MASSIVE | Annual Report 2013

Australian Synchrotron | CSIRO | MONASH University | VPAC | NCI | State Government Victoria

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Cover Image — Rat lung visualisation by Anton Maksimenko, Australian Synchrotron with editing by Symon McVilly. See page 26 for original image and description.

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From the Chair

In this, our third year of operation, our main goal was to complete installation and commissioning of the MASSIVE infrastructure that we embarked on in 2010. This was achieved in the first quarter of 2013 when the final parts of the stage-2 installation were handed over to MASSIVE for user access.

Throughout 2013 our user base has continued to grow. Over this 12-month period we have supported users from more than 70 different institutions (covering universities, research institutes, government departments, health services and private industry) — more than double the 2012 figure. The number of active MASSIVE user accounts has grown beyond 400, covering more than 120 different projects.

In 2012 MASSIVE was becoming recognised as an essential and integrated research tool for Australian researchers interested in imaging and characterisation. In 2013, this was amplified in many ways, with MASSIVE integrated into the research and data flow for major research organisations in Australia including the CSIRO, ANSTO, the Australian Synchrotron, Universities and several characterization facilities. This was achieved through a number of major collaborative efforts, including NeCTAR-funded projects, such as the Characterisation Virtual Laboratory (CVL), and eResearch Tools for the Australian Synchrotron Research Community, and contributions by MASSIVE partners.

The CVL has had a significant impact on the ease-of-use of the MASSIVE computers and nearly half of our users are now also users of the MASSIVE Desktop. The CVL has also facilitated MASSIVE's engagement with major Australian research infrastructure initiatives, such as the National Imaging Facility (NIF) and the Australian Microscopy and Microanalysis Research Facility (AMMRF), that have both developed bespoke software solutions within the CVL to help their respective users process and analyse data.

The MASSIVE team, led by Dr Wojtek James Goscinski, has been key to the success of the project, particularly as operations management transitioned from the Victorian Partnership for Advanced Computing (VPAC) to Monash University. This transition was handled well by both VPAC and Monash University and I thank both organisations for the professionalism and cooperation they showed.

My colleagues on the MASSIVE Steering Committee have also been essential to the continued success of MASSIVE. I thank the members for their support and enthusiasm for the project, including advocacy to the wider research community. The advice received from the two Scientific Advisory Committees has also been invaluable in guiding developments within the CVL and the Instrument Integration Program.

I am pleased with the development of the future MASSIVE3 project and am sure it's future impact on the Australian scientific community will be felt for many years to come.

Dr Robert Hobbs
Chair
MASSIVE Steering Committee

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Coordinator's Message

In 2013, MASSIVE cemented significant progress towards the founding partners' vision of creating an accessible, world-class imaging and visualisation facility.

In early 2013, MASSIVE operations transitioned from VPAC to Monash University. In a testament to the people involved at each organisation, this transition proceeded efficiently and professionally. This transition means MASSIVE is now co-located with other national computing projects at Monash, allowing savings to be reinvested into increased staffing. It has allowed us to increase our support across a range of services and collaborations — an important part of ensuring MASSIVE remains innovative and strategic in 2014 and beyond.

The Instrument Integration Program has impacted a large range of users across beamlines and instruments. Most significantly, 2013 was our first full year of operation of the Imaging and Medical Beamline Computed Tomography (CT) reconstruction service, which is now operating stably as part of the beamline. We are pleased to provide some early research outcomes within this annual report. We are also excited to be completing work to allow our partners to create and close projects dynamically. This will allow the Australian Synchrotron to allocate MASSIVE projects directly based on beamline merit allocation, create a more seamless user experience and provide researchers with an easier mechanism to continue access to MASSIVE after their synchrotron visit.

Once again training and outreach have been a prominent part of MASSIVE's engagement with the research community. This year we hosted OzViz 2013, which attracted over 120 attendees.

The initiation of the Characterisation Virtual Laboratory (CVL) has had a dramatic impact on our useage and provided a vehicle for us to develop key initiatives. Through the CVL, the AMMRF has been able to provide Australian and international researchers with access to unique analysis software for use with an atom probe (a specialised microscope capable of visualising individual atoms). Likewise, NIF is developing specialised neuroimaging analysis tools, as well as providing researchers across Australia with access to brain atlases.

More broadly, the CVL has provided an opportunity to vastly improve the MASSIVE Desktop by making it easier to access and use. This development alone has dramatically increased the accessibility of MASSIVE, opening it up to a wider range of researchers.

The staff of MASSIVE have been essential to the achievements of 2013 and created a fantastic springboard for growth in 2014. The support and guidance from the Steering Committee (Chaired by Dr Robert Hobbs), the Imaging and Visualisation Scientific Advisory Committee (Chaired by Professor Gary Egan) and the founding organisations helped to ensure the success of MASSIVE in 2013. They have all put MASSIVE in a position to build on the major achievements of 2013 and I look forward to working with them in 2014 and beyond.

The MASSIVE staff and I are excited to be working with the Steering Committee and our key stakeholders to develop a program for our future project, MASSIVE3.

Dr Wojtek James Goscinski
Coordinator
MASSIVE Project

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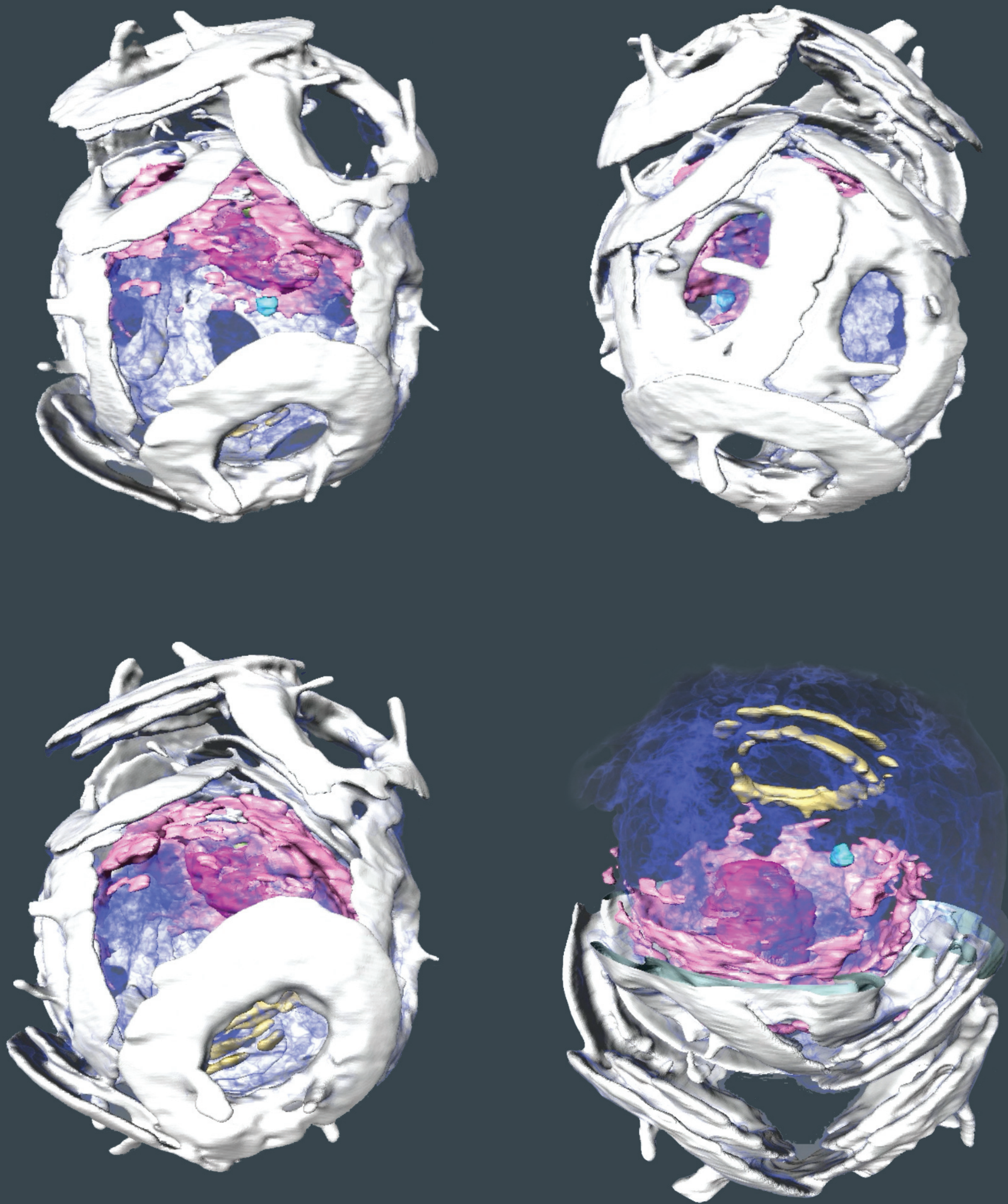

Coccolithosphores are single cell marine algae that capture carbon, locking it into calcite rings (white rings) that move from the centre of the cell to the outer shell and are then are shed to the ocean floor. These tiny structures (1/20th the width of a human hair) are captured using state-of-the-art X-ray computed tomography (CT), with the data processed and visualised using MASSIVE.

