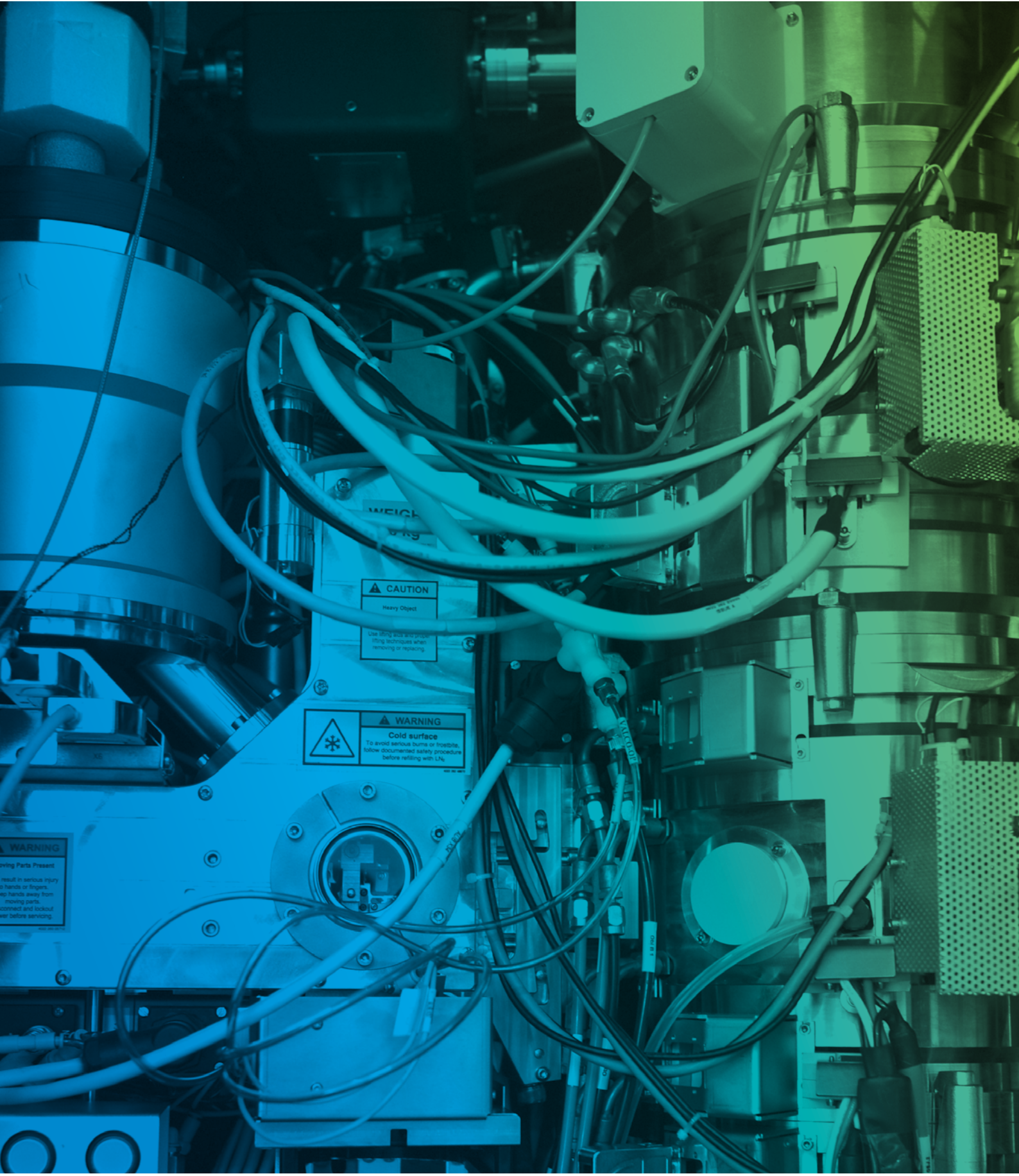

MASSIVE | Annual Report 2014

Australian Synchrotron · CSIRO · MONASH University · VPAC · NCI · Victoria

PARTNERS

AFFILIATE PARTNERS

INVESTORS

PROJECT FUNDERS

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From the Chair

It is with great pleasure that I can say MASSIVE has achieved what was intended of it four years ago in 2010. When it started MASSIVE had the ambitious vision to support a wide range of Australian instruments and the researchers using them with the capability to quickly process, analyse and visualise data. Indeed, MASSIVE remains a unique piece of infrastructure – not only in Australia, but also the world.

The founding partners – Monash University, Australian Synchrotron, CSIRO and VPAC – should all be proud of the journey they have embarked upon and the achievement of creating a world-class imaging and visualisation facility in MASSIVE.

In this report, we include highlights of the work and research conducted at the Australian Synchrotron, introduce new research partnerships and highlight significant research stories.

With the two foundation projects – MASSIVE1 and MASSIVE2 – complete, 2014 has seen MASSIVE switch focus to further growth and embark on the MASSIVE3 project.

This last year also saw the completion of the NeCTAR-funded Characterisation Virtual Laboratory (CVL) Project. The CVL – as you can read in this report – is a major undertaking to connect instruments to desktop computing facilities and provide easier mechanisms for researchers to process and analyse their data. The CVL is now available to all Australian researchers via the NeCTAR cloud – providing a cloud-based desktop environment for researchers in neuroimaging, structural biology, X-ray imaging, and atom probe microscopy. Key technologies developed under the CVL project are also run on the M1 and M2 computers. The project has made MASSIVE more accessible and usable to a large selection of researchers – including in key areas of the life sciences such as neuroscience and biochemistry.

In 2015 there will be new challenges and opportunities. Two new partners are joining the MASSIVE facility as affiliate partners: the ARC Centre for Advanced Molecular Imaging; and the ARC Centre for Integrative Brain Function. This provides an opportunity to progress the work underpinning neuroscience and structural biology that has been a major focus of the MASSIVE1 and MASSIVE2 projects. With more than eight national partners involved across the three Centres of Excellences (and a further 20 or so international partners) there is an opportunity to further the impact of MASSIVE.

I look forward to watching progress in 2015 and beyond as MASSIVE3 gets under way, the ARC Centres of Excellence reach maximum output and the CVL becomes a popular research tool.

Dr Robert Hobbs
Chair, MASSIVE Steering Committee

/02

Coordinator's Message

This year was particularly exciting for the MASSIVE team, with both the original MASSIVE1 and MASSIVE2 projects coming to a close and the CVL completing development.

It is timely to reflect on some achievements and highlights since the project began in 2011:

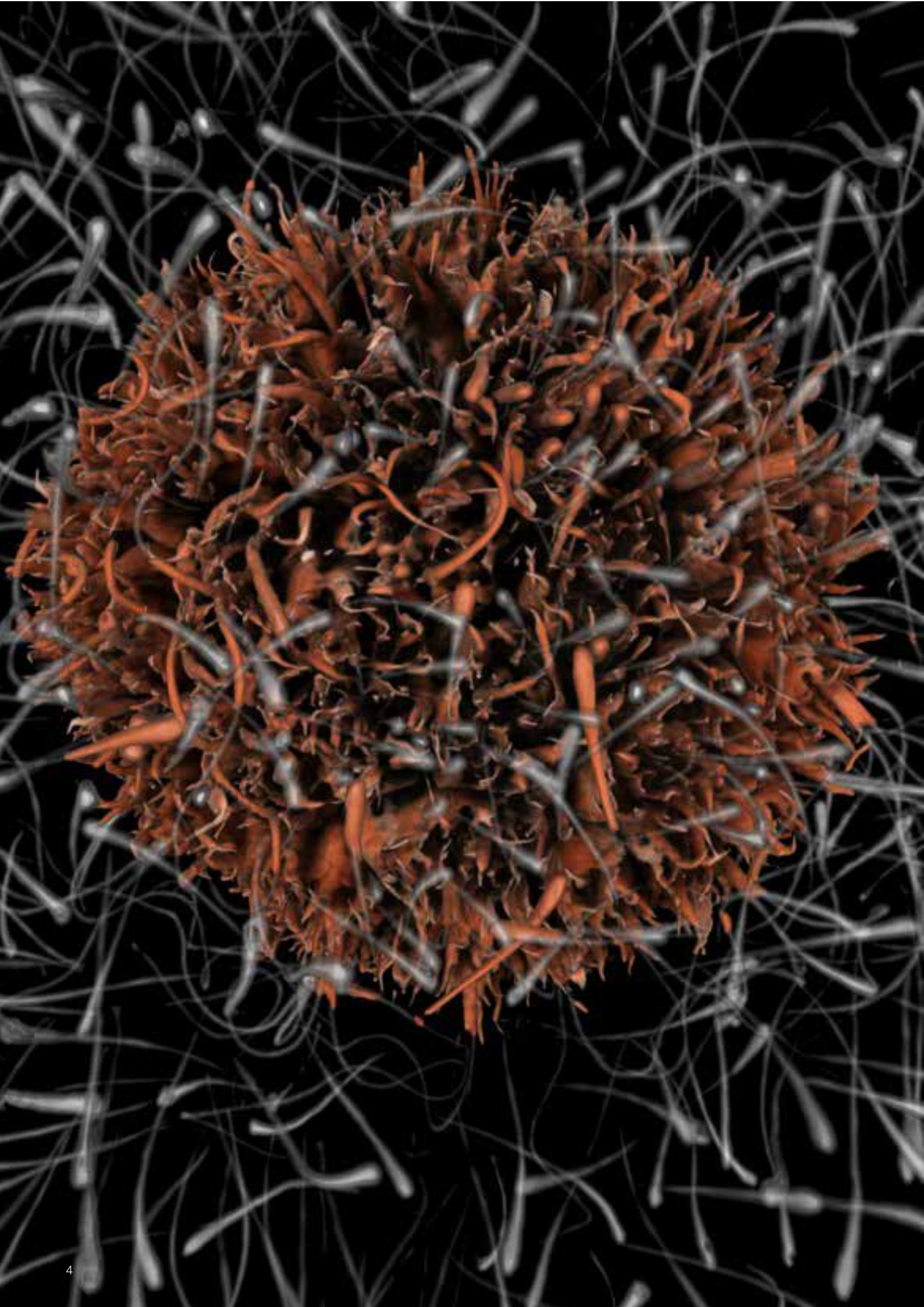
- MASSIVE has provided computing and data processing services to 270 projects through partner and merit based access, which includes 612 individual researcher user accounts.
- Our partnership with Australian Synchrotron has underpinned 446 Australian Synchrotron beamtime allocations, that have included more than 79 lead investigators, across 94 Australian and International research institutions and industry.
- The MASSIVE Desktop has proved an easy and effective way for non-expert researchers to begin using central computing and HPC. Over 300 researchers have used this capability and over half of these have remained long-term active users.
- The NeCTAR Characterisation Virtual Laboratory has developed software infrastructure that has been used by more than 450 researchers across major Australian facilities.

Most significantly, Monash University, CSIRO and the Australian Synchrotron formed a new collaboration, called MASSIVE3, to continue MASSIVE services till the end of 2016.

The new MASSIVE3 project has spurred us to undertake a major systems software upgrade. This upgrade will ensure that the M1 and M2 computers are state of the art and best configured to support future requirements – including aligning our software with the CVL software stack. This will provide an easier transition for users from CVL to MASSIVE and back.

We are excited that MASSIVE has two new affiliate partners: the ARC Centre of Excellence for Integrative Brain Function which is focused on 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. The year 2015 and beyond will see these new relationships provide opportunities for MASSIVE to develop new focus areas and expertise. The team and I look forward to the challenges that these opportunities will bring.

Dr Wojtek James Goscinski
MASSIVE Coordinator



/03

Achievements in 2014

In July 2014, MASSIVE completed the combined MASSIVE1 and MASSIVE2 projects and now continues under a new program of work, MASSIVE3. Section 6 of this report highlights the major achievements from 2010 to 2014.

In 2014, MASSIVE achievements included:

> Completion, with other partners, of the development of the Characterisation Virtual Laboratory (CVL), which is now available to all Australian researchers through the NeCTAR cloud.

  More than 450 registered researchers have used and benefited from the infrastructure developed by the CVL project. The software technology developed provides researcher with an easier mechanism by which to capture instrument data and process the data on centralised cloud and HPC infrastructure, including MASSIVE and the National Computational Infrastructure.

> Commencement of a major upgrade to ensure that systems software running the M1 and M2 computers are state of the art and best configured to support future requirements – including aligning MASSIVE software with the CVL.

> High demand for time as applications to use MASSIVE through the National Computational Merit Allocation Scheme again far outstripped the available hours. MASSIVE partners have allocated 10% of the facility to be distributed through the National Computational Merit Allocation Scheme (NCMAS) and in November 2014 requests for this time on the facility were 4 times what was available.

> Formation by Monash University, CSIRO and Australian Synchrotron of MASSIVE3 a program of work to continue services until the end of 2016. Partners have contributed $2.4M plus in-kind contributions to the project.

> The addition of two new partners to the MASSIVE collaboration. The ARC Centre for Integrative Brain Function, and the ARC Centre for Advanced Molecular Imaging each contributed to MASSIVE to become Affiliated Partners and receive a dedicated share of the facility and services.

OPPOSITE AND ABOVE: These images show developing infloresences of various species of mapaniid sedges (Cyperaceae, Mapanioideae). Species in this group possess unique floral forms, markedly different from stereotypic monocot flowers. State-of-the-art synchrotron techniques are helping to reveal the spatial and temporal development of the floral organs, that combined with gene expression studies are deciphering reproductive homologies and the evolution of these floral forms. The CT scans were performed as a part of an international project led by Professor Jeremy Bruhl (University of New England) who along with Dr. John Conran (University of Adelaide), Ms. Chrissie Prychid (University of New England) and Dr. Anton Maksimenko (Australian Synchrotron), participated in the beamtime sessions. Data processing and rendering was done by `Dr. A. Maksimenko (AS) on MASSIVE.

THIS PAGE: The Struthiolariidae ("ostrich-foot snails") are a Southern Hemisphere family of molluscs. Their distinctive shell forms have the potential to provide insights into both evolutionary processes and nearshore paleoenvironment. However, their early relationships, which are vital to understanding the origins and dispersal of the group between landmasses, have proven unresolvable using standard morphology and shell characters. Synchrotron microtomography will allow reconstruction of internal and external morphology, providing critical data for mathematical analyses of shape which will allow resolution of early struthiolariid evolution, and fundamentally underpin further study of their paleoenvironmental variation. This research was conducted by Katie Collins, Ian Schipper, Michael Gazley, James Crampton (Victoria Uni of Wellington). This shell was kindly by the Invertebrate Palaeontology department at Museum Victoria. Rendering by Anton Maksimenko at Australian Synchrotron.

/04

About Massive

The Multi-modal Australian ScienceS Imaging and Visualisation Environment (MASSIVE) is the Australian specialised high performance computing (HPC) facility for imaging and visualisation. The project is a collaboration between Monash University, CSIRO, Australian Synchrotron and VPAC.

MASSIVE provides hardware, software and expertise to drive research in disciplines such as biomedical science, materials research, engineering and geosciences.

The facility underpins a range of advanced imaging modalities, including synchrotron X-ray and infrared imaging, functional and structural magnetic resonance imaging (MRI), X-ray computer tomography (CT), electron microscopy and optical microscopy.

It provides an extensive program of user support and training in HPC and has an active outreach program to ensure that the MASSIVE stakeholders, Australian and international researchers, government and the broader community are aware of its benefits and achievements.

MASSIVE is unique in Australia with its focus on fast data processing, including processing data in-experiment, large-scale visualisation, and analysis of large-cohort and longitudinal research studies.

It offers Australian scientists access to two physically separate computer systems joined by a high-bandwidth communications link:

M1, located at the Australian Synchrotron at 800 Blackburn Road in Clayton

M2, located at the Monash University campus in Clayton.

In addition, MASSIVE offers services through the cloud as the lead developer and operator of the CVL.

The MASSIVE project aims to:

1. Provide a world-class imaging and data processing facility to research groups identified by the MASSIVE stakeholders.

2. Increase the uptake of imaging and visualisation services by research groups using the Australian Synchrotron and Australian research groups generally.

3. Increase Australia's characterisation capability by providing compute infrastructure for processing, analysis and visualisation.

4. Increase the skills of research groups to use and develop imaging and visualisation services.

5. Strengthen the partnership that supports the MASSIVE project.

6. Underpin the ARC Centre for Integrative Brain Function, and the ARC Centre for Advanced Molecular Imaging with computing expertise and HPC access.

In doing so, MASSIVE expects to:

1. Equip research groups with an extended capability to use and develop leading-edge imaging and visualisation facilities.

2. See substantial research achievements arising from the use and development of the MASSIVE facility.

3. Attract increased investments in the MASSIVE facility and related imaging and visualisation facilities.

/05

Service and Capability Development

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

Increasingly, 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 can be used for image processing and interactive analysis and visualisation of very large and multidimensional datasets in near real- time, including a library of specialised image 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 were designed specifically for their purpose with a number of features that fulfil the core data processing and visualisation requirements:

A high performance file system of 498 terabytes (TB) capable of combined write speeds of 5 gigabytes (GB) per second. Fast reading and writing of data is essential to enable image processing such as that required at the Imaging and Medical Beamline (IMBL).

The operating systems are designed for efficient data processing, including CT reconstruction, whilst being generic enough for the wide range of processing tasks undertaken.

Two graphics processing unit (GPU) co-processors are installed on each computer node of M1 and M2. GPUs are very effective for accelerating processing such as CT reconstruction. They are essential for fast rendering for visualisation, and are being applied in a wide range of fields, in imaging in particular, as well as high performance computing in general.

Specialised visualisation nodes on M2 have high memory (144 GB per node) and GPUs that are specifically designed for high-end visualisation and hardware rendering.

