	Beamline Project
Lamb lung imaging pilot study	Monash University, The Womens Hospital, The Hudson Institute	Douglas Blank, Genevieve Buckley, Graeme Polglase, Ilias Nitsos, James Pearson, Karyn Rodgers, Katie Lee, Kelly Crossley, Lauren Kerr, Linda Croton, Marcus Kitchen, Omar Kamlin, Robert Acres, Stuart Hooper, Valerie Zahra, Anton Maksimenko, Christopher Hall	Beamline Project
Large-scale probabilistic time series forecasting: applications to electricity smart meter data	Monash University	Souhaib Ben Taieb	Partner Share
Low dose mammography commissioning tests	Australian Synchrotron, University of Melbourne, Monash University, CSIRO	Darren Thompson, Matthew Dimmock, Robert Acres, Timur Gureyev, Yakov Nesterets, Anton Maksimenko, Christopher Hall	Beamline Project
Low Reynolds Number Aerodynamics of Flapping Wings	ADFA	John Young	National Merit Allocation
Machine Learning Theory and Its Application to Cyber Security	ADFA	Jiankun Hu, Jinwei Xu	National Merit Allocation
Melbourne Brain Centre 7T MRI Protocol Development	University of Melbourne	Amanda Ng, Jon Cleary, Peter Yoo, Sila Genc, Warda Syeda, Yasmin Blunck	National Merit Allocation
Memory models in spiking neural circuits with plasticity	University of Sydney	Adam Keane, John Palmer, Pulin Gong	Partner Share
Microtextural insights into the origin and significance of mafic components in a silicic ignimbrite from the worlds youngest supereruption			Beamline Project
Microwear imaging of the world's oldest potential bone tools from the hominin bearing paleocave site of Drimolen, South Africa	La Trobe University	Andy Herries, Rhiannon Stammers	Beamline Project
Modelling mixed cation sodalites for radioactive iodine-129 capture and disposal in the nuclear fuel cycle	ANSTO	Eugenia Kuo	National Merit Allocation
Analysis of instrumented ore car data	Monash University	Andrew Yuen, Wenyi Yan	Partner Share