Data provided by John Beardall, Philip Heraud and Stuart Larsen. Visualisation by Kaye Morgan

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01.

Achievements in 2013

In 2013, MASSIVE made significant advancements, including growing our user community and improving usability, to become a valuable tool for Australia's researchers.

The major achievements of 2013 include:

- MASSIVE is participant in, or supporting, three successful Australian Research Council (ARC) Centres of Excellence (awarded in December 2013):

  > The ARC Centre of Excellence for Integrative Brain Function led by Monash University will support neuroscience researchers tackling the challenging problems involved in understanding how the human brain works. MASSIVE Coordinator, Wojtek James Goscinski, is the Coordinator for Neuroinformatics and Computational Resources for this centre.

  > The ARC Centre of Excellence for Robotic Vision, led by Queensland University of Technology, is set to create robotic systems that can operate in the complex real world. MASSIVE is contributing High Performance Computing (HPC) time and expertise to help achieve this challenge.

  > ARC Centre of Excellence in Advanced Molecular Imaging, led by Monash University, will develop innovative imaging technologies to explore the immune system, leading to a better understanding of how the immune system functions. MASSIVE is working closely with this project to integrate Cryo-electron microscopy (Cryo-EM) imaging capabilities at The Clive and Vera Ramaciotti Centre for Structural Cryo-Electron Microscopy.

- More than 120 individual projects were undertaken using MASSIVE in 2013 and we reached a major milestone of 400 user accounts. We are developing particularly strong experience supporting neuroinformatics with over 25 neuroscience projects making use of MASSIVE in 2013.
- The stage-2 MASSIVE upgrade was completed in early 2013, significantly increasing the computational and data processing capabilities of our systems. As a result of the stage-2 upgrade our usage increased by 130%.
- The national share of MASSIVE administered through the National Computational Merit Allocation Scheme (NCMAS) once again saw demand significantly exceeding supply. MASSIVE received 19 applications through the NCMAS, with the majority of applications within our area of specialisation. This made MASSIVE the third most requested HPC facility in Australia, as measured by number of projects requested through NCMAS. 17 applications were allocated time on the facility.

More than 120 individual projects were undertaken using MASSIVE in 2013 and there are now more than 400 individual user accounts.

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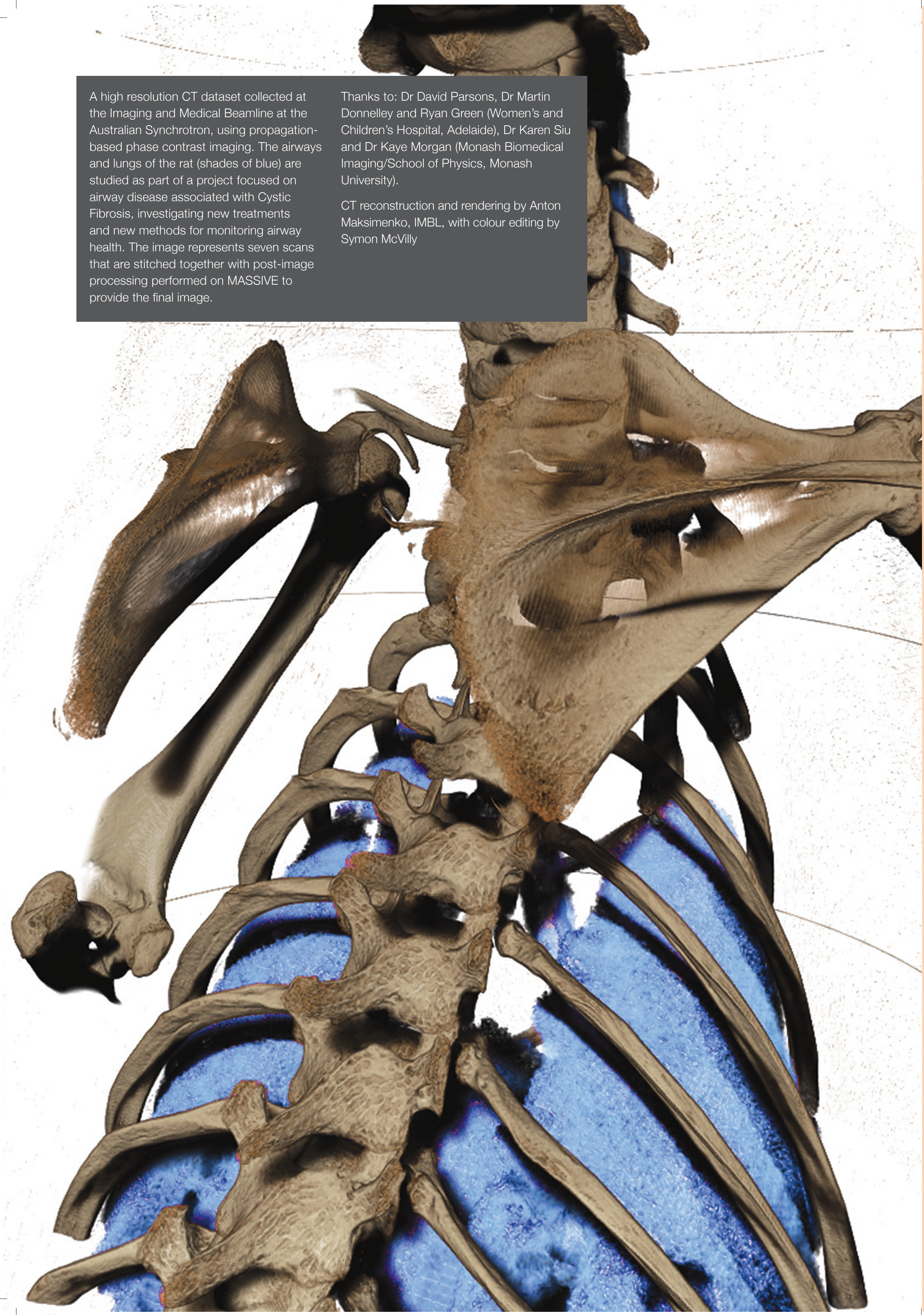


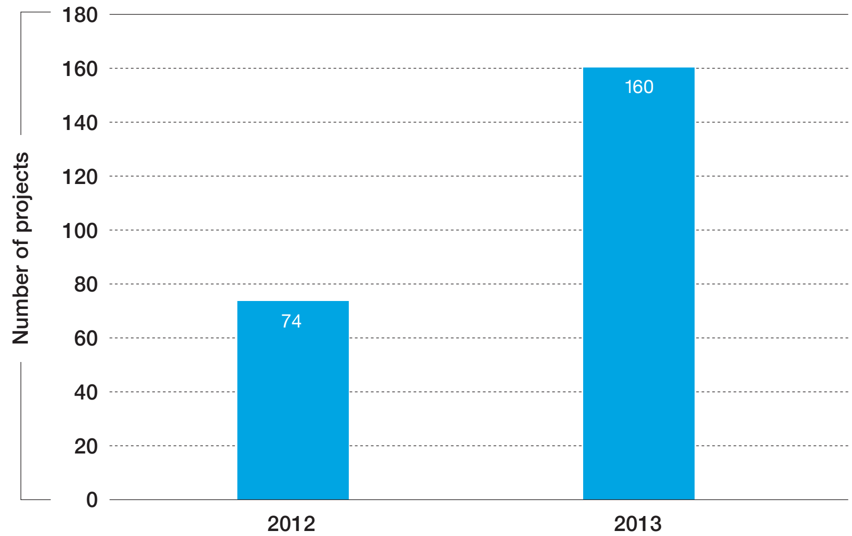
A high resolution CT dataset collected at the Imaging and Medical Beamline at the Australian Synchrotron, using propagation-based phase contrast imaging. The airways and lungs of the rat (shades of blue) are studied as part of a project focused on airway disease associated with Cystic Fibrosis, investigating new treatments and new methods for monitoring airway health. The image represents seven scans that are stitched together with post-image processing performed on MASSIVE to provide the final image.