Systems Upgrade

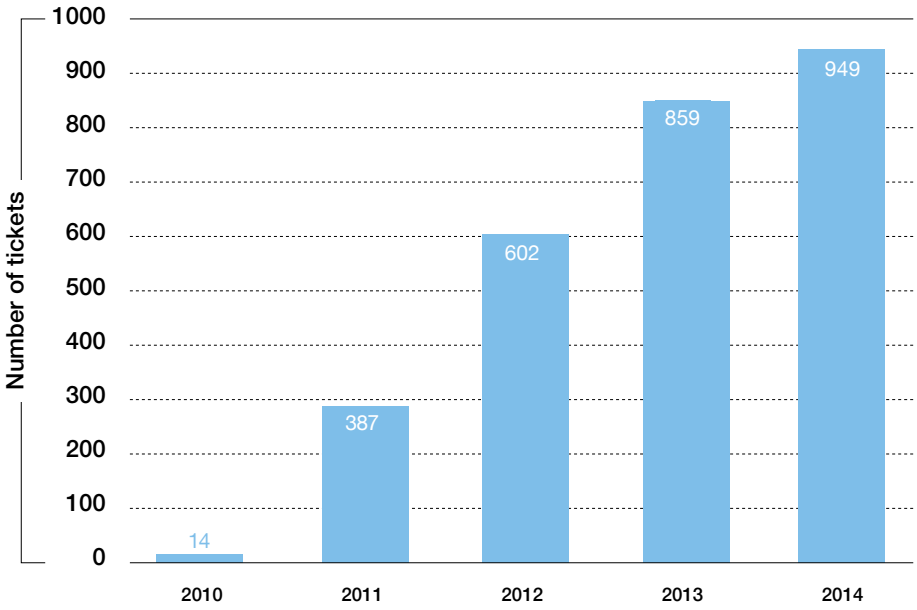
MASSIVE is undertaking an upgrade of systems software, including the scheduler and operating system. The upgrade will ensure that systems software running the M1 and M2 computers remain state of the art and best configured to support future requirements.

The upgrade will also align the computers with infrastructure developed for the CVL, which will make it easier for researchers to use the research cloud alongside MASSIVE. The upgrade is being undertaken in stages between June 2014 and June 2015 to minimise inconvenience to users.

General Support

In 2014 MASSIVE continued to provide significant help and support to users, answering over 900 help enquiries ranging from software installation requests to challenging computational problems (see Figure opposite).

MASSIVE support requests from 2010 to 2014



In 2014, the MASSIVE team answered over 900 support requests. This figure reflects the increased usage of the facility as more users rely on the instrument data processing workflows and MASSIVE Desktop environment.

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

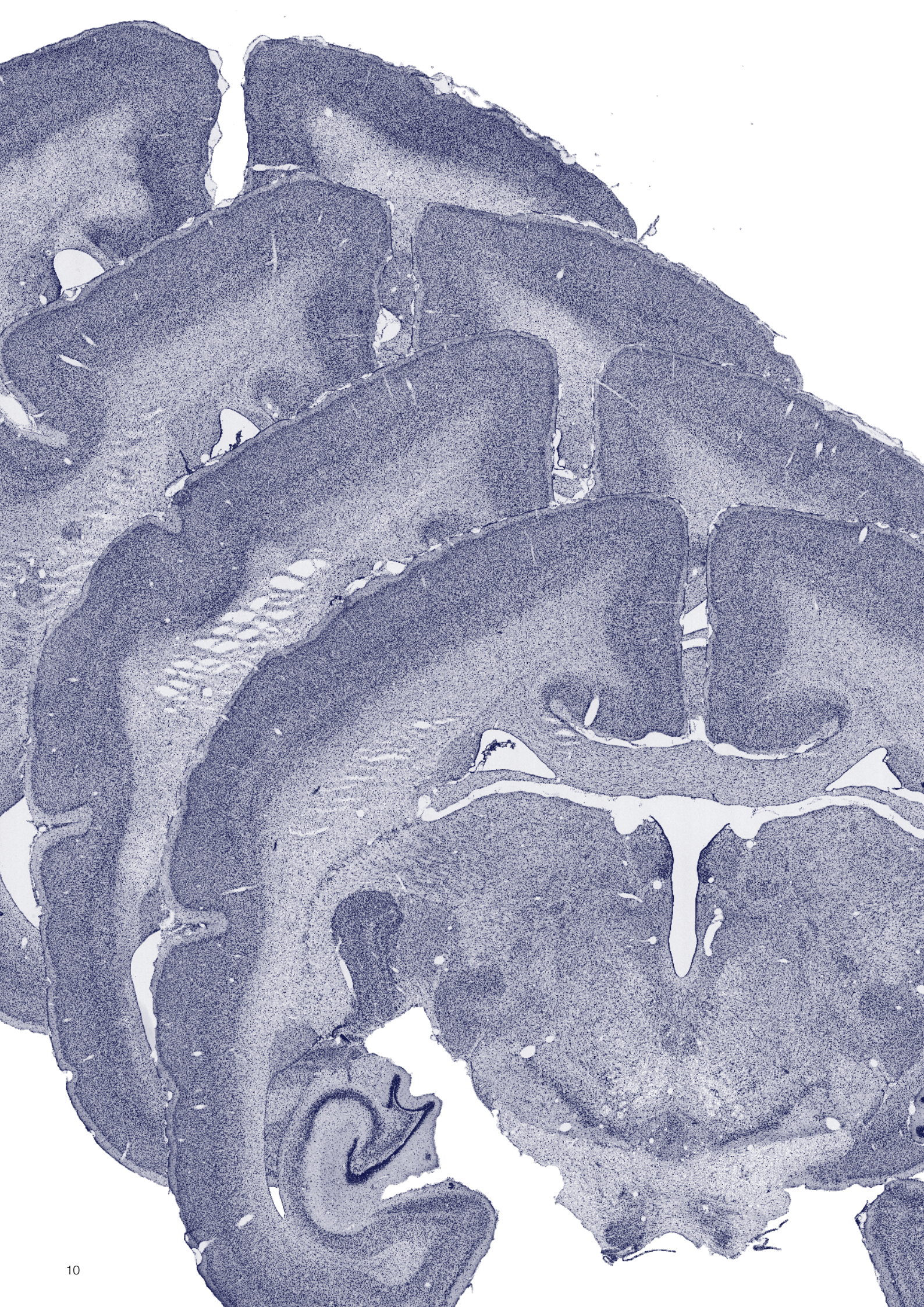
118 nodes (1720 CPU-cores total) in four configurations:

1. 32 with 12 cores per node running at 2.66GHz
   - > 48 GB 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)
   - > 192 GB 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
   - > 64 GB RAM per node
4. 20 nodes with 16 cores per node running at 2.66GHz
   - > 128 GB RAM per node
   - > 4x QDR Infiniband Interconnect
   - > 250TB + 95 TB of fast access parallel file system

CVL at 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
   - > 37 GB RAM per node
2. 4 nodes with 20 cores per node
   - > nVidia K2
   - > 75 GB RAM per node
3. 2 nodes with 64 cores per node
   - > 234 GB RAM per node
4. 15 nodes with 1 core per node
   - > 4 GB RAM
5. 6 nodes with 16 cores per node
   - > 64 GB RAM per node



/06

Outcomes of the MASSIVE Project: 2011 to 2014

In July 2014, the MASSIVE partners commenced a new program of work, called MASSIVE3, under partner funding. MASSIVE3 follows on directly from the combined MASSIVE1 and MASSIVE2 programs.

Highlights of the MASSIVE project from 2011 to 2014:

> MASSIVE supported a large cohort of researchers across a wide variety of research projects:

- Through direct access, MASSIVE provided computing and data processing services to **270** projects through partner and merit-based access. In total, it supported **612** individual user accounts.
- Through instrument integration work and workflows at the Australian Synchrotron, MASSIVE has underpinned **446** beamtime allocations for more than **791** investigators from **94** Australian and international research institutions and industry.

> MASSIVE has developed a unique Australian capability that supports an increasing number of researchers with the need to generate and process instrument data:

- The facility runs an instrument integration program to help in the movement of data to an HPC environment and provide in-experiment data processing. This capability is best demonstrated at the IMBL where fast CT reconstruction and visualisation is a fundamental part of the experiment workflow.
- The MASSIVE Desktop provides an easy way for researchers to begin using HPC. It has become an essential tool for scientists working with large datasets, including large images and other types of instrument data. Over **300** researchers have used the MASSIVE Desktop and more than **150** of them remain active users.

> MASSIVE has had a strong role in the development of eResearch software infrastructure. In particular, MASSIVE led the NeCTAR CVL, which has developed software infrastructure used by over **450** researchers. Other software projects, including the NeCTAR Australian Synchrotron Tools project, have significantly increased the capability offered on MASSIVE. The CVL represents a strategic collaboration between Monash University, University of Sydney, Australian National University, University of Queensland, National Imaging Facility, Australian Microscopy and Microanalysis Research Facility, Australian Synchrotron and ANSTO, with contributions from the CVL partners of over $3.2M.

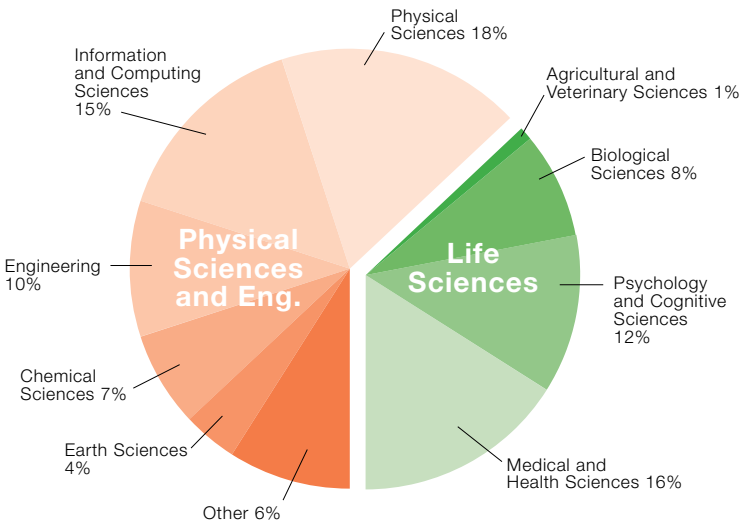
> The MASSIVE partners, Monash University, CSIRO, Australian Synchrotron and VPAC, have built a strong collaboration, which has received $5.6M of contributions plus significant in-kind contributions totalling over $8M.

> The MASSIVE3 project partners have committed $2.3M to the end of 2016 to continue operations. This new partnership will include new focus areas driven by the ARC Centre for Advanced Molecular Imaging, and the ARC Centre for Integrative Brain Function.

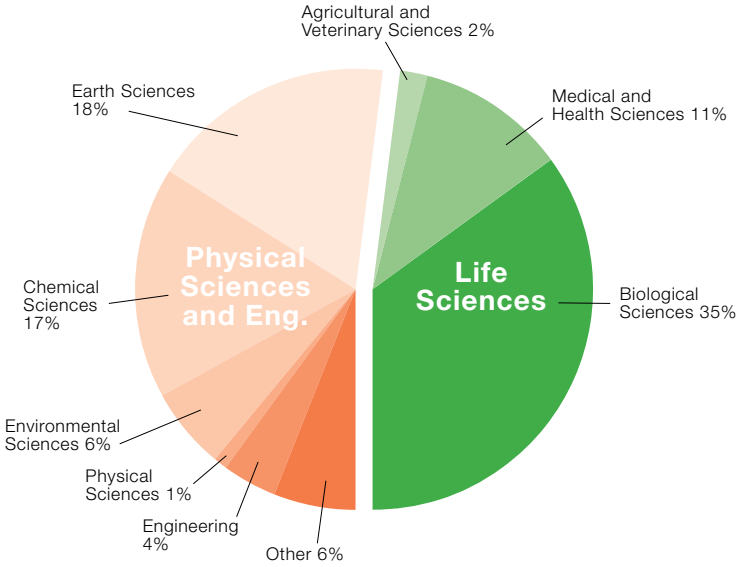
OPPOSITE: Professor Marcello Rosa (Monash University) and colleagues from the Wójcik Lab (Nencki Institute, Poland) are using MASSIVE to process and reconstruct high-resolution marmoset brain images in order to learn about the way the brain processes vision. High-resolution scans of marmoset brain tissue are used to reconstruct 3D volumes on MASSIVE. These reconstructed volumes are registered against a brain atlas so that data from many different cases can be compared.

Outcomes of the Massive Project: 2011 to 2014

Research undertaken using MASSIVE through direct access

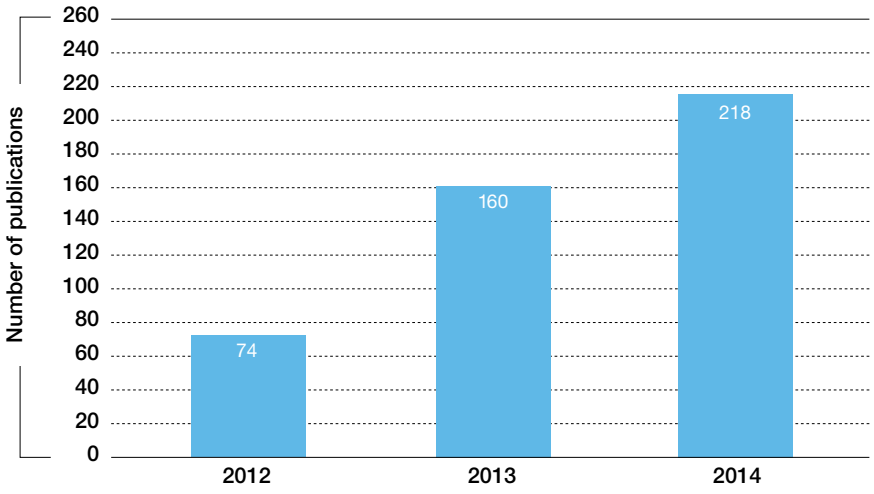


Research undertaken using massive through beamline access at Australian Synchrotron



User publications accepted or published, as reported in Project Leader Reports

MASSIVE underpins a wide range of research across the partners and nationally. This graph shows the aggregate publications in 2012, 2013 and 2014 across MASSIVE projects, as reported in annual Project Leader Reports.



MASSIVE through the National Computational Merit Allocation Committee

36 projects have been allocated on MASSIVE through the NCMAS

15 Australian institutions have accessed MASSIVE through the NCMAS

6m CPU-core hours have been allocated across a wide range of areas, including chemistry, astrophysics, engineering, physics and a wide range of the life sciences, including neurosciences, proteomics, anatomy, lung research and anatomy.

4x Requests for time on MASSIVE through the NCMAS have consistently been far more than what is available. For example, in November 2014 researchers requested approximately 4 times the total national share.

MASSIVE at the Australian Synchrotron

5 beamlines use MASSIVE to process user data during or after data capture

94 institutions have used MASSIVE through beamline allocations

28 research projects (non-beamline) have been allocated time on MASSIVE.

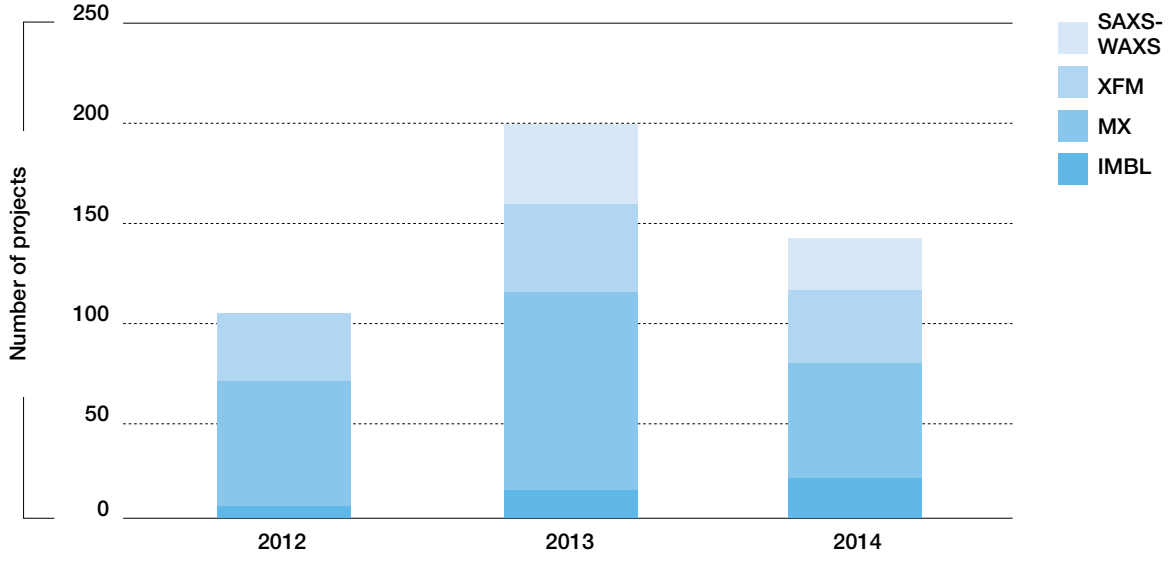
791 individual investigators across 446 beamline allocations have benefited from access to MASSIVE.

MASSIVE use at Australian Synchrotron is the result of a number of projects to integrate beamlines including the NeCTAR Australian Synchrotron Tools project, and CSIRO investment in X-TRACT CT reconstruction software.

The biggest users of MASSIVE through Australian Synchrotron were (beamtime projects allocated):

Monash Uni	71
CSIRO	34
Uni Queensland	33
Australian Synchrotron	29
Uni Canterbury	23
Uni Melbourne	22
St Vincent's Institute	15
Other Institutions	219

Australian Synchrotron Beamtime allocations underpinned by MASSIVE 2012 to 2014.



Research Stories

The Imaging and Medical Beamline

Combining the capabilities of MASSIVE, the Australian Synchrotron's Imaging and Medical Beamline (IMBL), and CSIRO's X-TRACT has created a CT Reconstruction Service able to create unique 3D imaging of live beings in intricate detail and in near real-time.

This harnessing of computing power for sophisticated imaging techniques is helping create 3D, high resolution imaging of otherwise invisible detail. The increased speed and accuracy is helping researchers see greater possibilities to answer harder questions, faster. An added benefit of the speed with which MASSIVE can process terabytes of information is the opportunity afforded researchers to make the most of limited beamline access at the Synchrotron.

The project is been a collaboration between Australian Synchrotron, Monash University and CSIRO.

Uncovering Ancient Fossils At IMBL

Associate Professor Kate Trinajstic of Curtin University, Western Australia is a palaeontologist with a strong research interest in the evolution of those parts of our skeleton that make us vertebrates.

In particular, she studies fossils of the ancient armoured fish collectively known as placoderms, the first vertebrates to possess a jaw. The subjects of her current research swam in the oceans about 380 million years ago in the Devonian Period.

The appearance of jaws signalled the development of a number of other defining features, including paired pectoral and pelvic fins, a neck and complex musculature.

Kate's focus is on the appearance of secondary sexual characteristics that signal the emergence of male and female forms of a species, known technically as 'sexual dimorphism'.