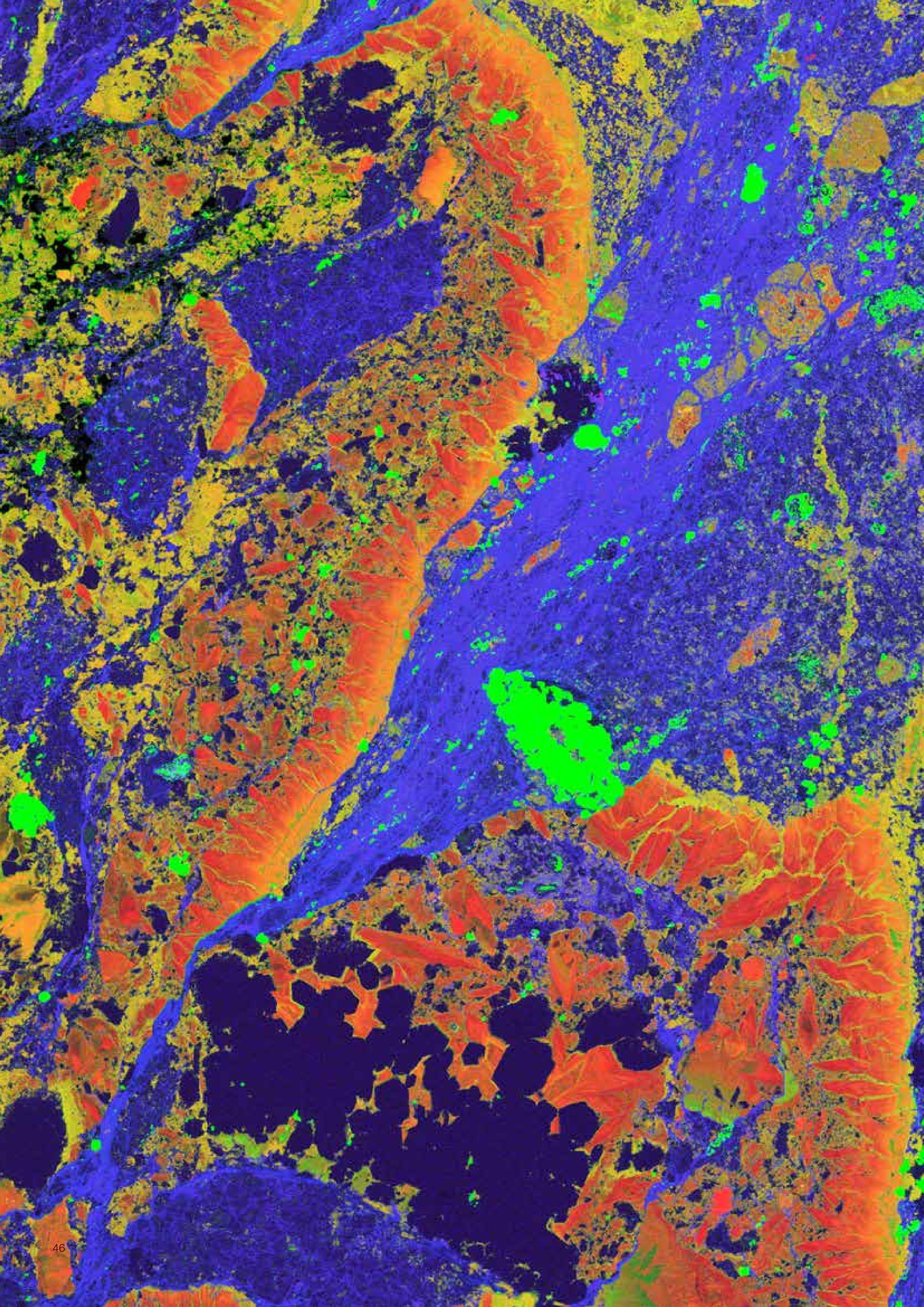
Title	Organisations	Users	Allocation
Multi-energy quantitative X-ray CT for mineral and energy resources rock samples	CSIRO, Australian Synchrotron	Adrian Trinchi, Andrew Stevenson, Anthony Hughes, David Molenaar, Miao Chen, Sam Yang, Sheridan Mayo, Vu Nguyen	Beamline Project
Mummificiation Process, Dental Decay and Possible Evidence of Interceptive Orthodontic treatment in a Mummified Child from Graeco-Roman Egypt			Beamline Project
Neural bases underlying individual differences in impulsivity and control	University of Queensland	Alexander Puckett, Georg Kerbler	National Merit Allocation
Neuroanatomical correlates of injury severity and outcome following TBI	Monash University	Gershon Spitz	Partner Share
Optimise RELION for use with different accelerators	Victor Chang Cardiac Research Institute	Callum Smits	Discretionary
Origins of the Struthiolariidae: Resolving the phylogeny of Cretaceous-Paleogene ostrich-foot snails using synchrotron micro-CT and three-dimensional shape analysis	Victoria University of Wellington, CSIRO, Australian Synchrotron	C Ian Schipper, Katie Collins, Michael Gazley, Robert Acres, Anton Maksimenko, Christopher Hall	Beamline Project
Post-cranial reconstruction of *Leaellynasaura amicagraphica*—towards completing the digital puzzle	Museum Victoria, Monash University, Australian Synchrotron	Alistair Evans, Anton Maksimenko, Benjamin Francischelli, James Rule, Karen Siu, Lap Chieu, Les Kriesfeld, Lesley Kool, Lisa Nink, Mike Cleeland, Oliver Gore, Patricia Vickers-Rich, Qamariya Nasrullah, Sally Davies, Thomas Rich, Tim Ziegler	Beamline Project
Protein RNA complexes	Monash University	Matthew Wilce	Partner Share
Rapid information processing in subcortical amygdala pathways	University of Queensland	Jessica McFadyen, Marta Garrido	Partner Share
Rational design of anti-microbial agents	Monash University	James Wettenhall, Matthew Belousoff, Mazdak Radjainia	Partner Share
Re-Action: innovations in motor and cognitive rehabilitation	Monash University	Karen Caeyenberghs, Kerri Wait	Partner Share
Seeking the First Treatment for Neonatal Pulmonary Arterial Hypertension: Studies at the Imaging and Medical Beamline (Submission 2)	Monash University, University of Otago, Australian Synchrotron	Christine Bui, Claudia A Nold, Daryl Schwenke, Ina Rudloff, James Pearson, Kirstin Elgass, Megan Wallace, Philip Berger, Robert Acres, Steven Shian Chin Cho, Anton Maksimenko, Christopher Hall	Beamline Project
SIMPAS research on particle science and technology	Monash University	Jieqing Gan, Jieqing Gan, Sida Liu, Siyuan He, Tengfang Zhang, Xuejiao Liu, Zheng Qi	Partner Share
SIMPLE image processing suite	Monash University	Frederic Bonnet, Hans Elmlund, Jarrod Voss, Mazdak Radjainia	Partner Share
Simulation and Modelling of Particulate Systems	Monash University	Jieqing Gan, Jieqing Gan, Zheng Qi	National Merit Allocation
Snapshot of termites nest for bio-inspired design of porous materials	CSIRO	Aaron Thornton	Beamline Project