Thanks to: Dr David Parsons, Dr Martin Donnelley and Ryan Green (Women's and Children's Hospital, Adelaide), Dr Karen Siu and Dr Kaye Morgan (Monash Biomedical Imaging/School of Physics, Monash University).

CT reconstruction and rendering by Anton Maksimenko, IMBL, with colour editing by Symon McVilly

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 and 2013 across MASSIVE projects, as reported in annual Project Leader Reports.



- The CVL has started to demonstrate impact across the characterisation user community:

  > Software developed under the CVL has made the MASSIVE Desktop significantly easier to use and has now been accessed by over 140 researchers. To support this increased demand, we have more than doubled the number of desktop nodes available to users (from 10 to 22 nodes). MASSIVE Desktop users now access it on average two times per week and over half of the users have accessed it more than 50 times. This capability is now a standard but important part of our users research workflow.

  > The ScienTific Remote DEsktop Launcher (STRUDEL) is a tool to make accessing remote desktops easier, that is now being adopted at a number of HPC facilities in Australia.

  > CVL projects in Neuroimaging, Structural Biology, Energy Materials (Atom Probe) and Energy Materials (X-ray) have commenced and are expected to make noteworthy impact in 2014.

- Throughout 2013, we were involved in 20 training or outreach events including the annual OzViz workshop which was attended by over 120 people and included an exhibition of work in Monash University's CAVE2™, with data processing provided by MASSIVE. A major part of the workshop was devoted to analysis and visualisation of 3D datasets.

- As part of our Instrument Integration Program, MASSIVE user projects have been integrated with Australian Synchrotron beamlines meaning that in 2014 projects will be automatically allocated, and closed, based on beamline merit allocation. Importantly, in the future this will provide Synchrotron users with a MASSIVE identity, allowing data processing and visualisation after their beamline visit.

MASSIVE Desktop users now access it on average two times per week and over half of the users have accessed it more than 50 times. This capability is now a standard but important part of our users research workflow.

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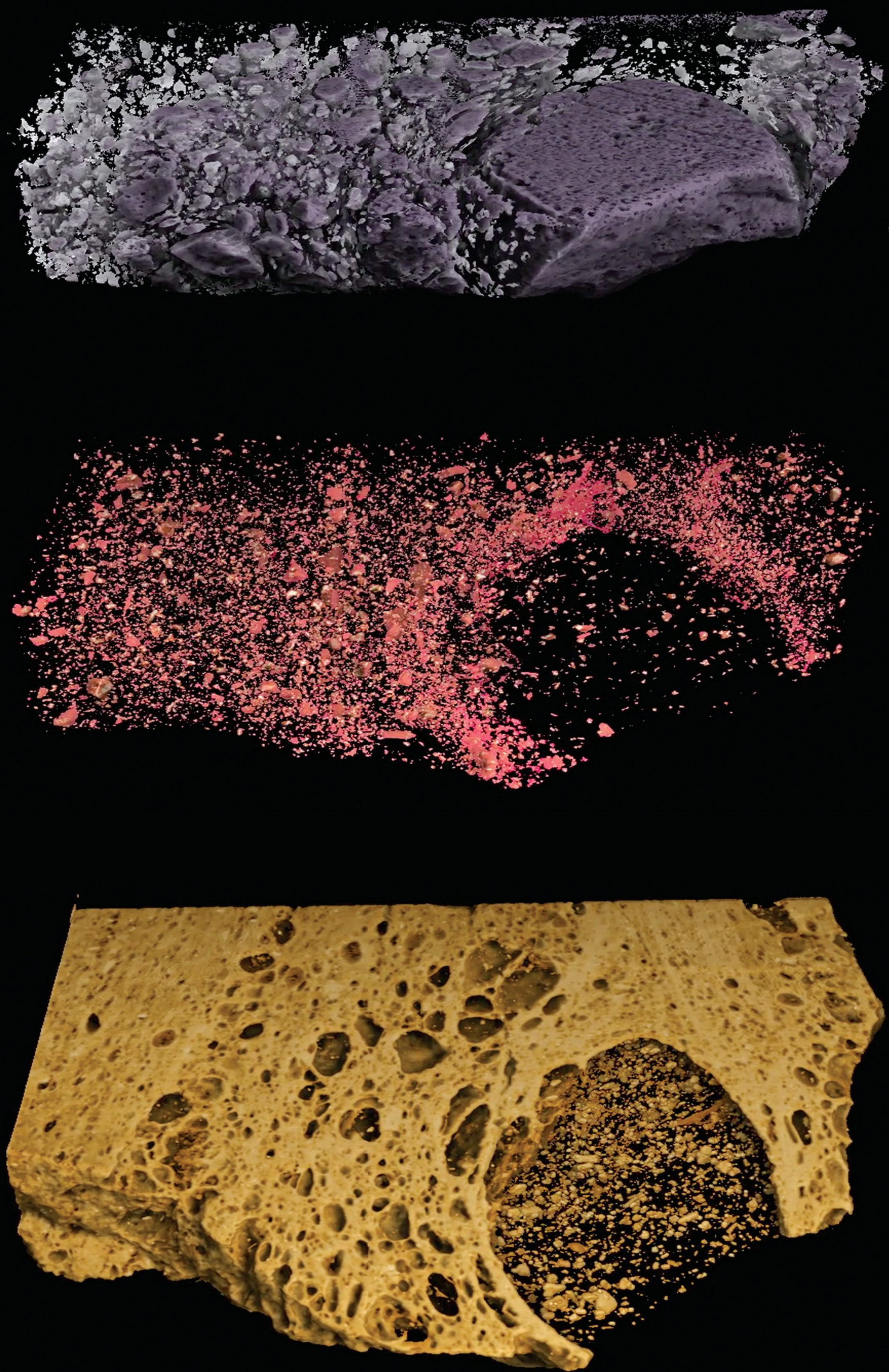

A composite volcanic bomb from Puyehue-Cordón Caulle, Chile. Pyroclasts (volcanic fragments hurled through the air by volcanic activity) were welded back together in the volcanic vent creating a composite volcanic bomb. The purple is pumice clasts and the yellow is welded glass margins. Captured on the Imaging and Medical Beamline at the Australian Synchrotron, the image represents ten scans that are stitched together to achieve the images above.

Image courtesy Ian Schipper of Victoria University of Wellington. Visualisation by Anton Maksimenko, Australian Synchrotron.

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02.

About MASSIVE

The Multi-modal Australian ScienceS Imaging and Visualisation Environment (MASSIVE) is the Australian specialised High Performance Computing facility for imaging and visualisation. This facility provides the hardware, software and expertise to drive research in disciplines such as biomedical science, materials research, engineering and geosciences.

MASSIVE stimulates advanced imaging research that will be exploited across a range of 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.

The facility provides an extensive program of user support and training in all aspects of HPC. It 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 a unique Australian facility with a 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 separate facilities with computer systems linked by a high-bandwidth communications link:

- M1, located at the Australian Synchrotron at 800 Blackburn Road in Clayton; and
- M2, located at the Monash University campus located in Clayton.

These two interconnected computers operate at over 5 and 30 Teraflops, for M1 and M2 respectively, using traditional Central Processing Unit (CPU) processing, and accelerated to over 50 and 120 Teraflops, respectively, using Graphical Processing Unit (GPU) co-processors. They are unique computers in Australia, tailored for fast data processing and visualisation. Both systems are enhanced by software optimised for the characterisation community.