Her interest in ancient species is long-standing. As an undergraduate student Kate worked as a volunteer at the Western Australian Museum where she met one of Australia's leading palaeontologists, Professor John Long, now at Flinders University, with whom she collaborates today.

With paired fins, came the first fish penises, or male 'claspers, which were also paired elements. Placoderm claspers are the first external structures known to function in vertebrates as specialised reproductive organs, so they play a significant part in the evolution of vertebrates.

Kate and her colleagues have been able to achieve what was previously impossible by combining the most advanced imaging facility in Australia, the Australian Synchrotron, with the computing capability and know-how of the MASSIVE cluster.

Until recently, research into fossils was hampered by the methods needed to prepare samples, which involved freeing the fossil from its rocky surrounds by treatment with acid. Unfortunately, the treatment removed not only the rock, but also any soft tissue, such as muscle or cartilage, that held together bony features including the vertebrae of the spinal column. As a result, acid treatment destroyed the integrity of the sample.

A modified preservation technique involved embedding one side of the fossil-containing rock in resin to keep the structure intact, and treating half of the sample with acid. This too had limitations in that it converted a 3-D sample to the flat 2-D face of the resin.

"I visit the synchrotron with my fossils and do the scan, then a nice image appears on my computer."
Associate Professor
Kate Trinajstic

ABOVE: Resin embedded placoderm (armoured fish) tail from the Gogo Formation of Western Australia. The anatomy of the tail on the resin embedded side could not be clearly determined and synchrotron scanning revealed the hidden parts of the pelvis.

And as Kate found “the most important bit that you wanted to see was in the resin”.

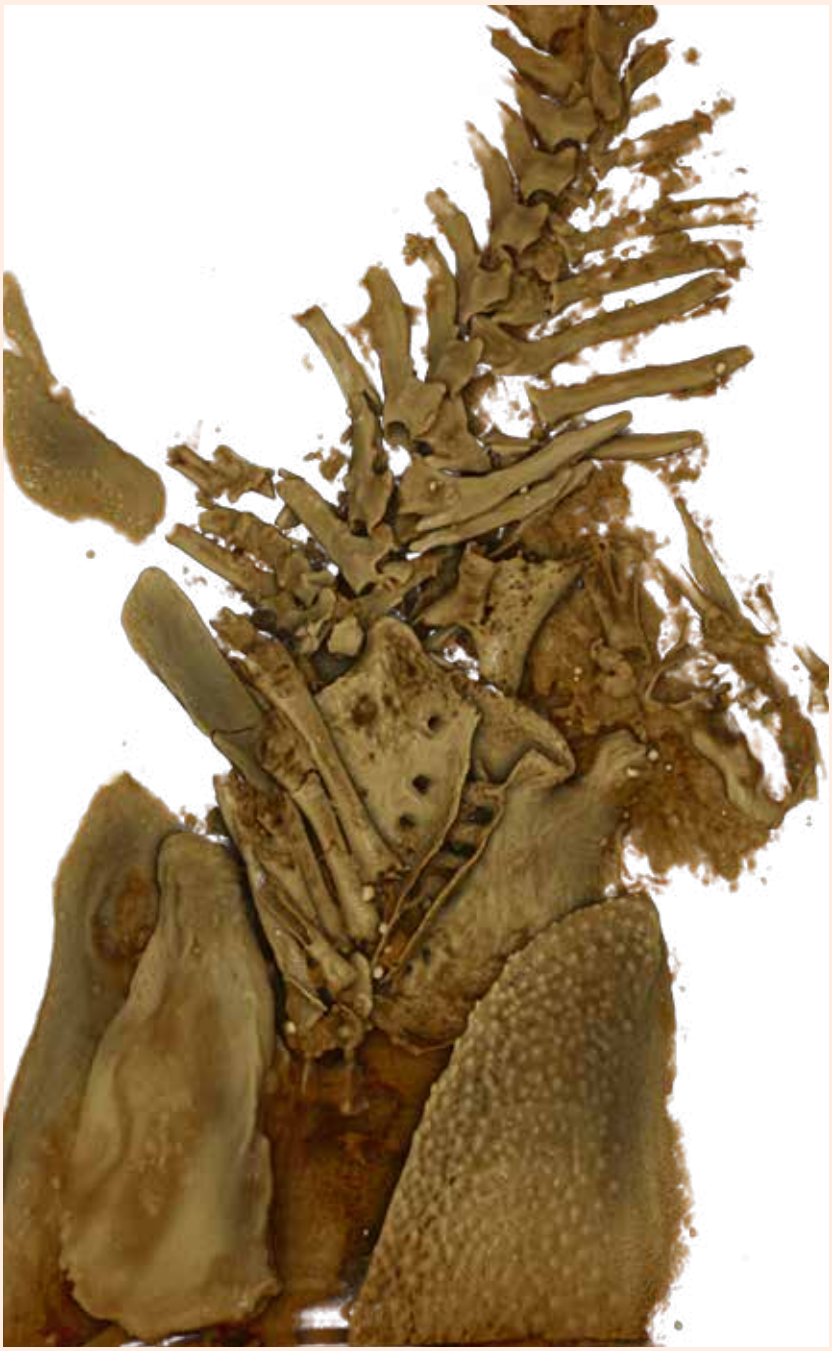
The advances in imaging provided by the synchrotron enable researchers to look into the resin, to re-create the 3-D structure. The synchrotron also made possible the imaging of preserved soft tissue, which, according to Kate, “is incredibly unusual” in the world of fossil research.

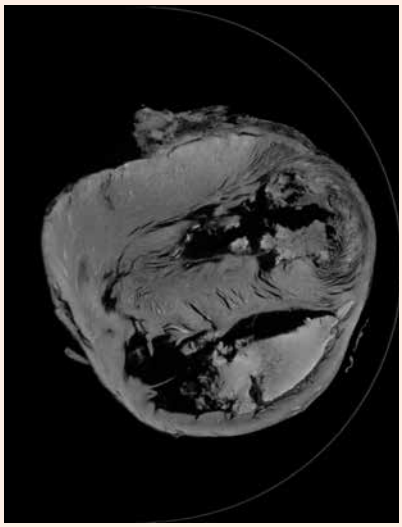
Kate has spent two scanning sessions using the synchrotron’s imaging beamline on fossil samples collected from the Gogo Formation in the Kimberley, where she and others travel to “go bush and break a lot of rocks”.

The Gogo site is special, as it preserves an ancient reef ecosystem, providing simultaneously both the context of the environment and the ecology of the time. It is essentially a snapshot of Australia’s first ‘Great Barrier Reef’.

Kate’s interaction with the MASSIVE cluster and the expertise of its personnel has been vital to the processing and reconstructing of the huge amounts of imaging data behind her discoveries.

It enabled her and her colleagues to discover that, contrary to current thoughts on the subject, the bony claspers of the placoderms are distinct in evolutionary terms from the cartilaginous claspers of modern sharks. The former paired appendages are separate from the pelvic fin, whereas the latter are a modified part of the fins, indicating that paired appendages evolved independently within the sharks and placoderms.





Vascular Imaging

X-ray imaging is useful for viewing whole organs or tissues where their composition is diverse, such as bone and muscle. However, soft tissues, such as muscles and organs tend to have much the same proportion of elements such as hydrogen, carbon, oxygen, sulphur and chlorine. The similarity in composition makes it difficult to use X-ray imaging to obtain useful information about tissues and pathological changes.

Light microscopy overcomes the problem by the use of staining techniques to differentiate tissue and cell types for histological and other analysis. However, light microscopy does not provide useful images of thick samples. The samples must be cut into slices thinner than a human hair, which destroys the original sample and creates the need to view and analyse lots of sections.

However, it is possible to use stains that enhance soft tissue contrasts when viewed via X-ray imaging in a process called microcomputed tomography, or microCT imaging. MicroCT-imaging can be used on intact organs.

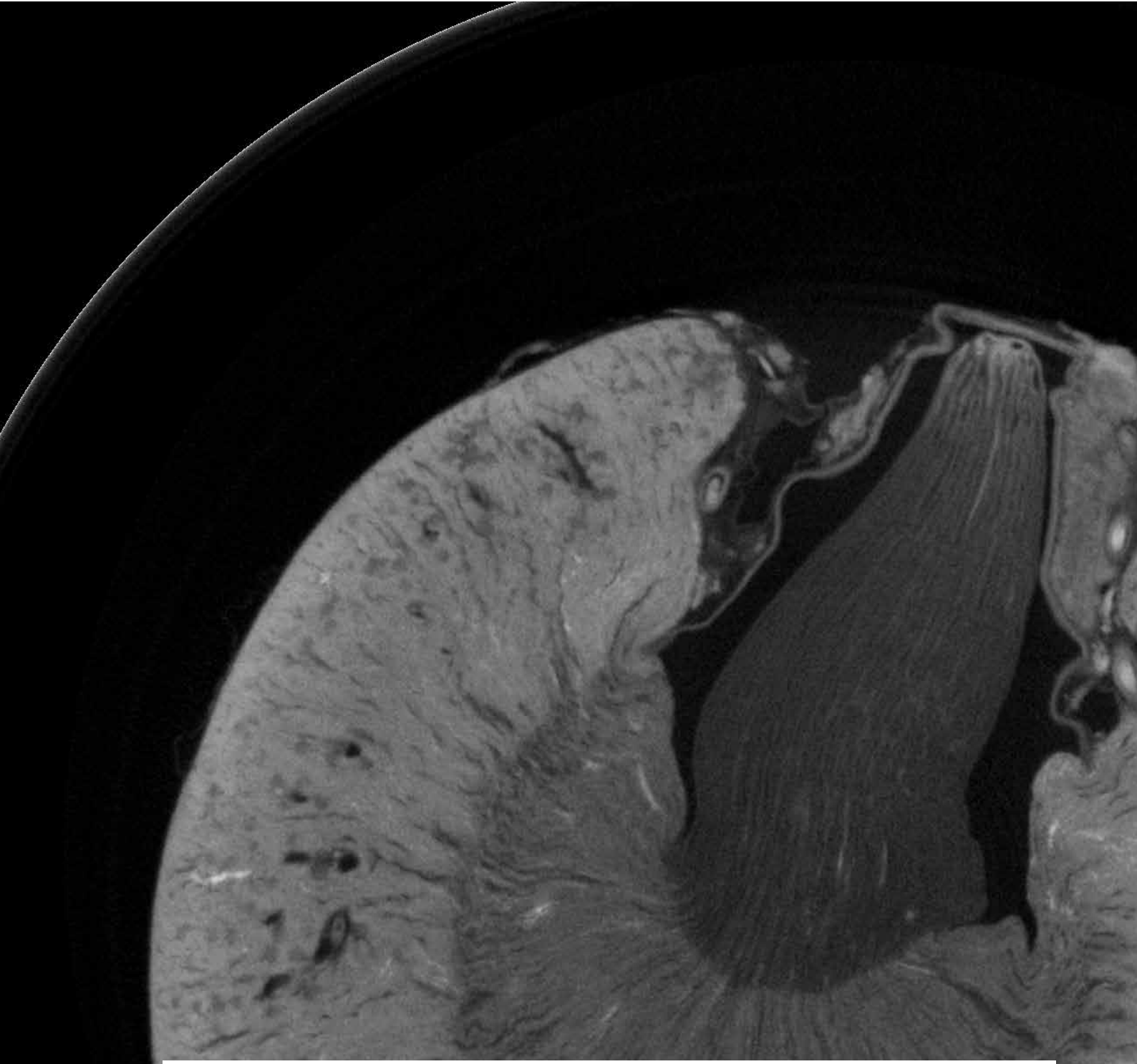
Dr James Pearson from Monash University and Dr Anton Maksimenko from Australian Synchrotron, are using an iodine-potassium idodide stain, also known as Lupol's solution, to visualise whole kidneys and hearts and create very high resolution micro-CT data sets.

Using the Australian Synchrotron Imaging and Medical Beamline and MASSIVE, Dr Pearson has been able to capture, process and visualise detailed 3D images of the kidney. The images include the extensive blood vessel network and the interwoven bulbous nephrons (filtration units of the kidney), and the long tubules that deliver filtered waste to the inner core of the kidney and ultimately to the bladder. The contrast of the images is so clear that it is possible to differentiate regions of the kidney and anatomical features such as the thickness of vessel walls. In 3D renderings selected components or regions of kidney can be viewed by virtual reslicing of the image data set in any desired direction.

This same technique is also being used to study models of heart disease. The images clearly show the region of heart attack and acute inflammation as a darker region with more disruption of muscle fibres than the healthy heart tissue. Furthermore, the 3D images of the heart give an estimate of the volume of the diseased heart tissue and the changes in blood vessel supply across the heart. Staining with Lupol's solution offers new possibilities for analysing organs or tissues before they are finally cut into sections for detailed microscopy studies.

The images clearly show the region of heart attack and acute inflammation as a darker region with more disruption of muscle fibres than the healthy heart tissue. Furthermore, the 3D images of the heart give an estimate of the volume of the diseased heart tissue and the changes in blood vessel supply across the heart.

CAPTION: microCT imaging of the heart (TOP) and kidney (OPPOSITE) using techniques developed by Dr James Pearson and colleagues at the Imaging and Medical Beamline and processed on MASSIVE.



CT Reconstruction at The Australian Synchrotron Imaging and Medical Beamline (IMBL)

The capabilities of MASSIVE, the IMBL and CSIRO's X-TRACT software have been combined to form a CT reconstruction service that can handle 3D imaging of samples such as biological systems, geological samples and other physical objects.

This harnessing of computing power to sophisticated imaging techniques is helping create 3D, high resolution images of details that would otherwise be invisible.

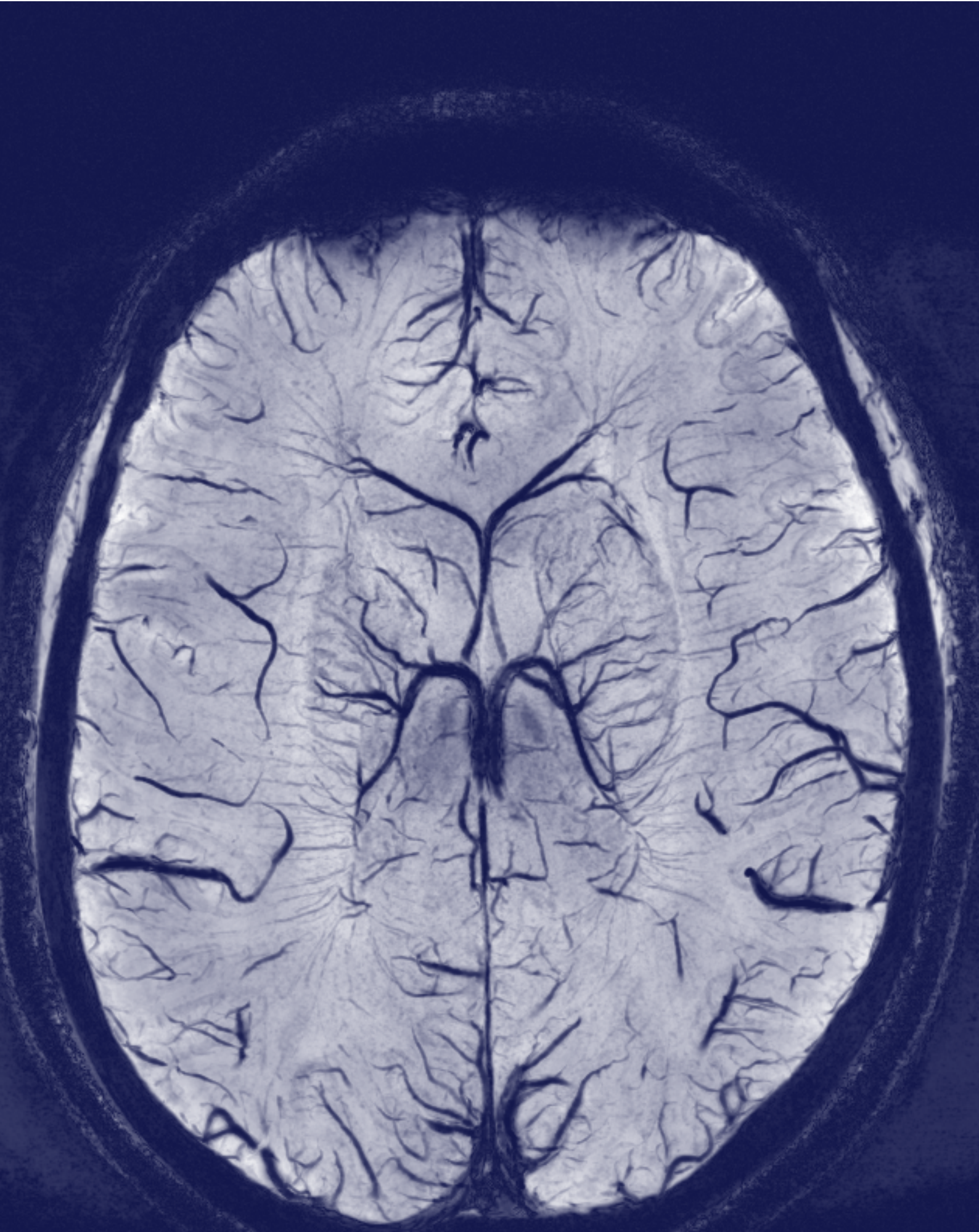
The increased speed and accuracy is helping researchers to ask harder questions and receive answers more quickly. The quicker turnaround means that researchers can make more effective use of limited beamline access at the synchrotron.

Future Steps

X-TRACT is an application for advanced X-ray imaging. It has been under development at CSIRO for over a decade and is the specialised software engine for CT reconstruction at IMBL.

Recently, several core modules have been ported from Windows to Linux and deployed in MASSIVE's desktop environment, giving synchrotron users an integrated HPC platform for image processing, including near real-time CT reconstruction and visualisation capabilities for large synchrotron datasets.

Integration between Australian Synchrotron and MASSIVE identity systems will be trialled in early 2015. Such integration will provide AS users with a MASSIVE project and user account from the moment they are allocated time on the beamline to months after their visit, giving them the opportunity to process and visualise their data.



Dr Amanda Ng at the Melbourne Brain Centre Imaging Unit is using MASSIVE to process brain data such as this 7 Tesla MRI susceptibility weighted image which shows minute venous vessels not visible at lower field strengths. Higher field strengths in MRI enhance the effects of magnetic susceptibility on image contrast, improving iron imaging methods such as susceptibility weighted imaging, T2 mapping and quantitative susceptibility mapping.*

/07

Characterisation Virtual Laboratory

In 2014, Monash University (through MASSIVE) and project partners, completed development of the NeCTAR-funded Characterisation Virtual Laboratory (CVL), a 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.