MASSIVE was used in determining the structure of human Complmenet Component 9 (C9) in a pore-like form. C9 is a major immune effector that normally functions in the elimination of pathogenic bacteria. Scientists within the Imaging Centre of Excellence are using this information in the development of molecules to enhance or inhibit C9 function in infection and inflammatory disease respectively.

Structure of the poly-C9 component of the complement membrane attack complex.
Dudkina NV, Spicer BA, Reboul CF, Conroy PJ, Lukoyanova N, Elmlund H, Law RH, Ekkel SM, Kondos SC, Goode RJ, Ramm G, Whisstock JC, Saibil HR, Dunstone MA.
Nat Commun. 2016 Feb 4;7:10588. doi: 10.1038/ncomms10588.

Title	Organisations	Users	Allocation
Stability and Control of Insect Flight	ADFA	Di Wu, John Young	Discretionary
Study of plasmonic devices	ANSTO	Eugeniu Balaur, Wye kit Leong	Partner Share
Synchrotron Imaging of an Endovascular Brain Machine Interface	University of Melbourne	Gil Rind, Nicholas Opie, Sam John	Beamline Project
Synchrotron micro-tomography imaging of aortic stent grafts in relation to the renal artery ostium	Curtin University	Albert Chong, Curtise Ng, Zhonghua Sun	Beamline Project
Teeth in placoderm fishes	Australian National University	Vincent Dupret	Beamline Project
Testing and evaluation of in-line phase-contrast CT imaging for mammographic applications	CSIRO	Darren Thompson, Yakov Nesterets	Beamline Project
Testing the metabolic theory of ecology using high throughput CT imaging	Monash University	Ben Wegener, Bernard Coetzee, Grant Duffy, Guillaume Latombe, Ian Aitkenhead, Jessica Hoskins, Katherine Moon, Rebecca Hallas, Robert Acres, Steven Chown	Beamline Project
The Characterisation Virtual Laboratory	Monash University	Various	Discretionary
The Characterisation Virtual Laboratory—Atom Probe EMAP	University of Sydney	Various	Discretionary



Title	Organisations	Users	Allocation
The effect of non-invasive respiratory support on pulmonary blood flow at birth	Monash University	Stewart Hopper	Beamline Project
The Neuroscience of Morality	Monash University	Ayushi Gupta, Felice van Nunspeet, Juan Dominguez, Pascal Molenberghs, Robert Eres, Stefanie Roberts	Partner Share
Titan Krios Core Facility	Monash University	James Wettenhall, Maryam Khoshouei, Matthew Belousoff, Mazdak Radjainia	Partner Share
Transition, stability and control of bluff body flows	Monash University	Mark Thompson	National Merit Allocation
Understanding the assembly of high electron affinity molecular acceptors on surfaces	La Trobe University	Chris Pakes (La Trobe University), Alex Schenk, Chris Wright	Partner Share
Understanding virus replication by Cryo-Em	Monash University	Alex de marco, DAMIA GARRIGA, Fasseli Coulibaly, Hans Elmlund, Joshua Hardy, Mazdak Radjainia	Partner Share
Unraveling the mysteries of Ediacaran fossils: internal morphology as key to understanding the evolution of complex macroscopic life	Museum Victoria, Monash University, Australian Synchrotron	Benjamin Francischelli, James Rule, Karen Siu, Les Kriesfeld, Lesley Kool, Lisa Nink, Patricia Vickers-Rich, Thomas Rich, Tim Ziegler	Beamline Project
Visualising water transport in plants: why are some species more drought resistant than others?	University of Western Sydney, University of Tasmania	Brendan Choat, Danielle Creek, Jennifer Peters, Rob Skelton, Rosana Lpez, Tim Brodribb, Anton Maksimenko, Christopher Hall, Robert Acres	Beamline Project

OPPOSITE:
Image across a whole thin-section sample from Sunrise Dam Gold Mine (Fisher et al., Miner. Deposita 50, 665-674 (2015); DOI: 10.1007/s00126-014-0562-z), showing a gold-bearing quartz-carbonate vein, acquired on the XFM beamline using the Maia detector system. Image displays Sr, Fe and Rb in RGB (66668 x 15001 pixels, 40.0 x 9.0 mm2, 0.13 ms/pixel, 1G pixels, 250 Gbytes).