The MASSIVE project aims to:

1. Provide a world-class imaging and visualisation 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 by Australian research groups generally.
3. Increase the performance and capability of 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 supporting the MASSIVE project.

In doing so, MASSIVE expects to:

- Equip research groups with an extended capability to use and develop leading-edge imaging and visualisation facilities.
- See substantial research achievements arising from the use and development of the MASSIVE facility.
- Attract increased investments in the MASSIVE facility and in related imaging and visualisation facilities.

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03.

Service and Capability Development

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

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 multi-dimensional 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 high performance computing 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 to develop research platforms, such as the CVL and to support other research infrastructure programs.

Hardware

The MASSIVE computers have been designed specifically for their purpose. They have a number of features designed to fulfil core data processing and visualisation requirements:

- A high performance file system (498 TB) capable of combined write speeds of 5 Gigabytes (GB) per second. Fast reading and writing of data is essential to enable fast 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. Two GPU co-processors are installed on each compute node across both M1 and M2. GPUs are very effective for accelerating techniques such as CT reconstruction. They are essential for fast rendering for visualisation, and are being quickly applied to a wide range of fields in imaging in particular as well as high performance computing in general.
- Specialised visualisation nodes on M2 with high memory (144 GB per node) and GPUs that are specifically designed for high-end visualisation and hardware rendering.

System Uptime

An important measure of the stability and availability of high performance computing systems is the proportion of time the system is available for use – also referred to as uptime. In 2013, MASSIVE uptime averaged 98.8%. This figure excludes scheduled downtimes for upgrade of the M1 and M2 systems.

General Support

In 2013 MASSIVE continued to provide significant help and support to users, answering over 850 help enquiries ranging from software installation requests to challenging computational problems (see Figure opposite).

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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:

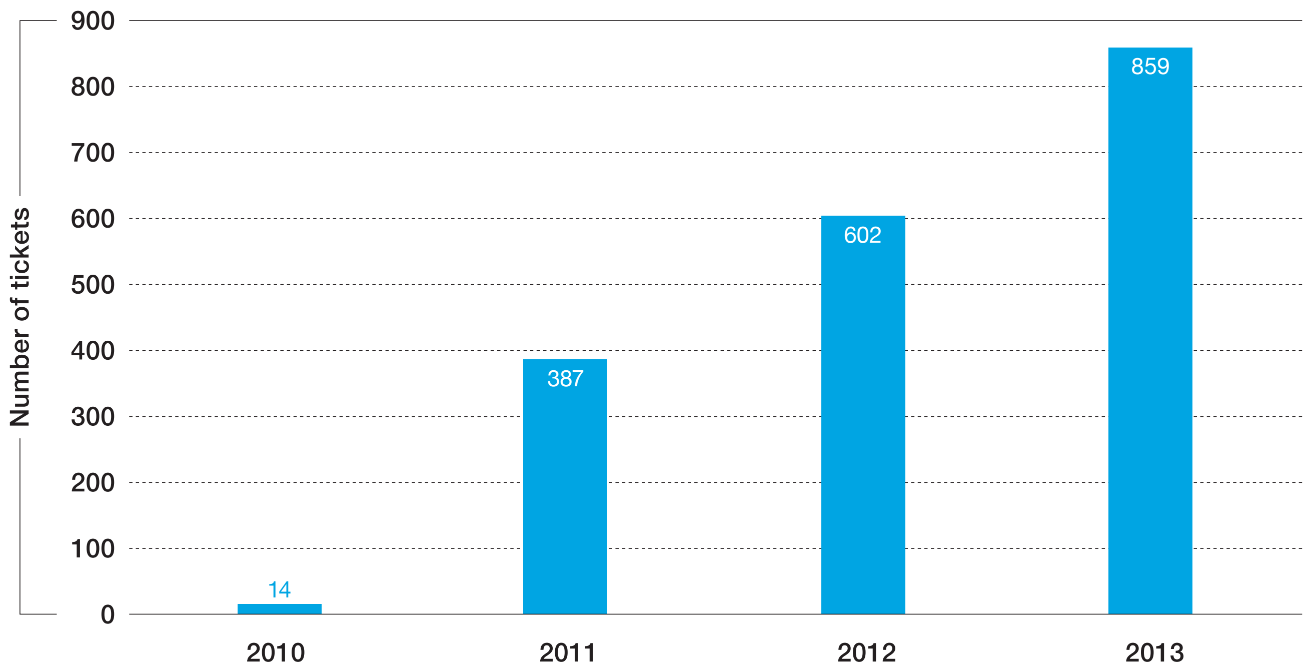
- 2 nVidia M2070 GPUs with 6GB GDDR5 per node
- 58TB + 95TB of fast access parallel file system
- 4x QDR Infiniband Interconnect

M2 at Monash University

118 nodes with a total of cores per node (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

MASSIVE support requests from 2010 to 2013



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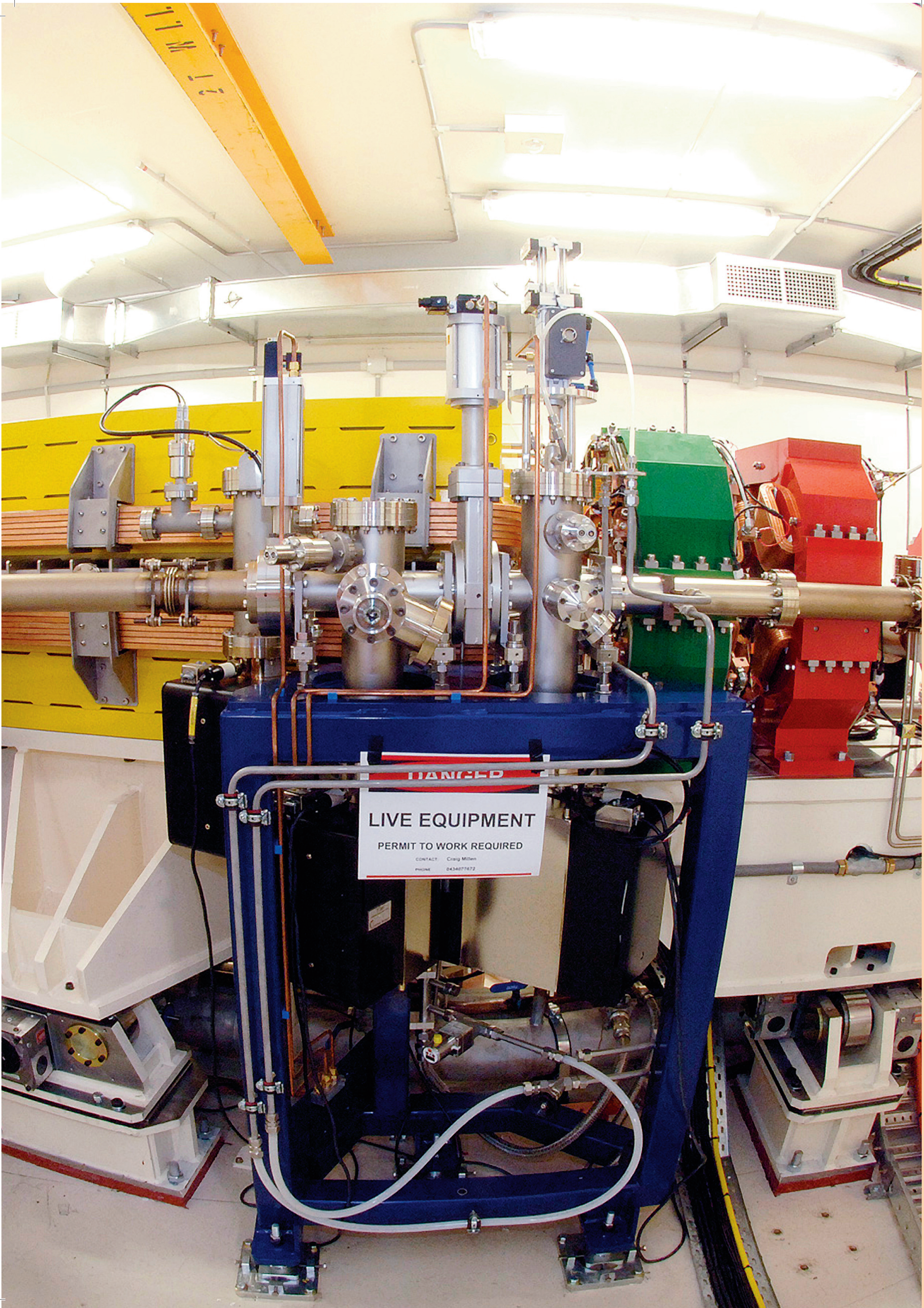

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04.