The CVL is a collaboration between Monash University, Australian Microscopy & Microanalysis Research Facility (AMMRF), Australian Nuclear Science and Technology Organisation (ANSTO), Australian Synchrotron, National Imaging Facility (NIF), Australian National University, the University of Sydney, and the University of Queensland.

The partners joined together around the CVL project with three major goals:

1. To integrate Australia's imaging equipment with specialised HPC capabilities provided by MASSIVE and National Computational Infrastructure (NCI) and with data collections provided by Research Data Storage Infrastructure (RDSI) nodes.

More than 450 registered researchers have used and benefited from the technology developed by the CVL project, providing them with an easier mechanism to capture instrument data and process that data on centralised cloud and HPC infrastructure, including MASSIVE and NCI.

2. To provide scientists with a common cloud-based environment for analysis and collaboration.

The CVL has been deployed across clouds at the University of Melbourne, Monash University, and QCIF. CVL technology has been used to provide easier access to HPC facilities at MASSIVE, NCI and Central Queensland University.

3. To produce four exemplar platforms, called Workbenches, for multi-modal or large-scale imaging in Neuroimaging, Structural Biology, Energy Materials (X-ray), and Energy Materials (Atom Probe).

The CVL environment now contains 103 tools for specialised data analysis and visualisation in Workbenches. Over 20 imaging instruments have been integrated so that data automatically flows into the cloud for management and analysis.

In addition, a number of specialised workflows have been developed and integrated, including atom probe data processing using galaxy, and automatic brain MRI and histology registration.

The newly developed infrastructure is also having an impact beyond the four workbenches. For example, HPC facilities across Australia, including facilities at Central Queenland University, the Brain and Mind Research Institute at University of Sydney and the Pawsey Centre, use software developed by the CVL to help a wider range of researchers access imaging and visualisation services.

More than 450 registered researchers have used and benefited from the technology developed by the CVL project

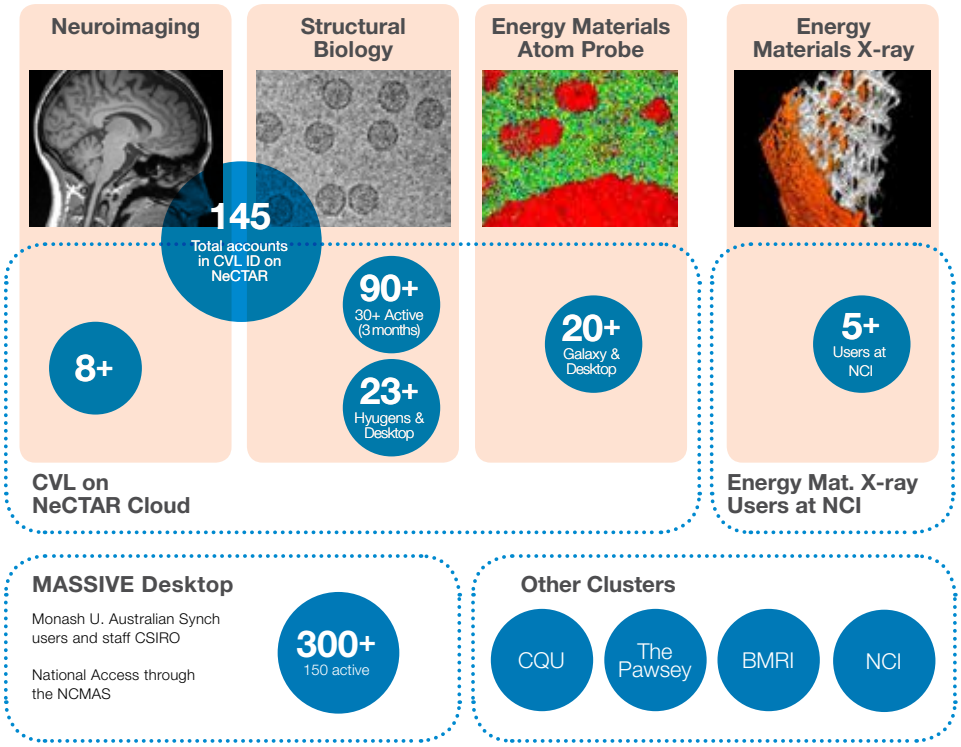
The technology developed under the CVL provides simple access to HPC resources by newcomers and inexperienced HPC users.

A range of tools developed as part of the CVL are now a core part of the MASSIVE service offering. Over 300 MASSIVE users have accessed the MASSIVE desktop environment, which has been significantly improved under the CVL program. Of the 300, over 60% have used this environment more than 10 times.

The CVL has provided MASSIVE users with a more usable environment to interactively view and analyse experimental data, or visualise simulated results.

Usage of CVL-developed technology and environments.

Technology developed as part of the CVL has been deployed on the NeCTAR cloud and other facilities, including MASSIVE, and used by a wide selection of researchers. The figure enumerates the number of researchers using CVL technology across Australia.



Recent advances in microscopy have enabled molecular processes to be seen in much greater detail, but they have also created challenges for scientists in how to work with such large amounts of data.

Structural Biology

The Characterisation Virtual Laboratory (CVL), funded through NeCTAR and project partners, provides a world-leading data management and workflow environment for scientists who use advanced imaging techniques.

Professor James Whisstock and the other researchers at the Whisstock Laboratory at Monash University study immune defence and blood coagulation, and how these processes relate to cancer, inflammatory diseases, and clotting related disorders.

They use X-ray crystallography and electron microscopy techniques to create images and molecular movies that allow them to watch these processes occurring.

"As we age almost all of us will be impacted by an aberrant effect of our immune system on our own bodies," says Professor Whisstock.

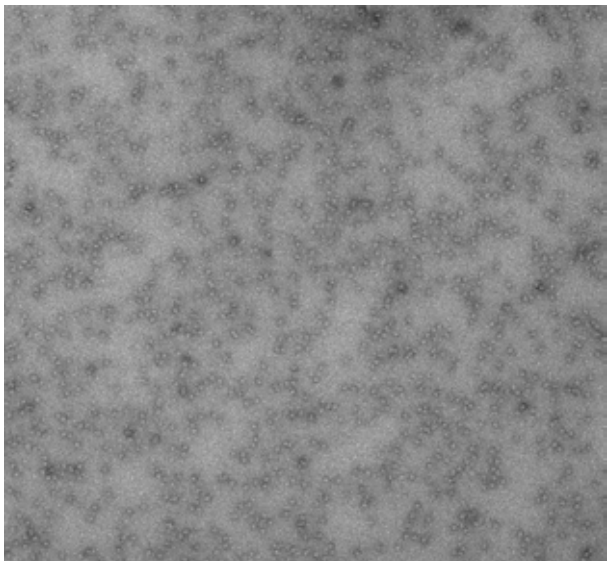
"If we're going to change the course of a particular molecular event, whether it be an aberrant immune response, or an out of control signalling response that occurs in cancer, we need to understand the mechanism. And a mechanism is never more clear than when you see it in glorious atomic detail."

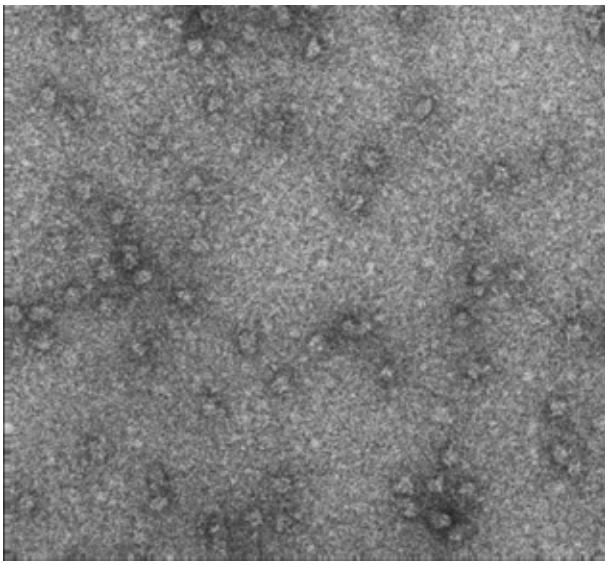
Recent advances in microscopy have enabled molecular processes to be seen in much greater detail, but they have also created challenges for scientists in how to work with such large amounts of data.

"To give you an example, a high-end electron microscope running in molecular movie mode might produce two terabytes of data per day, which may need to be processed while the instrument is running," Professor Whisstock says.

"So the workflow associated with imaging has moved from being the type of thing you could do manually with a laptop, to being a flood of information and a flood of data processing requirements.

"There are simple aspects to this, such as getting the data away from the microscope, backing it up, and making it available to the right people at the right time. And there are sophisticated aspects to it, such as applying the right software to the data in the right way at the right time to maximise both the productivity of the scientist and the productivity of the instrument.





"Because with an instrument that costs several thousand dollars a day to run, you don't want to be wasting time."

These challenges are faced not only by the Whisstock Laboratory but also by every researcher using imaging techniques—broadly known as characterisation—whether for structural biology, neuroimaging, or energy materials.

When the call for the NeCTAR virtual laboratories was announced, this community of scientists from major imaging facilities came together on a proposal for a Characterisation Virtual Laboratory to provide better data management and workflow for advanced imaging instruments.

As part of the Characterisation Virtual Laboratory (CVL) project, key instruments were integrated so that data is captured directly from the imaging instrument and placed in a managed environment, where it can be processed using software tools in the CVL and using either the NeCTAR Research Cloud or a high performance computing facility.

"It's like a scientific desktop," says Dr Wojtek Goscinski, Coordinator of the Multi-modal Australian ScienceS Imaging and Visualisation Environment (MASSIVE) at the Monash e-Research Centre. Dr Goscinski's team developed and operates the CVL.

"By capturing the data from the very point of generation, the workflow is set up from the start, and by the time the researcher gets back to their office their data is already there. It's already being managed, and it's in an environment with tools for doing their first set of processing."

Professor Whisstock says the CVL will be an essential component of the new Clive and Vera Ramaciotti Centre for Structural Cryo-Electron Microscopy, recently launched at Monash University.

"This will be the most sophisticated electron microscopy unit Australia has, and I hope it will be one of the lead microscopy units in the world.

"We've just finished an international, three-year program to prepare for running the facility. One of the things we noticed is that around the world ad hoc solutions have grown up around data management.

"We consulted widely in developing the computational aspect of the microscopy centre, and had many debates about many items. One of the things we are really pleased about is that researchers who have seen and worked with the system have all been impressed with the CVL, with Wojtek, and with the strategy, and they recognised the efforts that had gone into the process.

"In a sense that is ultimate peer review, if you like. International leaders in this field recognise the importance of this program and want to use it."

Dr Goscinski is now working to integrate more instruments with the CVL.

"Every lab that does microscopy imaging—and there are a lot of them across Australia—every one of those labs has a big, high-end PC sitting in the corner with a bunch of terabyte drives hanging off it, and that is their solution.

"Now they're approaching the point where that PC won't handle the workload anymore. It's also very wasteful. We can provide them instead with a shared resource, a managed environment, to replace that PC.

"As part of the CVL project we integrated just under 20 microscopes here at Monash University. But we very quickly realised that we can't scale any further because we don't have enough eResearch professionals to go in and configure the PCs that run those microscopes.

"So our next NeCTAR project is to develop some tools to put instrument integration into the hands of the instrument facility fellow—the person who runs the MRI machine or the microscope.

"We want to provide them with an easy way to connect their microscope to the CVL and central facilities. That's really promising to me because I think we can scale it to hundreds of instruments rather than tens of instruments."

SOURCE: WWW.NECTAR.ORG.AU/RESEARCHERS CHARACTERISATION-VIRTUAL-LABORATORY
AUTHOR: PATRICIA MCMILLAN

ABOVE: Examples of data generated by the FEI Titan Krios microscope installed as the flagship instrument at the Clive and Vera Ramaciotti Centre for Structural Cryo-Electron Microscopy. The image is a typical micrograph (2x2k) showing RNA plymerase II. The images illustrate the noisy nature of the data generated which requires a significant amount of data processing to resolve structures and gain insight.

Credit: Associate Professor Dominika Elmlund

New Partnerships

ARC Centre of Excellence for Integrative Brain Function

The ARC Centre of Excellence for Integrative Brain Function (CIBF) will address one of the greatest scientific challenges of the 21st century – understanding how the brain interacts with the world. CIBF will be a partner in the international neuroscience effort to achieve this goal.

The centre is a collaboration between researchers at Monash University, The University of Queensland, The University of Melbourne, The University of Sydney, Australian National University and The University of New South Wales. CIBF investigators are also based at Queensland Institute of Medical Research and 11 other partnering institutions in Europe, Japan and the US.

CIBF will investigate complex brain functions including attention, predictive coding and decision making that require the integration of information processing by many brain areas. Through understanding these complex functions, CIBF will gain unique insights into how the brain interacts with the world. CIBF researchers in cellular, systems and computational neuroscience, and neural engineering will actively pursue multidisciplinary approaches to investigate some of the most complex problems in neuroscience.

An essential part of CIBF is working with larger and larger datasets, created by imaging modalities such as MRI. MASSIVE is helping CIBF researchers to process, analyse and visualise their data.

Exploring the Patterns of Brain Connectivity

Professor Michael Breakspear, a psychiatrist and researcher, looks for unifying models to fit the complex neurophysiology of the brain and reveal how the brain works in time and space.

Michael's research covers wide-ranging aspects of brain function and neural connectivity networks - the so-called 'brain connectome'. Such knowledge could form the basis of a greater understanding of what can go wrong when the networks do not function properly, for example in schizophrenia, bipolar disorder, depression and dementia.

The handling and analysis of the large data sets generated by his research is 'computationally intensive', which is where MASSIVE comes in.

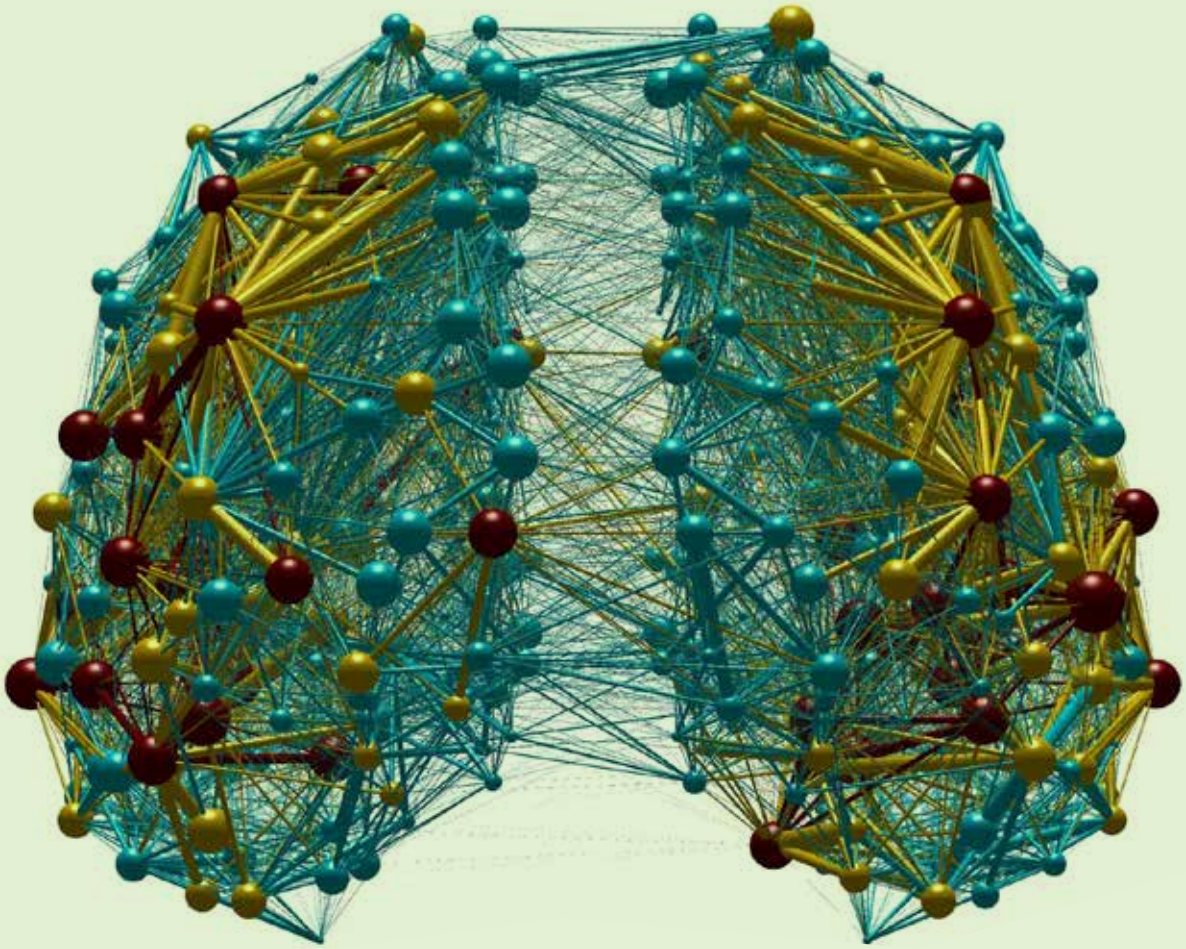
Michael's team designs brain imaging experiments capable of identifying signature patterns of connectivity across the population and how these changes might impact our 'normal' brain function. The models used take into account the relationships between brain structure, dynamics and cognitive function.

To validate some of the findings concerning the connectome, Michael and collaborators have shown by functional (f)MRI that certain areas of the brain differ between depressed and non-depressed people. They conducted fMRI on people who watched movie clips featuring that elicit emotions, for example, footage of a stand-up comedian.

The oxygen level in blood is a marker of metabolic activity and measurement of activity-related oxygen is a powerful tool in brain imaging. Functional MRI detects regions of the brain that 'light up' when they become more active due to changes in the proportion of oxygenated to deoxygenated haemoglobin in the local blood vessels. So fMRI can provide information about active neural networks.

While subjects viewed a movie, brain regions involved in higher order functions were shown by fMRI to become synchronised, allowing comparison of the brain function and connectome between different people.