/11

Financial Statement

			2015 12 months Jan to Dec	2016 6 months Jan to June
Brought Forward			**$205,906**	**($178,463)**
Income				
	Partner	Monash University	$2,100,000	$1,700,000
		CSIRO	$236,364	$200,000
		Australian Synchrotron	$203,400	$75,000
		CoE for Integrative Brain Function	$150,000	-
		CoE Molecular Imaging	$150,000	-
		Total	**$2,839,764**	**$1,975,000**
	Projects	NeCTAR - EIF		$132,000
		NeCTAR - NCRIS		$90,000
		Total		**$222,000**
	Other Income		**$5,314**	**$1,053**
	TOTAL		**$2,845,078**	**$2,198,053**

			2015 12 months Jan to Dec	2016 6 months Jan to June
Expenses				
	Projects	Desktops in the Cloud	$189,110	$109,899
		Characterisation Data Capture and Analysis	$228,986	$97,600
		CSIRO CAVE2 Access	$145,454	$94,546
		Total	**$563,550**	**$302,045**
	Facility			
	Management & Operations	Salary	$680,635	$332,172
		Governance	$4,500	-
		Total	**$685,135**	**$332,172**
	M3 Build	Compute and File System	$1,397,454	$499,763
		Installation & Services	-	$158,739
		Data Centre and Rack	$57,561	-
		Build Costs	$70,285	-
		Compute Costs	$18,863	-
		Total	**$ 1,544,162**	**$658,502**
	Hardware	Misc expenses	**$8,559**	**-**
	Utilities and Maint.	Power and hosting	$100,750	$50,375
		Hardware and Software maintenance	$160,000	
		Total	**$260,750**	**$50,375**
	Software	**Total**	**$72,662**	**$47,565**
	Training & Outreach	**Total**	**$96,373**	**$72,313**
	Other		**$1,088**	**($4,228)**
	TOTAL EXPENSES		**$3,232,280**	**$1,458,743**
Balance			($181,296)	$560,847
Interest			$2,834	-
Carried Forward			($178,463)	$560,847

Abbreviations

AMMRF Australian Microscopy and Microanalysis Research Facility

ANSTO Australian Nuclear Science and Technology Organisation

ARC Australian Research Council

CIBF Australian Research Council Centre of Excellence for Integrative Brain Function

CPU Central Processing Unit

CSIRO Commonwealth Scientific and Industrial Research Organisation

CT Computed Tomography

CVL Characterisation Virtual Laboratory

DIIRD Department of Industry, Innovation and Regional Development

EM Electron Microscope

GB Gigabyte

GPU Graphical Processing Units

HPC High performance computing

ImagingCoE ARC Centre of Excellence for Advanced Molecular Imaging

IMBL Imaging and Medical Beamline (at the Australian Synchrotron)

M1 the MASSIVE computer located at Australian Synchrotron

M2 MASSIVE computer located at Monash University

M3 MASSIVE computer located at Monash University

MASSIVE Multi-modal Australian ScienceS Imaging and Visualisation Environment

MASSIVE1 The program of work to provide HPC capability for the Australian Synchrotron and the Australian Synchrotron user community

MASSIVE2 the program of work to provide Australian researchers access to specialized HPC services for imaging and visualisation under the NCI Specialised Facilities Program.

MASSIVE3 The new collaboration and program of work funded by Monash University, CSIRO, Australian Synchrotron, and new partners, ImagingCoE and CIBF.

MRI Magnetic Resonance Imaging

NCI National Computational Infrastructure

NCMAS National Computational Merit Allocation Scheme

NeCTAR National eResearch Collaboration Tools and Resources

NIF National Imaging Facility

RDSI Research Data Storage Infrastructure

SAC Science Advisory Committee

SU System Units

TB Terabyte

XFM X-ray Fluorescence Microscopy

NOTES

NOTES

MASSIVE
Monash eResearch Centre
Ground Floor, 15 Innovation Walk
Monash University, Clayton Campus,
Victoria, 3800

E: coordinator@massive.org.au
W: www.massive.org.au