Instrument Integration Program

The Instrument Integration Program helps connect instruments to MASSIVE, thus providing scientists with the ability to perform sophisticated analysis of captured data. In some cases this allows researchers to analyse and visualise data as the experiment is in progress or shortly after it completes.

Providing access to HPC during an imaging experiment allows researchers to decide whether a scan has successfully produced the desired data – before proceeding with the next step of the experiment. In some cases the images captured by detectors are very large and necessitate the movement of datasets in the Terabyte range. These constraints dictate that significant computing power is available on demand and that the computer is tightly coupled to the instruments.

Australian Synchrotron

MASSIVE provides a computational platform for the Australian Synchrotron to deploy unique data processing workflows for beamline data processing.

Imaging and Medical Beamline (IMBL): Fast data storage and data reconstruction for CT using the X-TRACT software package. Development of this capability has been a collaboration between the MASSIVE partners: Australian Synchrotron, CSIRO, VPAC and Monash University.

The following capabilities at Australian Synchrotron have been developed as beamline initiatives and under the National eResearch Collaboration Tools And Resources (NeCTAR) funded eResearch Tools for the Australia Synchrotron Research Community project to target the MASSIVE systems.

Infrared Microspectroscopy: Extended Multiplicative Signal Correction of infrared (IR) hyperspectral images.

Macromolecular and Micro-Crystallography Crystallography (MX1/MX2): Protein structure determination from MX diffraction images using the Auto-Rickshaw software package.

Small and Wide Angle X-ray Scattering (SAXS/WAXS): Automated real-time data analysis pipeline for the generation of 'first look' results for protein Small Angle X-ray Scattering data to enable informed decision making about the course of the experiment.

X-ray Fluorescence Microscopy (XFM): Performing rapid quantitative and non-destructive Synchrotron X-ray Fluorescence (SXRF) analysis with the GeoPIXE software package on MASSIVE, enabling rapid concurrent analysis sessions (near real-time and post-experiment).

Monash University

Monash Biomedical Imaging: A number of data capture and processing workflows have been developed to support researchers analysing data collected on CT and MRI systems.

Laboratory for Dynamic Imaging: MASSIVE is collaborating with staff and postgraduate students to allow efficient transfer and processing of data from the Dynamic X-ray Imaging Facility, a first of its kind facility for realtime imaging of biological dynamics.

The Clive and Vera Ramaciotti Centre for Structural Cryo-Electron Microscopy. Through the CVL, MASSIVE staff have been assisting the design of the data management and processing environment for CryoEM instrumentation to be installed in 2014.

National Projects

Through the CVL, MASSIVE is supporting integration of a number of key exemplar instruments with analysis capabilities in the NeCTAR cloud. These capabilities will be available to users in 2014.

Atom Probe at the Australian Centre for Microscopy and Microanalysis at the University of Sydney: The University of Sydney is developing a toolkit and workflows for processing of atom probe data.

X-ray CT instruments at Australian National University: Australian National University (ANU) is using the CVL to deploy a number of existing analysis tools and workflows, including Mango.

MRI equipment at the Centre for Advanced Imaging, at the University of Queensland: The University of Queensland and University of Melbourne are using the DaRIS software to integrate MRI equipment with the CVL Workbench for neuroimaging.

Left — A photo of part of the accelerator at the Australian Synchrotron which accelerates electron beams for use in the generation of synchrotron light. Photo courtesy of the Australian Synchrotron.

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05.

Characterisation Virtual Laboratory

MASSIVE has a key role in the development of research infrastructure for the characterisation community.

Over the last ten years, governments and research organisations have made large investments in Australian imaging instruments. As a result, researchers now have access to powerful microscopes through AMMRF, high-resolution medical imaging equipment through NIF, unique nuclear capabilities through ANSTO and rapid acquisition X-ray imaging at the Australian Synchrotron. Each of these facilities enables researchers to acquire large amounts of data in a short space of time, all of which needs to be analysed and visualised. MASSIVE is helping to develop infrastructure that provides this data processing capability. In particular:

- MASSIVE is developing software as part of the $3.2M Characterisation Virtual Laboratory (CVL) project. This collaboration is composed of members of the Australian Characterisation Council, Australian Synchrotron, ANSTO, AMMRF and the NIF, along with Monash University, University of Queensland, Australian National University, and University of Sydney. MASSIVE participates in this project to build usage amongst the research areas of neuroscience, structural biology, and energy materials. MASSIVE is also participating in the CVL project to enhance interactions with the broader characterisation community, as well as to further develop the interactive analysis and visualisation capabilities of MASSIVE.
- MASSIVE and the CVL are platforms for a number of further projects funded by the NeCTAR initiative including Cloud-Based Image Analysis and Processing Toolbox (with CSIRO) and eResearch Tools for the Australian Synchrotron research community.

The CVL has three main functions:

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;
2. To provide scientists with a common cloud-based environment for analysis and collaboration; and
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). These domain-specific versions of the CVL will be completed (and handed over to end users for on-going development and maintenance), in mid 2014.

MASSIVE's major role in the CVL is the developer of the underlying software infrastructure, which will be complete in early 2014.

As at December 2013, the CVL project was approximately 60% complete and had already made an impact in a number of ways. Indeed, the CVL Workbenches have increased NeCTAR cloud uptake and reduced barriers to use amongst their respective communities.

Early highlights of the CVL project include the uptake of the Atom Probe Workbench (Page 15), the application of the MASSIVE Desktop to anatomy research (Page 16), the development of STRUDEL (Page 19), and applying the CVL to neuroimaging (Page 19).

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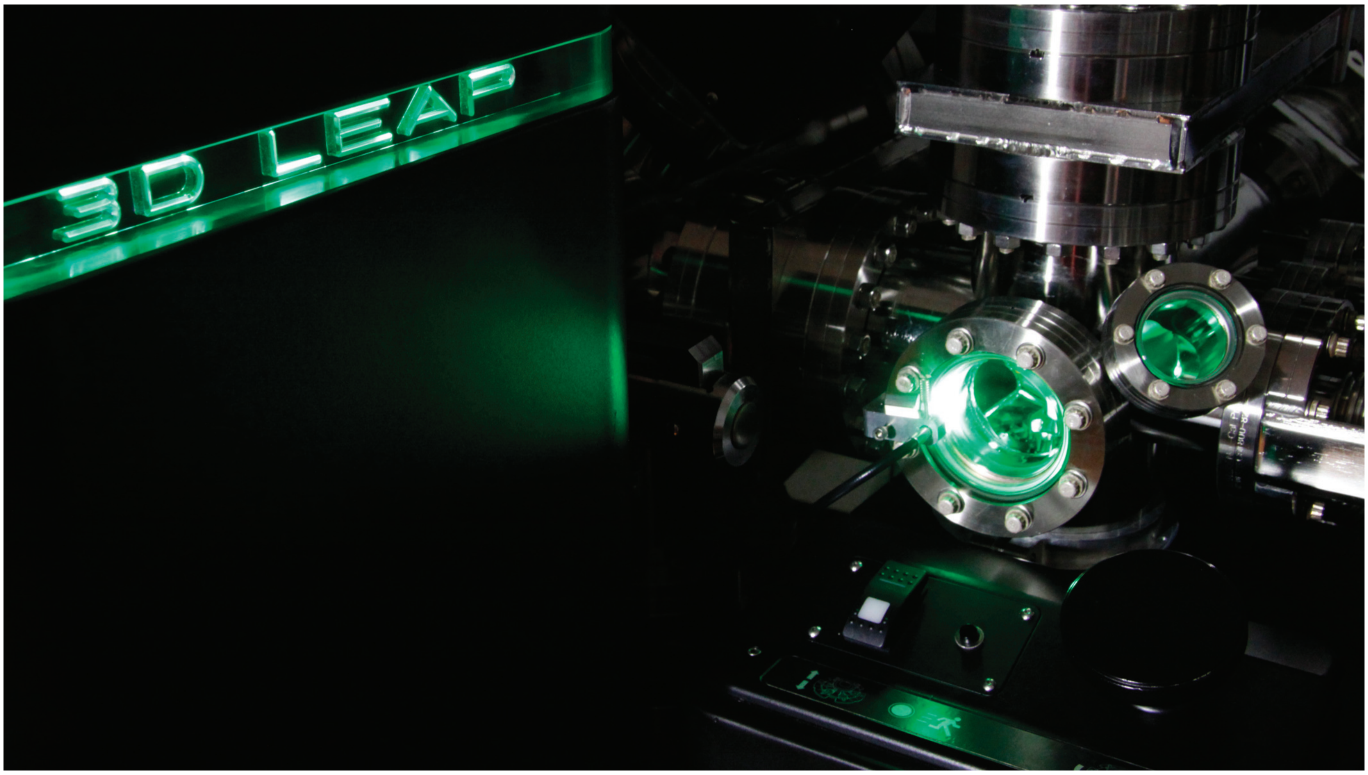