Michael's finding that the connectome varied between different groups could lead to changes in diagnosis and treatment of brain disorders in the future. Importantly, such imaging could improve our understanding of the complexities of normal brain function.



Among the many interests of Michael and colleagues is the relationship between physical wellbeing and mental health and gaining knowledge of the connectome to explore that relationship.

Normally, sitting people tend to stay seated and moving people tend to keep moving, which is more efficient than randomly switching between the two.

To measure patterns of movements and associated impact on the connectome and brain function, the researchers are collecting data from an 'accelerometer' belt that people wear while going about their daily lives.

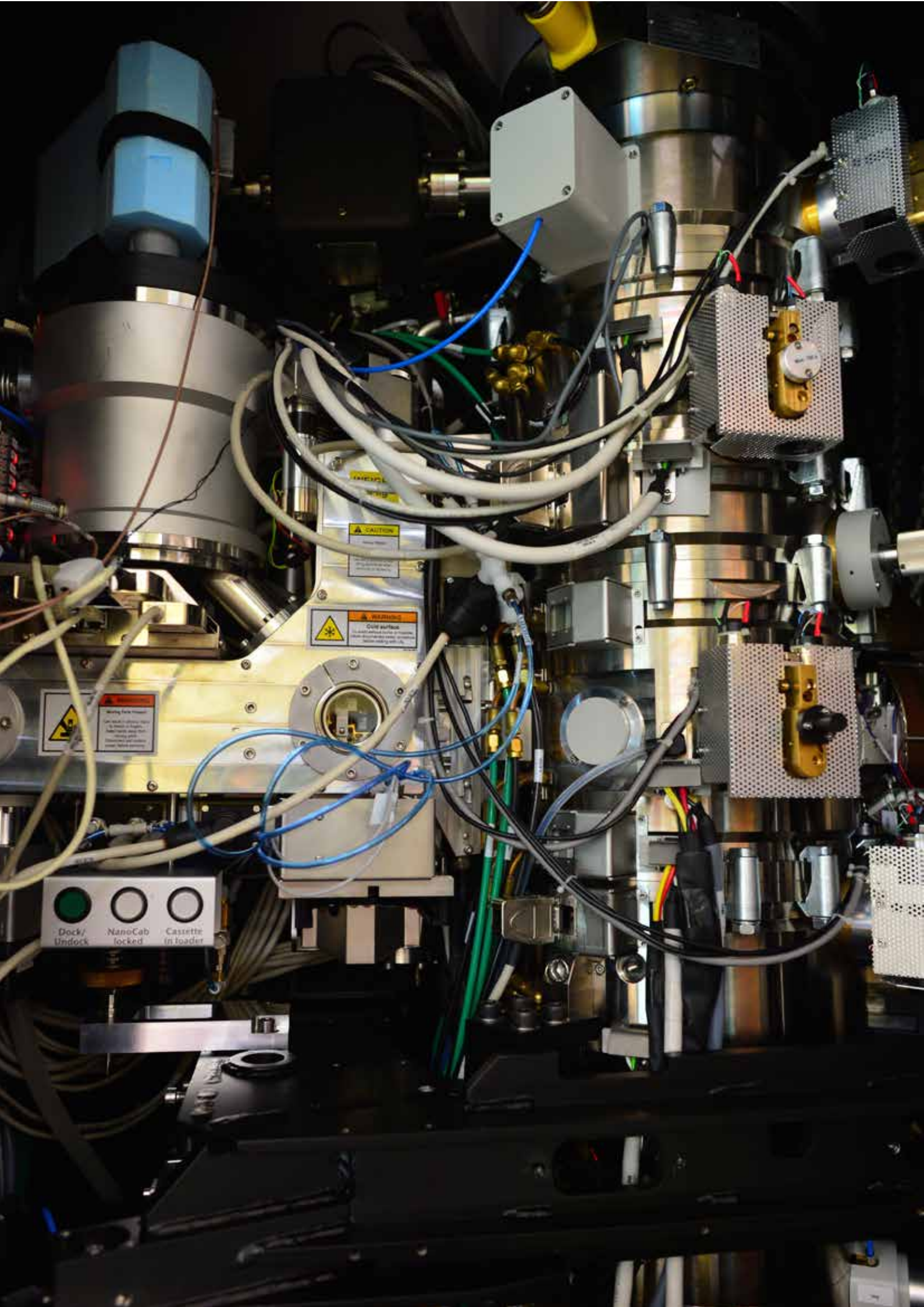
The resources and know-how of MASSIVE have been enlisted to analyse a vast amount of data against seven different models to find the best fit to the data collected from the belts.

In an unusual approach, the analyses involved applying to humans the type of approach used by physicists to study molecules, atoms and electrons.

Depending on the findings of this first study, Michael envisages adapting the design of the experiments to the use of smart phones instead of accelerometer belts and extending the study groups.

"There are parallels between our behaviour and an atom stuck in an electric field that jumps between low and high-energy states. Sitting can be viewed as the low-energy state and standing and walking represents the transition to the high-energy state".

CAPTION: Professor Michael Breakspear and his team are using MASSIVE to formulate models that take into account the relationships between brain structure, dynamics and cognitive function. van den Heuvel et al. (2011) J. Neuroscience, Harriger et al (2012) PLoS ONE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New Partnerships

ARC Centre of Excellence for Advanced Molecular Imaging

The ARC Centre of Excellence for Advanced Molecular Imaging (Imaging CoE) is a $39 million Centre of Excellence based at Monash University, funded by the Australian Research Council and collaborating and partner organisations including the Universities of Melbourne, New South Wales and Queensland, La Trobe University, the Australian Synchrotron, the Australian Nuclear Science and Technology Organisation, University of Warwick, UK, the Deutsches Elektronen Synchrotron, and commercial partners Leica and Carl Zeiss.

The Centre's aim is to develop and use innovative microscopy and imaging techniques to characterise the key interactions interactions that underpin immunity. To achieve this aim, the centre bring together expertise across physics, chemistry and biology and will utilise a wide range of imaging techniques that span from atomic imaging using X-ray diffraction to cellular and whole animal imaging using confocal and fluorescence imaging, all focused on furthering our understanding of how the immune system functions and sometimes malfunctions.

Australia's Most Powerful Biological Microscope

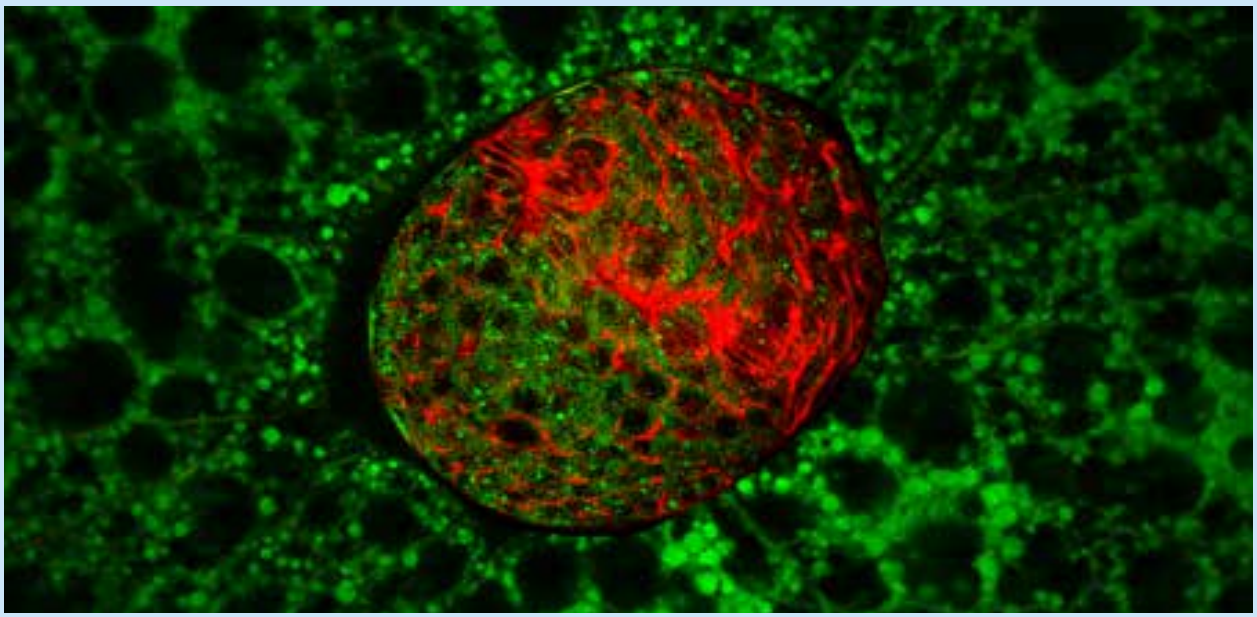
Life and health ultimately depend on the interactions of large biological molecules– proteins, lipids, carbohydrates and others. How those interactions are initiated and proceed depends on the 3D shapes and structures of the participating molecules.

In February 2015, Monash University unveiled the most powerful biological microscope in Australia. The microscope is capable of providing detailed images of molecular interactions. The $5 million FEI Titan Krios cryo-electron microscope will transform the way we view the human immune system, and enable Australian researchers to work towards better treatment for diseases of the immune system, which include cancer, malaria, diabetes, rheumatism and multiple sclerosis.

But the capacity of the new microscope to do its job, which is to provide extremely detailed images, is heavily dependent on how the associated huge amounts of data are processed, stored and analysed. The accurate, reliable handling of all the data hinges on MASSIVE and its integration with the new machine.

The $5 million FEI Titan Krios cryo-electron microscope will transform the way we view the human immune system, and enable Australian researchers to work towards better treatment for diseases of the immune system, which include cancer, malaria, diabetes, rheumatism and multiple sclerosis.

OPPOSITE: The inner workings of the FEI Krios electron microscope at the Clive and Vera Ramaciotti Centre for Structural Cryo-Electron Microscopy that is being launched in early 2015. Image: Philip Chan.



Along with the staff of MASSIVE, key players in this partnership will include A/Prof Hans Elmlund, director of the Clive and Vera Ramaciotti Centre for Structural Cryo Electron Microscopy, of which the Titan Krios is the centrepiece, and his wife A/Prof Dominika Elmlund. Both are members of the University's Department of Biochemistry and Molecular Biology and associate investigators of the Imaging CoE.

Dominika and Hans met while studying for their PhDs at the Royal Institute of Technology in Stockholm. They both undertook post-doctoral fellowships in the laboratory of Nobel Laureate Roger Kornberg at Stanford University in California where they developed their research expertise around cryo-EM technology—Hans on the computing side and Dominika in structural biology and the preparation of samples.

"Getting this data processing pipeline up requires new algorithms which take full advantage of MASSIVE", Hans said. *"We need to develop a lot of new code."*

Those algorithms will also be fine-tuned for each experiment. For instance, different kinds of data need to be collected to construct images of large, inflexible sub-cellular bodies such as ribosomes, as opposed to small highly flexible structures such as membrane receptors.

The relationship between the cryo-EM and MASSIVE extends to providing temporary increases in computing power to handle data-processing for specific jobs, and determining and arranging the storage needed to archive the enormous amount of data the cryo-EM produces.

"We are talking about petabytes of data—thousands of terabytes," Dominika explained.

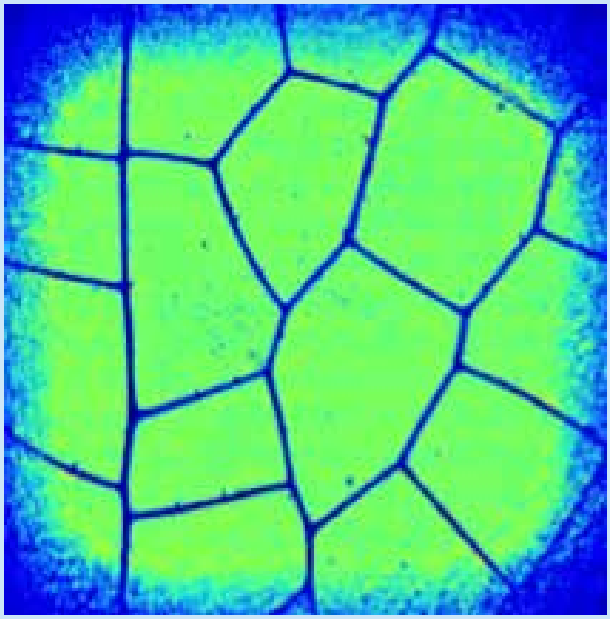
And to support its community of cryo-EM users, most of whom are life scientists rather than computer experts, MASSIVE has *"the most fancy remote desktop environment we've ever seen"* according to the Elmlunds.

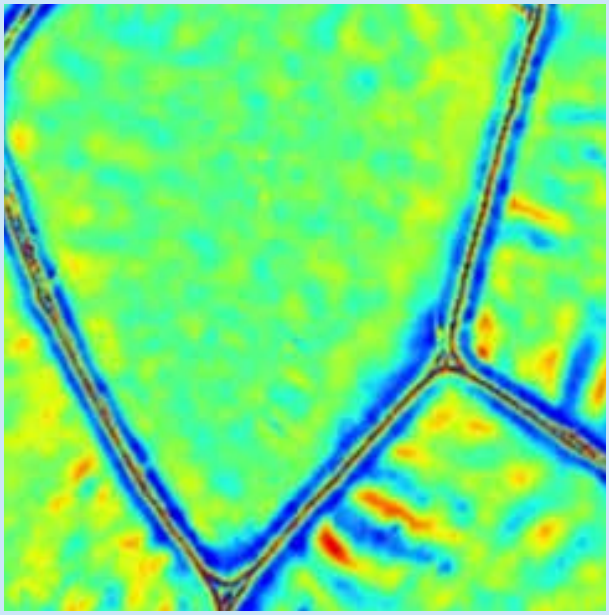
The major goal of the partnership between MASSIVE and the cryo-EM is to make the data-processing step easier and more efficient. That should result in users receiving their results—three-dimensional images of biomolecules—much more quickly, making them more competitive in the publication stakes. The aim is to decrease processing time from months to days.

MASSIVE is working with the Ramaciotti Centre to make processing and interpreting cryo-EM data as easy as possible. In future, when a researcher leaves the cryo-EM facility after capturing an image, the data should already be streaming to MASSIVE for processing, so that by the time they get back to their office, they are already in a position to start the first set of processing routines.

The major goal of the partnership between MASSIVE and the cryo-EM is to make the data-processing step easier and more efficient. That should result in users receiving their results—three-dimensional images of biomolecules—much more quickly, making them more competitive in the publication stakes.

ABOVE: A fluorescence image of Drosophila (fruit fly) fat body. Researchers in the Imaging CoE are using drosophila models to discover new roles for perforin-like immune effectors in developmental and neuro-biology.





Using MASSIVE to Develop Atomic Imaging Techniques

Uncovering the secrets of the immune system, one molecule at a time.

MASSIVE is playing a key role in the global quest to map the molecular mechanics of the immune system, enabling discoveries that will contribute to the development of a wide range of vaccines and therapeutics.

"From my point of view the task of making sense of the enormous datasets we are required to work with as part of our everyday research would be impossible without a resource such as MASSIVE," said Dr Brian Abbey, Associate Professor and ARC Future Fellow based at Victoria's La Trobe University.

Brian is also a Chief Investigator at the Imaging CoE, a $39 million Australian Research Council Centre of Excellence formed to develop novel imaging and microscopy techniques to further our understanding of how the immune system functions.

Dr Abbey is seeking to understand the molecular interactions and cellular responses that underpin immunity. The traditional approach of determining the atomic structure of proteins through X-ray crystallography is limited by the need for large crystals in order to achieve sufficient light refraction.

Dr Abbey's team is applying next generation imaging techniques, including those provided by MASSIVE, to the study of immunological assemblies at the atomic level.

"We currently have two main research projects on MASSIVE," he said. "The first is led by Dr Connie Darmanin, a former group leader of the membrane protein group at CSIRO. Dr Darmanin is now helping us to build an X-ray Free Electron Laser (XFEL) nanocrystallography program here in Australia.

"The second project involves a technique for high-resolution microscopy known as 'Coherent Diffractive Imaging' (CDI). CDI permits the reconstruction of samples with extreme sensitivity and, when combined with X-rays, achieves spatial resolution on the nanometer scale. This program is led by Dr Guido Cadenazzi."

The international XFEL community is moving rapidly towards developing the capability to image single molecules. The Imaging CoE is relying on the facilities at MASSIVE to respond to the urgent need to develop a suitable theoretical framework for interpretation the relevant data.

"We are already seeing order-of-magnitude improvements in the reconstruction times for our existing CDI datasets," said Dr Abbey.

"The times will continue to come down as we optimise our code. Meanwhile, our simulations of three-dimensional diffraction patterns from nanocrystals, would not be feasible without implementation on MASSIVE."

Access to the HPC powers of the facility provides a practical method of handling the gigantic (10-terabyte) datasets generated by each of the team's XFEL experiments. It also brings project-enabling economic efficiencies.

"Rather than outlaying the large cost of developing our own hardware solutions to the problem of sorting and analysing the datasets, we are taking advantage of the opportunities afforded by having access to external high-performance computing facilities such as MASSIVE," said Dr Abbey.

"Parallel computing in general is becoming a staple of modern experimental research. The datasets we are collecting using modern detectors and X-ray sources are beyond anything I could have imagined when I began in X-ray science more than 10 years ago."

ABOVE: Optical Fresnel coherent diffraction ptychography of dragonfly wing. A 9 x 9 ptychography scan (eighty-one individual projections) was recorded to create a high resolution image over a large field of view. This imaging method produces native phase contrast which allows for the possibility of quantitatively imaging structure and composition changes throughout the sample.

Guido Cadenazzi, Nicholas Anthony, Brian Abbey
Physics Department, La Trobe University

Research Stories

The X-ray Fluorescence Microscopy Beamline

Iron Work to Boost Rice Diets

Alex Johnson of the University of Melbourne and his colleagues used the Australian Synchrotron to demonstrate that their new strain of rice had higher levels of iron and zinc than ordinary rice, particularly in the endosperm – the part of the rice grain that most people eat.

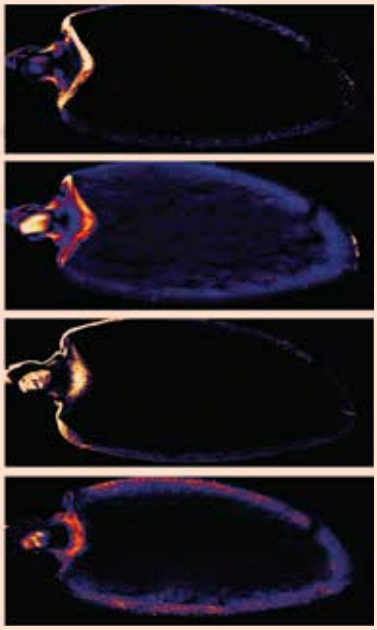
The team used the X-ray fluorescence microscopy beamline at the synchrotron and GeoPIXE on MASSIVE to produce detailed maps of where iron and zinc were found at resolutions down to sub-micron levels. At this resolution, each grain of rice can be analysed in great detail – 7 million pixels of visual information per grain brings very high accuracy to the imaging.

It is now known that the new rice variety has up to four times the iron content and twice the zinc content of ordinary rice grains.

The work is significant because in many regions of the world where rice is the major food source the levels of iron, zinc and pro-vitamin A are insufficient to meet daily nutritional requirements.

The new iron-enriched rice variety developed by Melbourne and Adelaide researchers could help solve iron problems of iron deficiency that affect more than two billion people. According to the World Health Organization, iron deficiency is the world's most common nutritional disorder.

SOURCE: WWW.SYNCHROTRON.ORG.AU/AUSSYNCBEAMLINES/X-RAY-FLUORESCENCE-MICROSCOPY/HIGHLIGHTS-XFM/IRON-WORK-TO-BOOST-RICE-DIETS



Synchrotron X-ray Fluorescence Beamline Data Processing using GeoPIXE on MASSIVE

Synchrotron based X-ray fluorescence microscopy (XFM) is a non-destructive technique used to map elements (such as gold, copper, zinc and iron) present in a sample, along with their locations and chemical form.

XFM can resolve details as small as 0.1 micrometres across and detect much lower concentrations of elements than laboratory-based techniques.

At the Australian Synchrotron, XFM data are collected using the Maia detector which has a total of 384 individual detectors and each X-ray identified by one of them represents one fluorescent event. The sample is scanned through the focussed X-ray beam and each event is tagged by the XY coordinate in the scan.

Given the number of detectors and events, a lot of data needs to be resolved in space and time. Using the XY coordinate in the scan to provide the coordinate on the sample, X-ray events energies from all detectors can be analyzed to generate spatial distribution maps of the component elements in the sample.

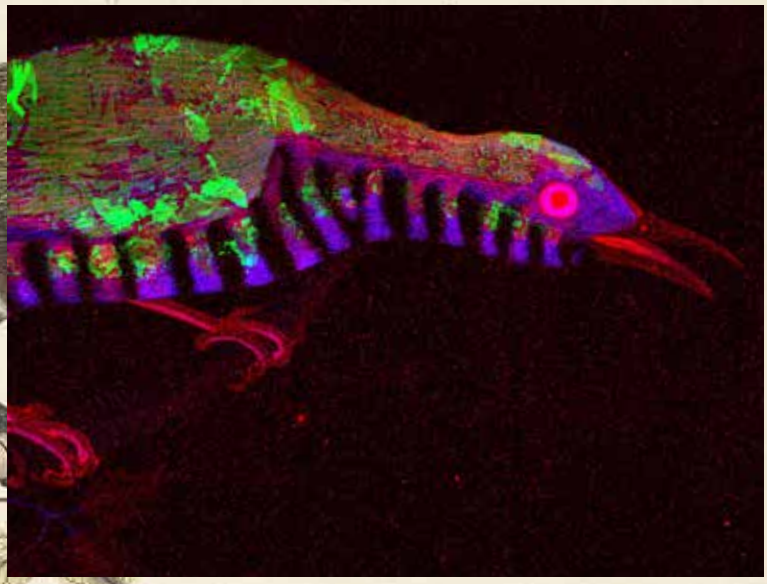
Thus, there is a major computational challenge to analyse the spectra from 384 detectors, and to combine them in a meaningful way, perhaps for more than 100 million pixels, and extract measures of the concentration of major and trace elements in each pixel to form element images.

GeoPIXE

To process XFM data, researchers use the CSIRO-developed software package GeoPIXE on MASSIVE. GeoPIXE allows scientists to examine the detailed spectral data and construct images of element distribution.

Users of the software examine and fit representative XFM spectral data that GeoPIXE uses to construct a dynamic analysis (DA) transform matrix for imaging. Using DA, raw data events are processed and transformed into separate images for each element (essentially their location within the sample). The DA method is equivalent to performing a linear least-squares fit to the spectral data in each pixel only orders of magnitude faster.

Using the matrix approach and parallel processing on MASSIVE, DA achieves the result at rates of around 108 events into 10^4-10^5 pixels per second. Further tools in GeoPIXE permit the reconstruction of XANES image stacks for speciation analysis and their correction, for example for spatial drift. Users then explore this multi-element or speciation image space using GeoPIXE and extract spectra from specific features for further quantitative analysis or to verify the accuracy of imaging.



Early Drawings Reveal their Secrets

Artists regularly use metals in their inks to create vivid and iridescent effects. The State Library of New South Wales is using the presence of metals to assess the provenance of over 700 early scientific drawings of birds and flowers created between 1791 and 1792.

X-ray fluorescence microscopy (XFM) can be used to scan delicate drawings at 0.1 micrometre resolution, or less than one-thousandth the diameter of a typical human hair. XFM can indicate if gold, copper, zinc or iron, amongst other metals, are present.

As the technique is developed, the library will create signatures for the various inks used and use them to determine rapidly and accurately the provenance of the early artwork that forms part of Australia's history.

SOURCE: WWW.SYNCHROTRON.ORG.AU/AUSSYNCBEAMLINES/X-RAY-FLUORESCENCE-MICROSCOPY/HIGHLIGHTS-XFM/DRAWING-SECRETS-REVEALED

/08

Training and Outreach

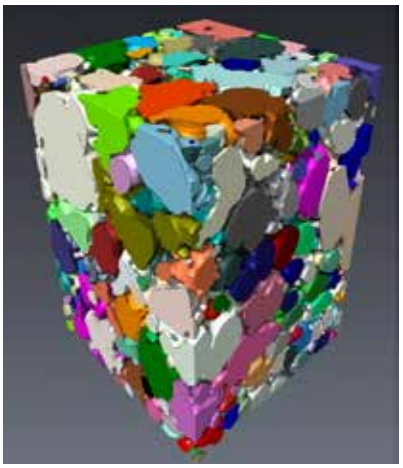
In 2014 MASSIVE focused on training events that prepare users groups to the new systems software environment being rolled out in late 2014 and early 2015.

INCF

The Victoria, Australia node of the International Neuroinformatics Coordinating Facility (INCF) was established in 2012 by Monash University and the University of Melbourne, through MASSIVE and VLSCI, respectively. The Victoria, Australia INCF node is a component of the MASSIVE Training and Outreach program.

In 2016 the Victoria, Australia node will grow to become an Australia-wide node. Funding for this initiative has been secured through CIBF. 2015 is the second year of node operations and the focus of activity has been on:

- Assisting neuroscientists, including researchers from the ARC Centre of Excellence for Integrative Brain Function (CIBF), to begin using HPC systems for data processing and analysis.
- Managing research data space for neuroinformatics researchers. A grant of $1M for data storage space has been successfully funded through the RDSI program and will be dedicated to characterisation researchers, including a specific data space allocation to CIBF and neuroinformatics researchers.
- Preparing for the Neuroinformatics 2015 Congress to be hosted by the Victoria, Australia node and held in Cairns (http://neuroinformatics2015.org/) in August 2015.



CAPTION: Researchers at CSIRO are using MASSIVE to look at the effect of different salt additives on the structure and porosity of bread-dough made from high and low protein flour. For each of 16 samples we acquired a micro-CT scan every 5 min during a 2.5 hour rising and baking cycle. This resulted in over 460 tomographic datasets, which required tomographic reconstruction and 3D data analysis to extract structural data and statistics. The image shows segmented data illustrating the structural complexity of the sample. The experimental work was carried out by Sherry Mayo, Thu McCann and colleagues from CSIRO at the Australian Synchrotron's Imaging and Medical Beamline.

Training Events

Title		Location	Date/s
Introduction to HPC and Linux	MASSIVE team	Bungle Bungle Meeting Room, Australian Regenerative Medicine Institute (ARMI), Level 1, Building 75, Monash University, Clayton Campus VIC	01/04/14
Introduction to HPC and Linux	MASSIVE team	Level 2 Boardroom (Rooms 204/205), School of Biomedical Sciences, Building 76/77, Monash University, Clayton Campus VIC	21/05/14
			09/07/14
Introduction to Linux	Monash eResearch Centre	Computer Lab G11, Faculty of Engineering, Building 60, Monash University, Clayton Campus VIC	11/07/14
Introduction to NCI	National Computational Infrastructure (NCI)		14/07/14
SLURM Workshop	MASSIVE team	Room G98, Building 75, Monash University, Clayton Campus VIC	23/12/14

Outreach Events

Title		Location	Date/s
Monash Technology Research Platforms Showcase	MASSIVE team (Representation at shared showcase stand)	Foyer & Room G19, Building 75, Monash University, Clayton Campus VIC	28/03/14
Imaging Informatics Workshop	Sponsored & MASSIVE team	Auditorium, Monash Biomedical Imaging (MBI), Building 220, 770 Blackburn Rd, Monash University, Clayton Campus VIC	21/08/14
Victorian Platform Technologies Network (VPTN) Showcase	MASSIVE team (Representation)	National Centre for Synchrotron Science (NCSS), Australian Synchrotron, 800 Blackburn Rd, Clayton VIC	11/09/14
Monash University Innovation & Technology Expo	MASSIVE team (Representation at shared exhibition booth)	Campus Centre Banquet Hall, Building 10, Clayton Campus VIC	29/09/14 - 30/09/14
Launch of the ARC Centre of Excellence for Advanced Molecular Imaging	MASSIVE team (Presentation and Booth)	Foyer, Building 75 Monash University, Clayton Campus VIC	15/10/14
XRM 2014 Satellite Workshop “The Big Data in X-Ray Microscopy”	Sponsored & MASSIVE team (Presentation)	Laby Theatre, The University of Melbourne, Parkville Campus VIC	25/10/14 - 26/10/14
eResearch Australasia 2014	MASSIVE team (Representation at Monash eResearch Centre’s exhibition booth)	Pullman Melbourne Albert Park, 65 Queens Road, Albert Park VIC	28/10/14 - 30/10/14
Supercomputing 2014	MASSIVE team (Representation at Australian HPC booth)	The Ernest N. Morial Convention Centre, New Orleans Convention Centre, USA	17/11/14
New User Symposium: Synchrotron, Accelerator and Neutron Techniques 2014	Sponsored	National Centre for Synchrotron Science (NCSS), Australian Synchrotron, 800 Blackburn Rd, Clayton VIC	19/11/14
Australian Synchrotron User Meeting 2014	Sponsored	National Centre for Synchrotron Science (NCSS) , Australian Synchrotron, 800 Blackburn Rd, Clayton VIC	20/11/14 - 21/11/14

/09.

Usage and Users

Since its inception, MASSIVE has steadily grown the number of institutional users from 11 (2011) to over 100 (2014). The organisations involved cover research institutes, hospitals, universities, private industry and government departments across Australia and internationally. In 2013, this equated to supporting over 110 active projects and more than 500 individual user accounts. The table below lists the institutions which have users of MASSIVE.

Institutional users can be categorised into three groups, those directly accessing MASSIVE through a merit allocation or partner project (Linux), those accessing MASSIVE through integration with an instrument (Instrument) or those accessing MASSIVE through both methods.

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, 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.

Institutions
Researchers from the following institutions have used MASSIVE since the start of the project:

University

Australian National University
Curtin University
Deakin University
James Cook University
La Trobe University
Massey University
Monash University
Queensland University of Technology
RMIT
Southern Cross Uni
University of Adelaide
University of Hawaii at Manoa
University of Melbourne
University of New South Wales
University of Newcastle
University of Otago
University of Queensland
University of South Australia
University of Sydney
University of Technology Sydney
University of Wollongong
Western Australia

Australian Defence Force Academy
Birbeck University of London
Imperial College London
RIKEN Yokohama Inst
Stockholm University
Swinburne University
Universidad de Granada
Universidad Politécnica de Madrid
Università di Trento
Universität Heidelberg
Universität Leipzig
University of Amsterdam
University of Birmingham
University of California San Diego
University of Illinois Chicago
University of Manchester
Victoria University

Charles Sturt University
Dartmouth College
Flinders University
Griffith University
Katholieke Universiteit Leuven
Lancaster University
Macquarie University
Nanyang Tech University
Sunshine Coast
University Antwerp
University New England, Aus
University Oxford
University Reading
University Saskatchewan
University Trieste
University Western Sydney
University of Auckland
University of Canterbury
University of Sassari
University of Tasmania
University of Waikato
Victoria University of Wellington

Research Institute

ANSTO
Australian Synchrotron
CSIRO
Garvan Institute of Medical Research
Baker IDI
Bionics Institute
Brain Research Institute de Bascule
Indian Institute of Astrophysics
Institute of Nuclear Physics, Polish Academy of Sciences
Neuroscience Research Australia
QIMR Berghofer
QIMR Berghofer Medical Research Institute
Russian Academy of Sciences
Synchrotron Light Research Institute
VERSI
Victorian Partnership for Advanced Computing

Academia Sinica
AgResearch Ltd
Burnet Institute
Callaghan Innovation
Centenary Institute
DLS (Diamond Light Source)
Elettra, Sincrotrone Trieste
Ian Wark Research Inst
Institut de Physique du Globe de Paris
Korea Advanced Inst Sci Tech
Ludwig Institute
Monash Institute of Medical Research
Nanjing Uni Infor Sci & Tech
RIKEN Yokohama Institute
St Vincent's Institute
The Florey Institute of Neuroscience and Mental Health
Uni Michigan
Uni Oulu
Victor Chang Cardiac Research Institute
Walter and Eliza Hall Institute of Medical Research

Medical

Alfred Health
Eastern Health
GGZ inGeest
Melbourne Health
IRCCS Burlo Garofolo Hospital
Peter Mac
QLD Health
Royal Adelaide Hospital
The William Buckland Radiotherapy Centre
Women's and Children's Hospital, Adelaide

Industry

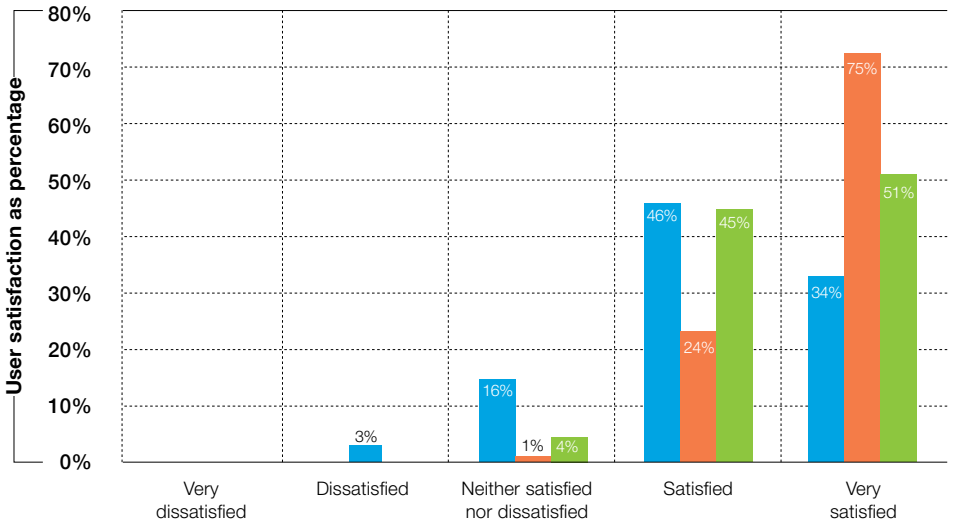
IBM
4DX
Australian Red Cross Blood Service
AgResearch Ltd
Carrick Gold Ltd
GNS Science

Government

Ames Laboratory
IVEC
Department of Primary Industries
Museum Victoria
State Library New South Wales
Western Australian Museum
DSTO
NGV (National Gallery Vic)
Synchrotron SOLEIL
SA Museum
Natural History Museum, UK

Key
Linux and Instrument
Linux
Instrument
Bold indictates new additions in 2014

User Satisfaction with MASSIVE



In 2013, MASSIVE undertook a User Satisfaction Review, the results of which is summarised in this graph. The next User Satisfaction Review is scheduled for 2015.

MASSIVE Usage Data for 2014 (in system units)

			Jan-Jun 2014	Jul-Dec 2014	Totals 2014
Total Available			**9,741,120**	**9,741,120**	**19,482,240**
Dynamically Scheduled	Monash	58 projects	296,358	705,565	1,001,923
	Victorian	4 projects	640,496	346,282	986,778
	NCMAS	14 projects	434,643	370,344	804,987
	Synchrotron	19 projects	1,468,528	1,313,840	2,782,368
	CSIRO	8 projects	15,229	64,696	79,925
	Discretionary	13 projects	690,683	1,001,926	1,692,609
	Total	**105 projects**	**3,545,937**	**3,802,653**	**7,348,590**
	System Testing & Maintenance	6 projects	8,441	49,067	57,508
On-Demand Processing and Visualisation	CT processing at IMBL beamline	10 nodes	525,600	525,600	1,051,200
	GeoPIXE processing at XFM beamline	3-4 nodes	157,680	210,240	367,920
	AutoRickshaw at MX1 and MX2 Beamlines	1 node	52,560	52,560	105,120
	MASSIVE Desktop	25 nodes	1,314,000	1,314,000	2,628,000
Total Used			**5,604,218**	**5,905,053**	**11,500,830**
Unused			**3,649,846**	**3,349,011**	**7,007,298**
Percentage Unused #			**39%**	**36%**	**38%**

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.

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Governance

MASSIVE is governed by a Steering Committee, which is advised by a Science Advisory Committee representing the MASSIVE researcher community.

Steering Committee

The Steering Committee is chaired by an independent member elected by the representatives of the partners on the committee — since 2012, this position has been held by Dr Robert Hobbs.

MASSIVE is managed within an associated legal entity, known as the Coordinating Institution, documented within the Collaboration Agreement which is Monash University.