Working with Atoms

The Australian Microscopy and Microanalysis Research Facility (AMMRF) has a broad vision that includes being the characterisation facility of choice for researchers in Australia. Part of achieving this vision includes providing researchers with access to world-class imaging and associated analysis infrastructure.

For their part in the AMMRF, the University of Sydney has an atom probe — an advanced type of microscopy platform allowing visualisation of individual atoms and 3D reconstruction of the surface of materials. Atom probes are particularly useful in the fields of metallurgy, to determine chemical composition of alloys, and semiconductors to help design nanometre scale electronics.

As a visualisation platform, an atom probe has what might be described as mechanical components and software components. The mechanical components provide opportunities to visualise structures at the atomic scale, and the software components reconstruct the data into a form that can be visualised in 2D or 3D. Thus, the software component, and the associated computational infrastructure, are essential parts of the atom probe.

Over the past few years, researchers at the University of Sydney, led by Professor Simon Ringer, have been developing specialist computer programs to aid in data analysis. Indeed, they are a world-leading research group in the development of computational atom probe microscopy techniques. As other groups do not have the capacity to program these tools themselves, the atom probe group at the University of Sydney brings important capabilities to researchers worldwide. However, so far these capabilities have only been enjoyed by University of Sydney atom probe researchers and their direct collaborators. This is beginning to change as a result of development of the CVL and the associated Atom Probe Workbench.

By deploying these computer programs within the Atom Probe Workbench as part of the CVL, the programs are available to the wider atom probe community, not just Sydney University researchers. “It is this increased availability that will make the most impact,” said Dr Anna Ceguerra (a member of Professor Ringer’s team), “as people around the world will be able to use the specialist programs without having to invest in programming these codes themselves.” Added to this, the CVL is connected to MASSIVE and therefore able to provide the computational resources required to perform the 2D and 3D reconstructions.

Although these changes are having a world-wide impact in the atom probe community, they are also facilitating local change. For example, summer scholarship students within Professor Ringer’s team are offered research projects related to computational atom probe microscopy. Previously they were given access to a shared linux server. Now, with the Atom Probe Workbench within the CVL they are given a CVL account and join the existing projects related to their work. Dr Ceguerra praised this arrangement for two reasons. Firstly, it gives students “access to their own virtual machine with their own computational resources” (i.e. their own work environment they can access from any computer). Secondly, the CVL is able to provide the students with access to “experimental versions of the computer programs they are developing along with versioning control” (i.e. they can see the previous versions of code and their impact on the program as a whole). “The CVL project is leading the effort to move science data analysis to the cloud and thus provide a more flexible and more powerful environment”.

Above — The Atom Probe microscope at the University of Sydney. Photo courtesy of Jennifer Whiting and Anna Ceguerra.

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Making Research Computing More Accessible

Software developed under the CVL has made MASSIVE a more user-friendly environment and is allowing a broader range of researchers to exploit the facility. This includes anatomy researchers at the Department of Anatomy and Developmental Biology at Monash University's School of Biomedical Sciences.

Dr Justin Adams, Ms Michelle Quayle and colleagues are using MASSIVE to achieve 3D digitisation of human anatomy and thus provide access to anatomical information that is otherwise not easy to visualise — such as the ventricles of the brain. The project involves segmenting imaging data from equipment such as MRI machines or Positron Emission Tomography/Computed Tomography (PET/CT) scanners and reconstructing it into electronic 3D models. These 3D electronic models are further processed to create real 3D printed models of the anatomical region of interest.

Using MASSIVE the researchers can access specialised segmentation software and create the necessary 3D constructions from a standard desktop computer with access to the internet.

As testament to the usability of MASSIVE and the impact of the CVL, this project was undertaken by undergraduate biomedical science students enrolled in summer internships with Dr Adams and Ms Quayle. "We would not have pitched segmentation projects (for summer students) if not for MASSIVE and the CVL" said Dr Adams. Ms Quayle, added "prior to MASSIVE and the CVL, if such a project were provided to summer students, the laboratory would have needed a high-end visualisation workstation for each student". That amount of infrastructure is impractical for most laboratories.

"We would not have pitched segmentation projects (for summer students) if not for MASSIVE and the CVL"

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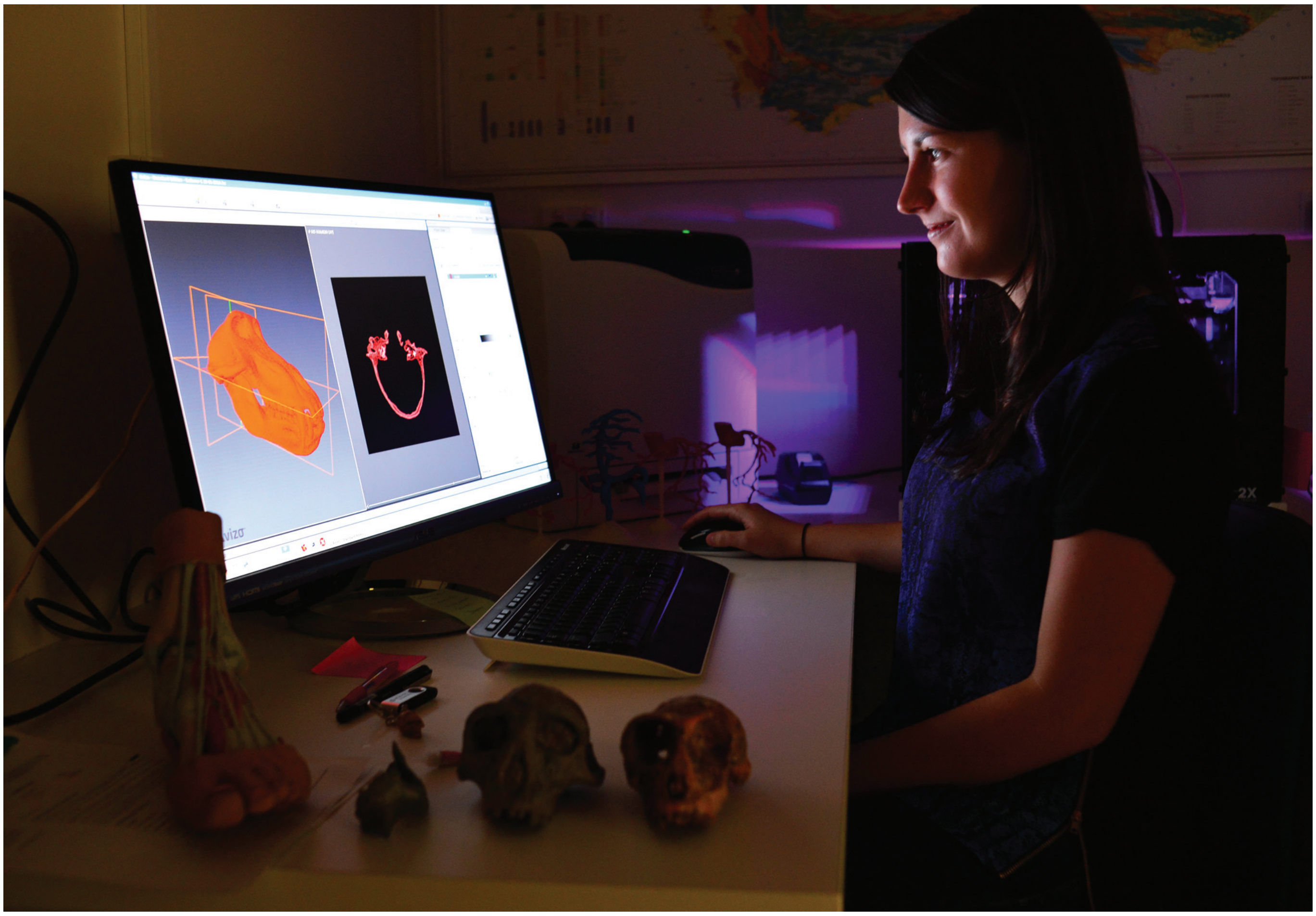

Through MASSIVE research have access to a high-performance desktop environment. Data stored on MASSIVE can be analysed using interactive desktop tools underpinned by a fast parallel file system, high memory and fast GPU rendering.

For the anatomy group, this has provided a high powered environment with shared software licenses that would not otherwise be available. Moreover, students could share their work with each other, and their supervisors, and training could be provided in a standard computer lab with each student operating their own machine.

The MASSIVE Desktop

The MASSIVE Desktop has proved to be popular amongst a range of MASSIVE users, including those analysing images in neuroscience, geology, materials science, palaeontology, and biological fluid dynamics. Remote desktop access to MASSIVE is essential because:

- Many of our users work with big data collections – as data and study sizes increase it becomes more practical to perform data analysis and rendering at the very location where the data is stored;
- Performing analysis and visualisation centrally allows researchers to access performance hardware, including a fast file system and GPUs;
- A remote desktop allows us to support a wide range of analysis tools and does not require wrapping or re-engineering of those tools. Users have access to the desktop tools they know and understand.

We expect this will allow scientists to focus on using tools and applying sophisticated analysis techniques, rather than on installing and configuring software or copying data, and will provide a wider range of researchers access to high-end computing.

Left — 3D printed models are one of the products of Dr Justin Adams' and Ms Michelle Quayle's work with anatomy students. These models will be used in teaching.

Above — Ms Michelle Quayle manipulating one of her 3D scans using the MASSIVE Desktop.

Photos courtesy of Philip Chan.

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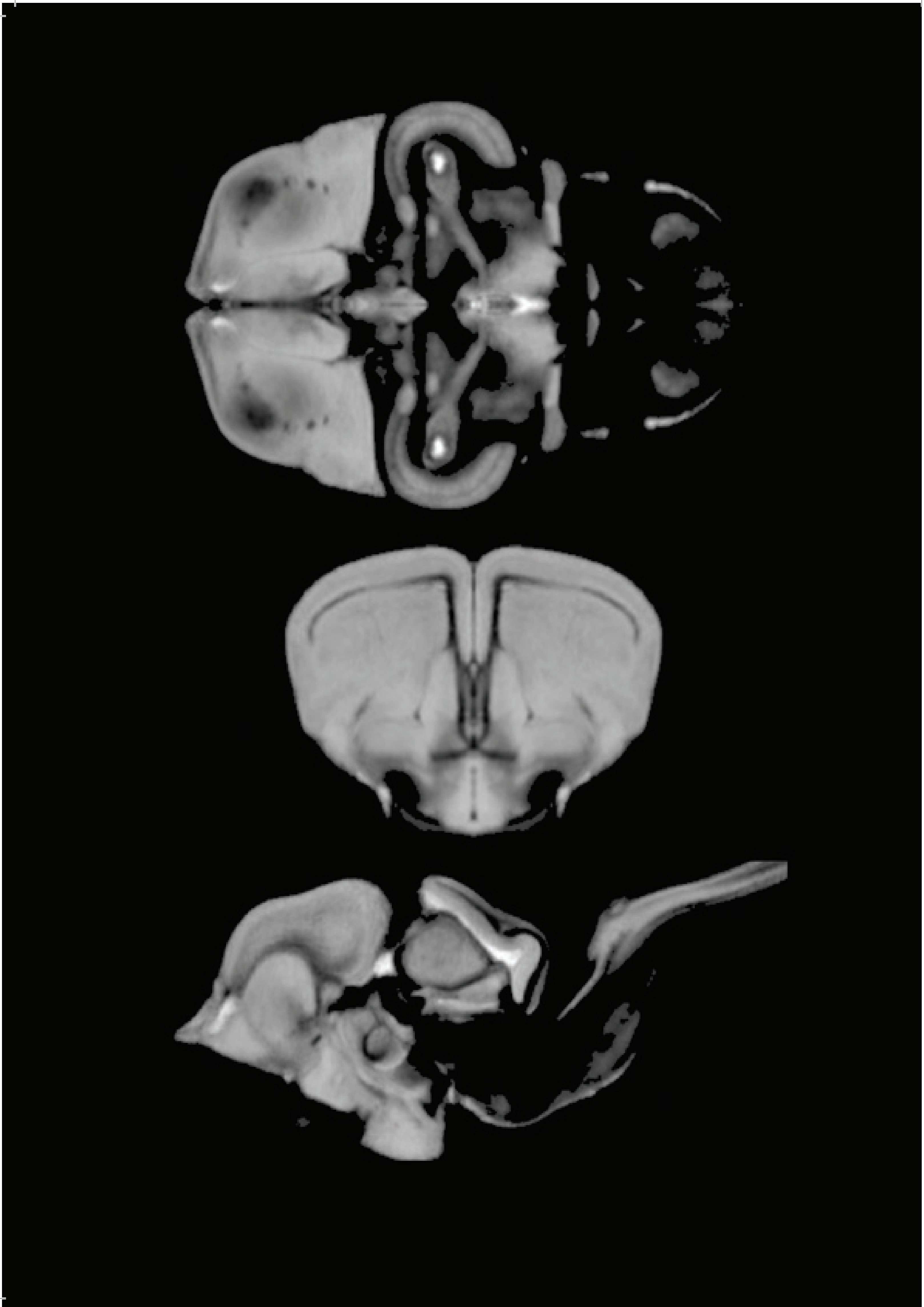

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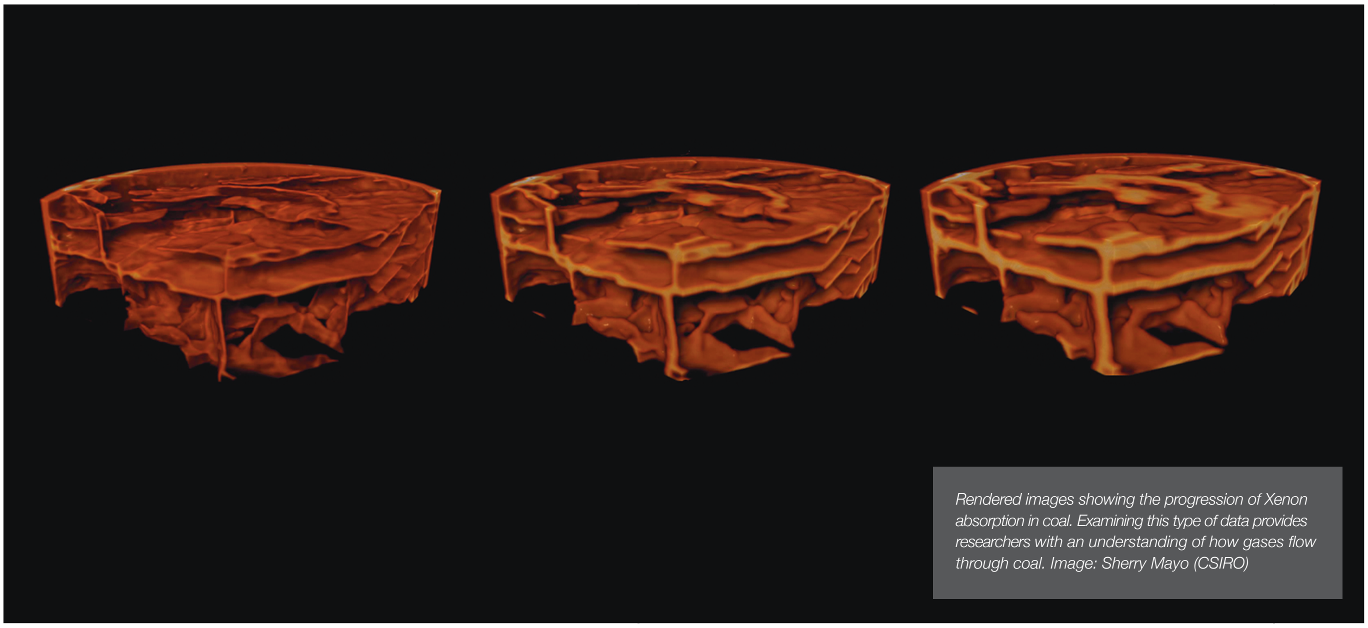