At January 2015, the MASSIVE Steering Committee comprised:

Dr Robert Hobbs,
Chair

Professor Paul Bonnington,
Monash University

Professor Andrew Peele,
Australian Synchrotron

Dr Alfred Uhlherr,
CSIRO

Dr Wojtek James Goscinski,
MASSIVE Coordinator (ex officio)

Science Advisory Committee

The Imaging and Visualisation Scientific Advisory Committee (IVSAC) comprises representatives of significant user groups as well as scientists conducting imaging and visualisation using HPC (and includes at least one member each from Australian Synchrotron, Monash and CSIRO).

At January 2015, the MASSIVE IVSAC Committee comprised:

Professor Gary Egan
Monash University, Chair

Dr Andreas Fouras,
Monash University

Dr Christopher Fluke,
Swinburne University

Dr Olivier Salvado,
CSIRO

Dr Chris Hall,
Australian Synchrotron

Professor David Sampson,
UWA

Dr Paul McIntosh,
MASSIVE representative

Dr Wojtek James Goscinski,
MASSIVE Coordinator (ex-officio)

ABOVE: MASSIVE Steering Committee meeting on the 30th March 2015. Members and observers from left to right:

Alfred Uhlherr PhD
CSIRO representative
Uli Felzmann PhD
Australian Synchrotron observer
Michael James PhD
Australian Synchrotron representative for Prof Andrew Peele
Wojtek James Goscinski PhD
Coordinator, MASSIVE
Robert Hobbs PhD
Chair
Paul Bonnington PhD
Monash University representative

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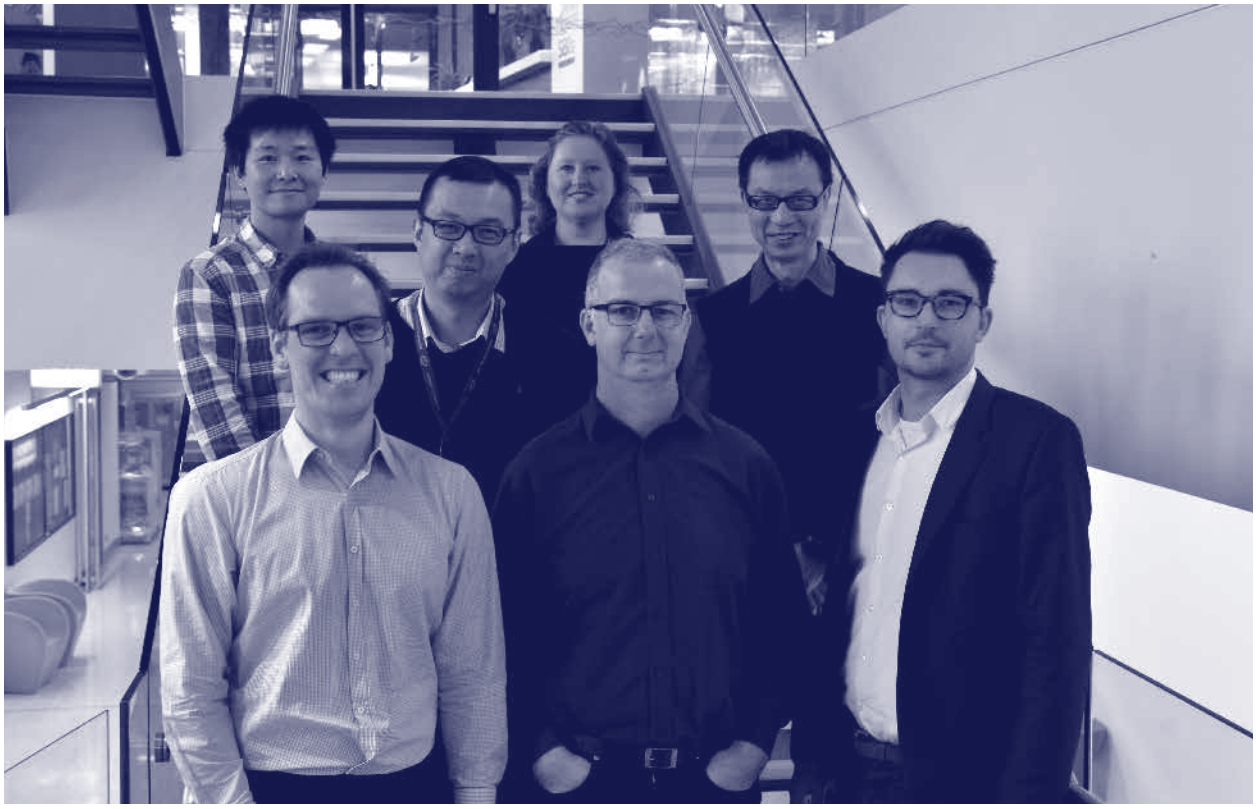
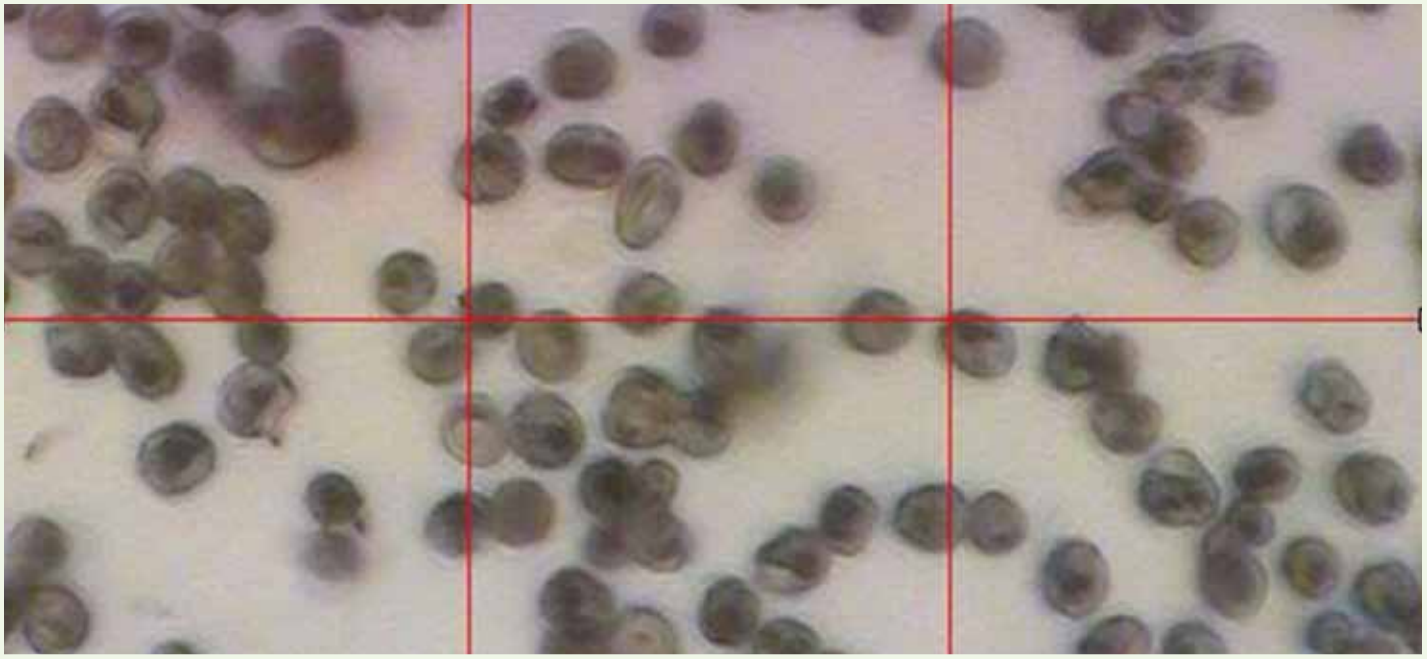
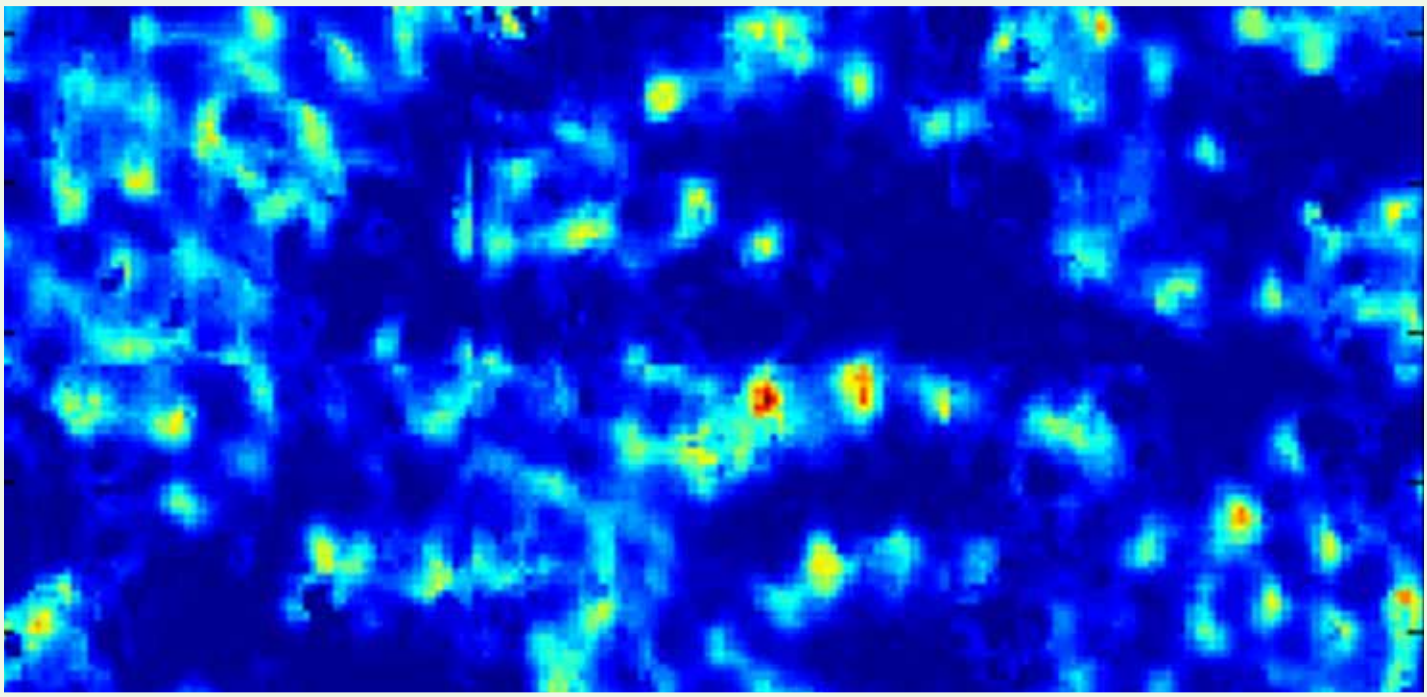
Team and Operations

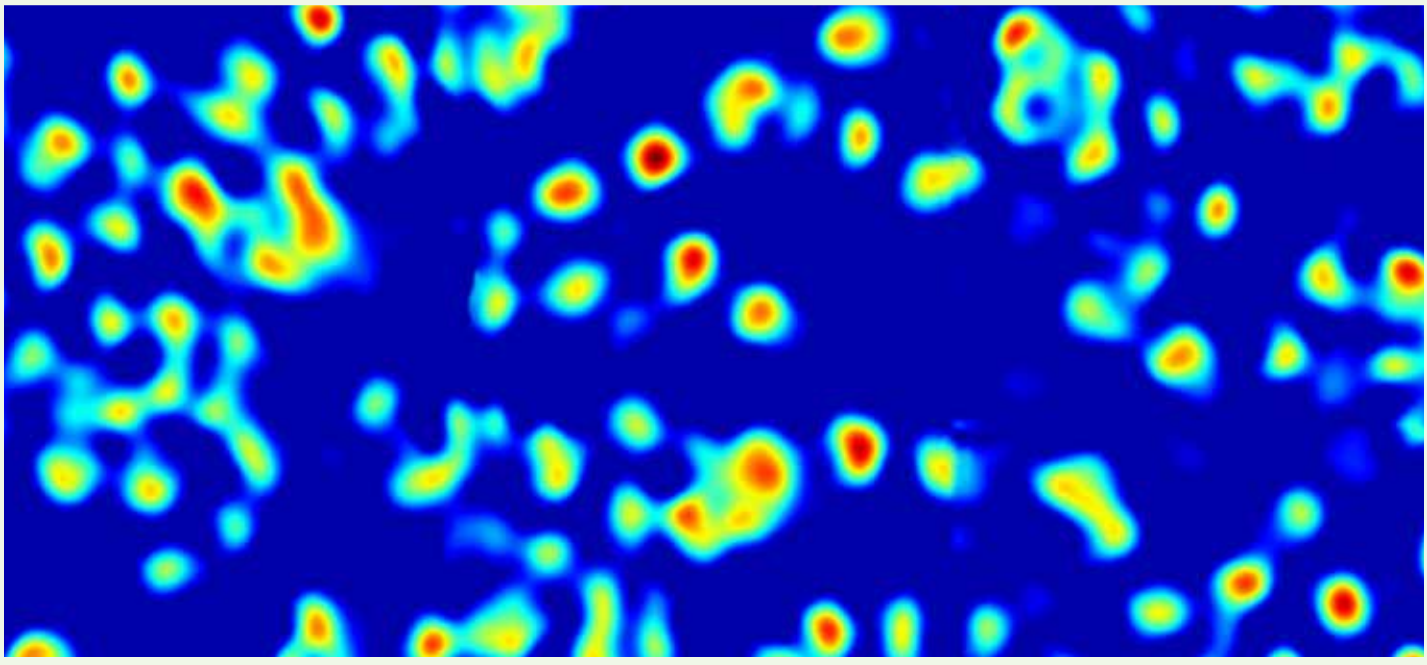


The MASSIVE team is the most vital part of the project. Members of the team possess a wide range of expertise, including skills in high performance computing, software development, systems administration and project management. A number of staff members possess higher graduate degrees in visualisation,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

ABOVE: 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







Research Stories

Diagnosing Malaria

Blood smears are the diagnostic method of choice for confirming a malaria infection, particularly in developing countries. The unit cost is low and the method is highly sensitive.

However, as the infection load decreases, more blood smears are needed to confirm the complete absence of malaria from the patient, rather than from a single sample. Although other more sensitive techniques could be used, such as polymerase chain reaction (PCR), immunofluorescence assays (IFA) or enzyme-linked immunosorbent assay (ELISA), they are often impractical due to time, cost or equipment constraints, especially in the field.

Researchers from the University of Melbourne, Monash University, Karlsruhe Institute of Technology (Germany) and the University of Wisconsin-Milwaukee (USA) are aiming to overcome such problems.

Associate Professor Bayden Wood (Monash University) and his team have used Fourier transform infrared (FTIR), to spatially resolve malaria in a blood smear. The use of infrared light absorption and reflection can confirm the presence of malaria in a blood sample. Furthermore, by combining data for all cells identified, they have identified the malaria stage of development with high accuracy in independent trials.

The FTIR analysis of blood smears requires sophisticated technology, including a synchrotron beamline and a high-performance computer to analyse the data. In a team effort, MASSIVE was able to provide the latter.

Associate Professor Wood's team wrote processing scripts to pass the data through the RMie-EMSC algorithm for correction of the spectroscopic scatter i.e. how the light is reflected by the malaria parasite and infected blood cells. The MASSIVE facility enabled the characterisation to take place in the cloud, so that results could be shared in real time with the collaborators in Australia, USA and Germany. MASSIVE not only saved time during analysis, but also that associated with securely transferring data between laboratories around the world.

The results generated from the synchrotron and MASSIVE have led to the development of a portable Attenuated Total Reflection (ATR-FTIR) spectrometer capable of of performing rapid diagnosis in the field. The MASSIVE computing facility will be further applied to store and process the ATR data in a virtual laboratory and provide a continually evolving data model.

Background

Scientists at the Infrared Microscopy Beamline on the Australian Synchrotron are using MASSIVE to help in the analysis of spectra recorded from biological samples. Synchrotron Fourier transform infrared (sFTIR) microspectroscopy can be applied to diverse areas of biological and medical research. This synchrotron technique provides a direct, and rapid probe of the chemical composition of biological tissues and cells without the need for pre-treatment of samples pre-treatment with stains or external markers. However, light scattering effects can hamper or interfere with the analysis of these sFTIR spectra.

MASSIVE is being used to computationally model and correct for light scattering effects in spectra and images generated using sFTIR microscopy spectra and images. The correction uses an algorithm developed in Europe known as Resonant Mie Scattering modelling through Extended Multiplicative Signal Correction (RMieS-EMSC).

Parallel computing on the MASSIVE HPC facility allows RMieS correction to be performed about 100 times faster than is possible on high-performance desktop computers. Extremely rapid RMieS-EMSC correction significantly reduces time spent on analysis of synchrotron IR microspectroscopic images and datasets to increase research output.

Performing RMieS-EMSC correction of sIR images and spectral libraries often reveals previously hidden information on the variation of chemical constituents within samples and so can lead to improved automated classification of the same samples.

The fast data analysis and improved accuracy of automated classification are particularly attractive to medical researchers interested in applying IR spectroscopy to the diagnosis of disease.

(A) Photomicrograph of a blood film with malaria parasites. (B) Hyperspectral Infrared Synchrotron chemical image showing a region of the spectrum related to lipids before MASSIVE correction. (C) The same image data as shown in (B) but after deconvolution and RMieS-EMSC correction using MASSIVE.

/12.

Projects

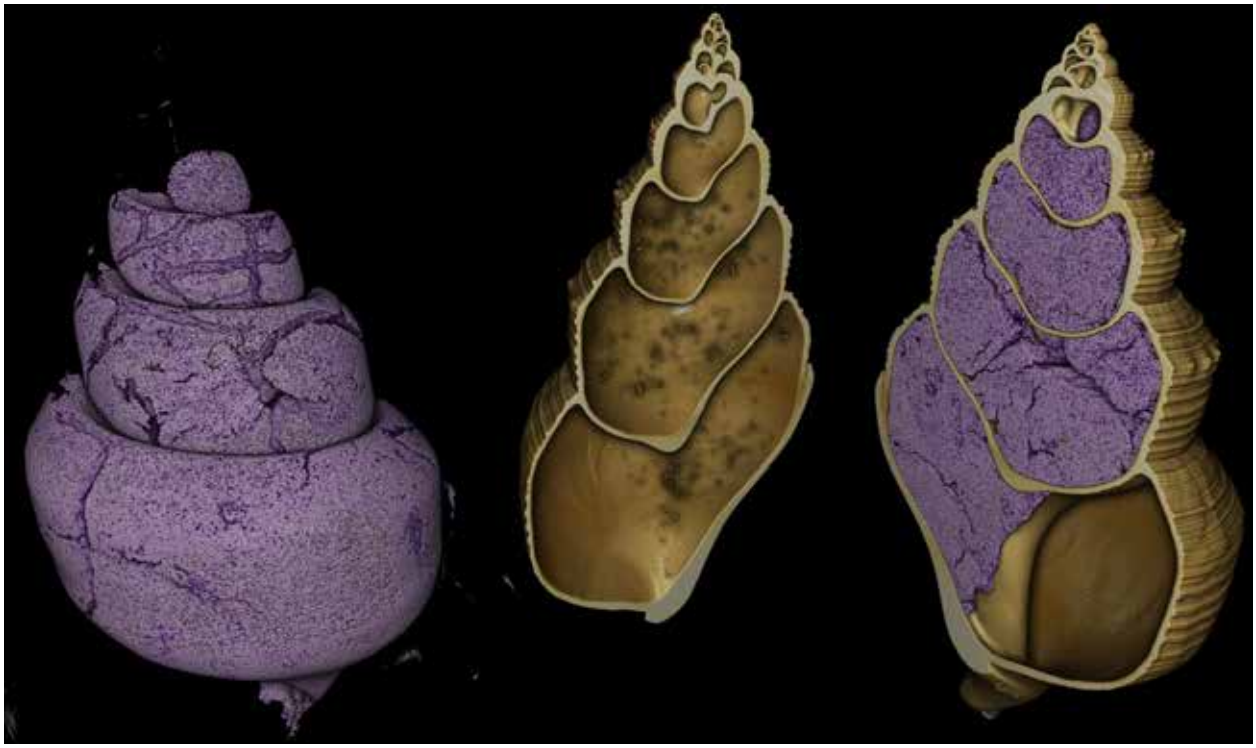
The following is a list of projects which have used MASSIVE in 2014, inclusing merit allocated projects through NCMAS. Merit allocation projects that use MASSIVE through beamline access at Australian Synchrotron are not listed.

Project Title	Chief Investigator(s)	
A functional magnetic resonance imaging (fMRI) study addressing cognitive function in individuals with Friedreich Ataxia	Nellie Georgiou-Karistianis, Monash University	Partner Share
A new, high spatial-resolution, dataset on internet use in Australia	Simon Angus, Monash University	Partner Share
A pilot project of automated analysis of confocal time series in leukocyte tracking	Graham Lieschke, Monash University	Partner Share
Accurate Monte Carlo Dose Calculations for Microbeam Radiation Therapy at the Imaging and Medical Beamline	Iwan Cornelius, University of Wollongong	Partner Share
ADS	Alex Fornito, Monash University, Chao Suo, Monash University, Murat Yucel, Monash University	Partner Share
An investigation of the effects of intranasal oxytocin on socio-emotional brain regions in Huntingtons disease	Govinda Poudel, Monash University, Izelle Labuschagne, Monash University	Partner Share
An MD study of radiation effects in candidate structural materials for demanding engineering applications	Roman Voskoboynikov, ANSTO	Partner Share
Analysis of Brain MR images for the study of Alzheimer's disease	Pierrick Bourgeat, CSIRO	Partner Share
Analysis of longitudinal structural MRI for TasCOG and CDOT studies	Richard Beare, Murdoch Childrens Research Institute and Monash University	NCMAS
Anatomical Image Processing and Biomechanical Modelling	Christopher Walmsley, Monash University, Colin McHenry, Monash University, Michelle Quayle, Monash University	Partner Share
Atomistic simulations for physical and electronic properties of nanomaterials	Nikhil Medhekar, Monash University	NCMAS
Australian Synchrotron Scientific Programming Group	Ulrich Felzmann, Australian Synchrotron	Partner Share

Project Title	Chief Investigator(s)	
Automated detection of cervical spine fractures in computed tomography images of the spine in trauma patients	Jarrel Seah, Monash University, Wai Ho Li, Monash University	Partner Share
Automation, processing and visualisation of large multi-dimensional micro-imaging datasets generated at Monash Micro Imaging	Keith Schulze, Monash University	Partner Share
Beryllium intermetallics for fusion applications	Simon Middleburgh, ANSTO	Discretionary
CF PCXI	Kaye Morgan, Monash University, Martin Donnelley, University of Adelaide	Partner Share
CoE Robotic Vision	Thomas Drummond, Monash University	Partner Share
Cognitive Control in Youth Obesity	Murat Yucel, Monash University	Partner Share
Coherent Diffraction Imaging	Grant van Riessen, La Trobe University	Partner Share
Computational approaches towards the neuronal basis of consciousness	Dror Cohen, Monash University, Mana Fujiwara, Monash University, Miao Cao, Monash University, Naotsugu Tsuchiya, Monash University, William Wong, Monash University	NCMAS
Computational investigations of solid state electrolytes	Fangfang Chen, Deakin University	Partner Share
Computed Tomography of Ceramic Matrix Composites During Mechnical Loading	Mitchell Sesso, Swinburne University of Technology	Partner Share
Conformational properties of bacterial toxins	Cyril Reboul, Monash University	Partner Share
Connectome mapping	Alex Fornito, Monash University, Ben Fulcher, Monash University, Chao Suo, Monash University, Murat Yucel, Monash University	Partner Share
Counting nephrons in the kidney via micro-CT	James Armitage, Deakin University, Karen Siu, Australian Synchrotron	Partner Share
Cross-channel analysis of multi-channel elecrtophysiological data in space, time and frequency	Dror Cohen, Monash University, Jochem van Kempen, Monash University, Naotsugu Tsuchiya, Monash University	Partner Share
CVL Energy Materials (X-Ray)	Adrian Sheppard, Australian National University, Stuart Hungerford, Australian National University	Discretionary
Decoding perceptual decisions from simultaneously recorded EEG and fMRI data	Carsten Murawski, University of Melbourne	Partner Share
Deep Learning Theory and Applications	Jiankun Hu, Australian Defence Force Academy	Discretionary
Depth Resolution In X-ray Fluorescence Microscopy (DXFM)	Matthew Dimmock, Monash University	Partner Share
Determining protein structures using transmission electron microscopy	James Wettenhall, Monash University	Discretionary
Development of New Thermoelectric Materials Based on the Defect Pyrochlore Structure	Elvis Shoko, ANSTO	Partner Share
Direct simulation Monte-Carlo for ultracold spinor gases	Chris Watkins, Monash University, Lincoln Turner, Monash University	Partner Share
Dopamine	Alex Fornito, Monash University, Chao Suo, Monash University, Murat Yucel, Monash University	Partner Share
Dynamic computed tomography of lungs in motion	Andreas Fouras, Monash University	NCMAS

Project Title	Chief Investigator(s)	
Electromagnetic Structure of Matter	Derek Leinweber, University of Adelaide, Waseem Kamleh, University of Adelaide	NCMAS
Electronic and thermal properties of 2D transition metal dichalcogenides	Nikhil Medhekar, Monash University	Partner Share
Embryo	Rajeev Samarage, Monash University	Partner Share
Evolutionary influence and phylogenetic constraints on morphology	Scott Keogh, Australian National University	Partner Share
Exhaustive Search for 3-way Genomic Interactions Associated with Disease	Qiao Wang, University of Melbourne	NCMAS
Functional brain imaging of interoception	Michael Farrell, Monash University	Partner Share
Genetic and environmental influences on brain structure and function	Alex Fornito, Monash University, Chao Suo, Monash University, Murat Yucel, Monash University	Partner Share
Genetics of brain structure and function	Katie McMahon, University of Queensland	NCMAS
GeoPIXE software AS Users Access	Chris Ryan, CSIRO	Partner Share
Graphene Electromechanical Actuation: Origins, Optimization, and Applications	Zhe Liu, Monash University	Partner Share
Gravitational Waves from Turbulent Neutron Stars	Andrew Melatos, University of Melbourne	NCMAS
High Entropy Alloys for Advanced Nuclear Applications	Simon Middleburgh, ANSTO	Discretionary
Human Brain Dynamics: Beyond the Connectome	Michael Breakspear, QIMR Berghofer Medical Research Institute, Sascha Frydman, QIMR Berghofer Medical Research Institute	Discretionary
ImageHD	Govinda Poudel, Monash University	Partner Share
Imaging and Medical Beamline	Andreas Moll, Australian Synchrotron, Ulrich Felzmann, Australian Synchrotron	Partner Share
Improving capabilities for tomographic reconstruction	Darren Thompson, CSIRO, Sheridan Mayo, CSIRO	Partner Share
Investigating neural mechanism of problem gambling and obsessive-compulsive disorder using MRI	Alex Fornito, Monash University, Chao Suo, Monash University, Leah Braganza, Monash University, Murat Yucel, Monash University	Partner Share
Investigations into the sturtcure and function of the pacemakers driving pyleoureteric peristalsis	Richard Lang, Monash University	Partner Share
Investigations of transitional and turbulent shear flows using direct numerical ...	Julio Soria, MonashUniversity, Omid Amili, Monash University	NCMAS
large scale 3D reconstruction for electron imaging	Jing Fu, Monash University	Partner Share
Magnetic Properties of Tc Oxides and Tc Metal	Eugenia Kuo, ANSTO	Discretionary
MBI testing and development (MOSP support)	Parnesh Raniga, Monash University	Partner Share
Modeling generative mechanisms underlying network changes observed in people with schizophrenia	Murat Yucel, Monash University	Partner Share
Modelling G protein-coupled receptors for drug discovery	David Chalmers, Monash University	Partner Share
Modelling Nanoscale Materials	Michelle Spencer, RMIT	Partner Share

Project Title	Chief Investigator(s)	
Modelling the Subsurface Structure of Sunspots	Hamed Moradi, Monash University	Partner Share
Molecular Dynamics Simultions on radiation damage of nuclear materials	Meng Jun Qin, ANSTO	Discretionary
Molecular simulations of proteins	Ashley Buckle, Monash University	Partner Share
Monash Biomedical Imaging Small Projects	Parnesh Raniga, Monash University	Partner Share
Monash CAVE2 rendering and data organisation	David Barnes, Monash University	Partner Share
Monash Clinical & Imaging Neuroscience (MCIN) group	Alex Fornito, Monash University, Chao Suo, Monash University, Murat Yucel, Monash University	Partner Share
Monte Carlo Calculations for Quality Assurance of Microbeam Radiation Therapy at the Australian Synchrotron	Iwan Cornelius, University of Wollongong	NCMAS
Multimodal Kidney Image Analysis	Parnesh Raniga, Monash University	Partner Share
MX Group Access	Tom Caradoc-Davies, Australian Synchrotron	Partner Share
Neural and physiological correlates of somatic contagion: A multidimensional model of empathy for pain	Melita Giummarra, Monash University	Partner Share
Neuroimage biomarker for vulnerability to psychosis in young adults	Alex Fornito, Monash University, Chao Suo, Monash University, Murat Yucel, Monash University	Partner Share



CAPTION: The Struthiolariidae ("ostrich-foot snails") are a Southern Hemisphere family of molluscs. This image was captured by the Imaging Beamline at Australian Synchrotron, with processing and rendering on MASSIVE. Research by Katie Collins, Ian Schipper, Michael Gazley, James Crampton (Victoria Uni of Wellington). This shell was kindly by the Invertebrate Palaeontology department at Museum Victoria. Rendering by Anton Maksimenko at Australian Synchrotron.

Project Title	Chief Investigator(s)	
New Methods for Probabilistic Single-particle Cryo-EM 3D Reconstruction at Near-atomic Resolution	Hans Elmlund, Monash University	Partner Share
Numerical modelling of solar photospheric magnetic activity	Sergiy Shelyag, Monash University	Partner Share
Numerical search of better radiotherapy protocols using genetic algorithms	Simon Angus, Monash University	Partner Share
Parameter Estimation of Stochastic Volatility Models using Particle Filtering	Kenneth Lindsay, Queensland University of Technology	Discretionary
Comprehensive study of the background for the Pixel Vertex Detector at Belle II	Andreas Moll, Australian Synchrotron	Partner Share
Quantifying the effects of partially coherent X-rays in coherent diffractive imaging	Giang Tran, La Trobe University	Partner Share
Quantum Simulation of Condensed Matter for Direct Comparison to Soft X-Ray Synchrotron Experiments	Bruce Cowie, Australian Synchrotron, Kane O'Donnell, Australian Synchrotron	Partner Share
Radiation effects in advanced oxides, carbides and nitrides for high temperature applications	Simon Middleburgh, ANSTO	Discretionary
Recontruction of 3D mice aortic arches with atherosclerotic plaques	Pauline Assemat, Monash University	Partner Share
Resonant Mie Scatter Correction for FTIR Microspectroscopy - IR Beamline Users	Keith Bambery, Australian Synchrotron	Partner Share
SAXSWAXS Autoprocessing Pipeline	Stephen Mudie, Australian Synchrotron	Partner Share
Simulations and visualisation of star and planet formation	Daniel Price, Monash University	Partner Share
Single projection and tomographic x-ray imaging with the Australian Synchrotron's Imaging and Medical Beamline	Jeremy Brown, Monash University	Partner Share
Small projects at BMRI	William Ryder, University of Sydney	Discretionary
STARImaging	Richard Beare, Murdoch Childrens Research Institute and Monash University	Partner Share
Statistics of Magnetised Supersonic Turbulence in the Interstellar Medium	Daniel Price, Monash University, Terrence Tricco, Monash University	NCMAS
Structure, dynamics and interactions of malaria surface proteins as vaccine candidates and drug targets	David Chalmers, Monash University	NCMAS
Supersymmetry at the Large Hadron Collider	Csaba Balazs, Monash University	Partner Share
Synchrotron Cretaceous Mammals	Alistair Evans, Monash University	Partner Share
Synchrotron-based phase contrast x-ray imaging of the lungs	Marcus Kitchen, Monash University	Partner Share
Tandem Maia-Geopixe real-time fluorescence analysis	Martin de Jonge, Australian Synchrotron	Partner Share
The association between neuroanatomical correlates of attention and working memory, and response to methylphenidate in traumatic brain injury rehabilitation	Catherine Willmott, Monash University	Partner Share
The Characterisation Virtual Laboratory Test and Development	Paul McIntosh, Monash University	Discretionary
The comparative physiology of oxygen delivery to the kidney	Roger Evans, Monash University	Partner Share

Project Title	Chief Investigator(s)	
The effect of cannabis on hippocampal morphometry and volume	Chao Suo, Monash University, Murat Yucel, Monash University, Valentina Lorenzetti, Monash University	Partner Share
The Industrial Ecology Virtual Laboratory	Arne Geschke, University of Sydney, Tim Baynes, CSIRO	Partner Share
Thermoelastic properties of hydrated sulphates	Helen Brand, Australian Synchrotron	Partner Share
Three-dimensional (3D) Cellular Imaging and Visualization with Computational Tomography	Shan Shan Kou, University of Melbourne	Partner Share
Thrombus Reconstruction	Josie Carberry, Monash University	Partner Share
Towards large-scale calculations of ionic liquids	Ekaterina Pas, Monash University	Partner Share
Trials for Monash Clinical & Imaging Neuroscience	Alex Fornito, Monash University, Chao Suo, Monash University, Murat Yucel, Monash University	Partner Share
Understanding the assembly of high electron affinity molecular acceptors on surfaces	Chris Pakes, La Trobe University	Partner Share
Visualisation Evaluation	Tomasz Bednarz, CSIRO	Partner Share
Visualising Culture by Revealed Preferences Harvested from Internet Search	Simon Angus, Monash University	Partner Share
Visualization of soft tissue from synchrotron x-ray phase contrast tomography	Daniele Pelliccia, Monash University	Partner Share
Visualization of the Radiation Dose Deposition in Synchrotron X-ray Microbeam Radiation Therapy	Iwan Cornelius, University of Wollongong, Michael Lerch, University of Wollongong	Discretionary
Vocal cord movements in Parkinson's disease	Dominic Thyagarajan, Monash Health and Monash University	Partner Share
X-Ray computed tomography imaging and modelling the microstructure of artificially cemented acid sulphate soils	Asadul Haque, Monash University	Partner Share
X-ray Phase Imaging	Aidan Carroll, La Trobe University, Andrew Peele, Australian Synchrotron	Partner Share

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Financial Statement

			MASSIVE1 AND MASSIVE2 Project Total 2010 to 30th June 2014
Income			
	Partner and Investor		
		Australian Synchrotron / DIIRD	$1,450,000.00
		CSIRO	$1,200,000.00
		Monash University	$900,000.00
		NCI	$1,200,000.00
		VPAC	$800,000.00
	Project Funding		
		NeCTAR	$118,965.00
		TOTAL Income	**$5,668,965.00**
Expenditure			
	Machine Specific		
		Hardware Procurement	$2,576,355.00
		Non-tender equip	$82,911.39
		Facilities	$201,111.34
		Software licenses	$201,250.68
		Subtotal	**$3,061,628.41**
	MASSIVE		
		Operations, Staff and Management	$2,411,116.96
		Steering Committee Costs	$27,362.61
		Training and outreach	$267,810.54
		Establishment and Other	$137,590.50
		Subtotal	**$2,843,880.61**
	Misc		
	TOTAL		**$5,905,509.02**
Interest			**$249,094.45**

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Abbreviations

AMMRF	Australian Microscopy and Microanalysis Research Facility
ANSTO	Australian Nuclear Science and Technology Organisation
ARC	Australian Research Council
CDI	Coherent Diffractive Imaging
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
EMSC	Extended Multiplicative Signal Correction
FTIR	Fourier transform infrared
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)
INCF	International Neuroinformatics Coordinating Facility
IR	Infrared
IVSAC	Imaging and Visualisation Scientific Advisory Committee
M1	the MASSIVE computer located at Australian Synchrotron
M2	MASSIVE computer located at Monash University
MAS	Merit Allocation Scheme
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
RMieS	Resonant Mie Scattering
SAC	Science Advisory Committee
SAXS/WAXS Scattering	Small Angle X-ray Scattering / Wide Angle X-ray
SSAC	Synchrotron Scientific Advisory Committee
SU	System Units
SXRF	Synchrotron X-ray Fluorescence
TB	Terabyte
VLSCI	Victorian Life Sciences Computation Initiative
VPAC	Victorian Partnership for Advanced Computing
XFEL	X-ray Free Electron Laser (XFEL)
XFM	X-ray Fluorescence Microscopy

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