Rendered images showing the progression of Xenon absorption in coal. Examining this type of data provides researchers with an understanding of how gases flow through coal. Image: Sherry Mayo (CSIRO)

Attracting Users with STRUDEL at CQU

Central Queensland University's (CQU) Research Technology Support have deployed STRUDEL on their local CQU HPC system. Since this deployment, STRUDEL has dramatically simplified HPC access for CQU researchers.

Previously, accessing remote desktops at CQU was achieved using the command line which created an unintended barrier to use. Feedback suggested a user-friendly point-and-click interface would improve use and provide a stepping-stone to accessing the full HPC capabilities.

In late-2013, STRUDEL was launched at CQU and has assisted in HPC user uptake, especially in regards to users not familiar with HPC or command line environments. STRUDEL has been one of a number of key strategies that have helped to increase the number of unique users. The last half of 2013 saw a doubling on unique users when compared to the previous half-year.

The deployment of STRUDEL had further positive consequences. "Most notable was a reduction in the amount of HPC support required, particularly relating to establishing user accounts and refresher training" said Jason Bell, Research Technologies Officer at CQU. The success of STRUDEL at CQU has raised the profile of STRUDEL, the CVL and MASSIVE amongst Queensland universities, with many showing interest in deploying STRUDEL to improve the HPC experience for their users

What is STRUDEL?

STRUDEL is a tool developed by the MASSIVE team to make it easier to access remote desktop environments running on an HPC or cloud. It is developed under the CVL and is used to access CVL workbenches across Australia, the MASSIVE systems in Melbourne, and now also at CQU. The MASSIVE team is continuing to develop the tool in 2014 and is actively working with other sites to deploy it locally to their users.

Neuroimaging using the CVL

Since its inception the National Imaging Facility has identified that one of the barriers that researchers need to overcome in modern imaging is access to sufficient computer power with the necessary software to perform analyses on very large data sets. Professor Galloway, Director of Operations for the National Imaging Facility, joined with other colleagues from Characterisation to advocate for computing infrastructure, to be made available to the wider research community. NIF welcomed the opportunity to work with MASSIVE to develop the CVL to provide an environment where researchers could connect these large datasets with appropriate compute facilities, and the necessary software.

Animal models are a critical part of understanding physiology, as well as developing novel therapies, but this research is often underpinned by identifying quite subtle changes in tissue structure and function. For statistical significance this research often utilises large numbers of animals, which greatly increases the amount of data, which required specialised computing facilities.

Mouse models are the commonest mammalian model for understanding many diseases, especially those that arise from genetic variation. Imaging is an important tool in characterising genetically modified animals. If there is access to a probabilistic model, then this can be compared, computationally with the variant, and small unanticipated changes can be identified. The development of the Mouse Brain atlas by the Australian Mouse Brain Mapping Consortium, led by Professor David Reutens from The University of Queensland, is one such tool. This data will be made available on the CVL, providing researchers from around Australia with the model, with which to compare their genetic variants. Furthermore, the CVL has, preinstalled, the software tools for the researcher to use to make those comparisons.

Opposite — Daniel Hoops (Australian National University), working with the National Imaging Facility and software integrated under the CVL Neuroimaging Workbench, generated this, the first 3D MRI-based model of a lizard brain. The model is based on MRI images of the brains of 14 individuals lizards and has a voxel size of less than 25 um. In collaboration with NIF researchers, he is using this model to measure differences in the brains of a variety of Australian dragon lizards. This involves processing MRI images of the brains of almost 300 lizards, towards the goal of better understanding evolutionary and ecological influences on variation in brain structure.

Image: Daniel Hoops & Scott Keogh (Australian National University), and Jeremy Ullmann & Andrew Janke (University of Queensland).

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06.

Research Stories

Neuroimaging

To study diseases of the brain, scientists commonly turn to MRI, a non-invasive scanning method, allowing researchers to undertake large studies or multiple scans with no negative effects. Researchers are able to scan a large population to ensure a strong statistical analysis, and patients can be scanned multiple times to capture change across a human timescale.

Large MRI studies require vast amounts of processing to analyse all of the data collected and to unlock the knowledge within. MASSIVE is helping neuroscientists to tackle this processing problem by providing tailored environments for high throughput neuroanalysis. MASSIVE currently supports over 25 Australian neuroscience research projects that include scientists who are making significant Australian-led advances in neuroscience.

In two separate projects that make use of MASSIVE, Australian researchers are making an impact on the world stage. In one study, University of Queensland and CSIRO researchers (including Associate Professor Katie McMahon) have demonstrated that some connections in the brain are strongly influenced by genes; suggesting some areas of the brain are more likely to be impacted by genetic diseases. This research is part of a world-wide collaborative called ENIGMA — Enhancing Neuro Imaging Genetics through Meta Analysis. ENIGMA combines the research efforts and data from large neurological research studies from across the world. Such a large dataset allows the identification of small (genetic) changes on brain development and function.

For their part in the research, Associate Professor McMahon and her collaborators scanned the brains of over 1,150 identical twins. The images were then compiled into a brain network representation that was able to reveal the relationship between genes and brain structure (i.e. the areas that are inherited versus those that are not). The findings have implications for the study of genetic disorders of the brain including Alzheimer's and Huntington's Disease. The computing power of MASSIVE was essential to project success.

Associate Professor McMahon and her collaborator Mr Strike agreed "there was no means us to duplicate the processing power available through MASSIVE, and it is possible that the analysis may not have been deemed feasible without MASSIVE".

Dr KaiKai Shen (a collaborator from the CSIRO) praised the data computing power of MASSIVE noting it performed the "major heavy lifting task [of the research] involving a large number of image registrations" (6,000 registrations at four to ten hours each).

In the second project, Professor Nellie Georgiou-Karistianis (Monash University) and her team are using MASSIVE to help conduct a longitudinal study — The IMAGE-HD study.

This project aims to track the onset and progression of Huntington Disease (HD), which will help us to understand how the disease develops over time. Through this research, the team found the number of poorly connected neural networks increased in people diagnosed with HD, compared to those without the disease. They also found that as the disease develops, the changes in the brain become more widespread.

These findings have important implications for drug development, particularly in terms of treatments geared toward preventing loss of neural connections, strengthening neural connectivity, and/or improving functional outcomes.

Dr Poudel, senior research fellow of the IMAGE-HD team, noted that "in the absence of MASSIVE our analysis pipeline would have significantly slowed down — approximately 20 times". He went on to say the "Parallel processing [capabilities of MASSIVE] allowed us to obtain results for 108 subjects over three time points in a couple of hours rather than days". MASSIVE has become a significant part of Dr Poudel's research tool kit. "MASSIVE is an impressive tool, which not only allows rapid analysis but also allows visualisation at a level not possible with other systems."

Opposite: images of the brain, showing connectivity between various regions, based on MRI data and computed using MASSIVE.

Image supplied by Kai Kai Shien (CSIRO)

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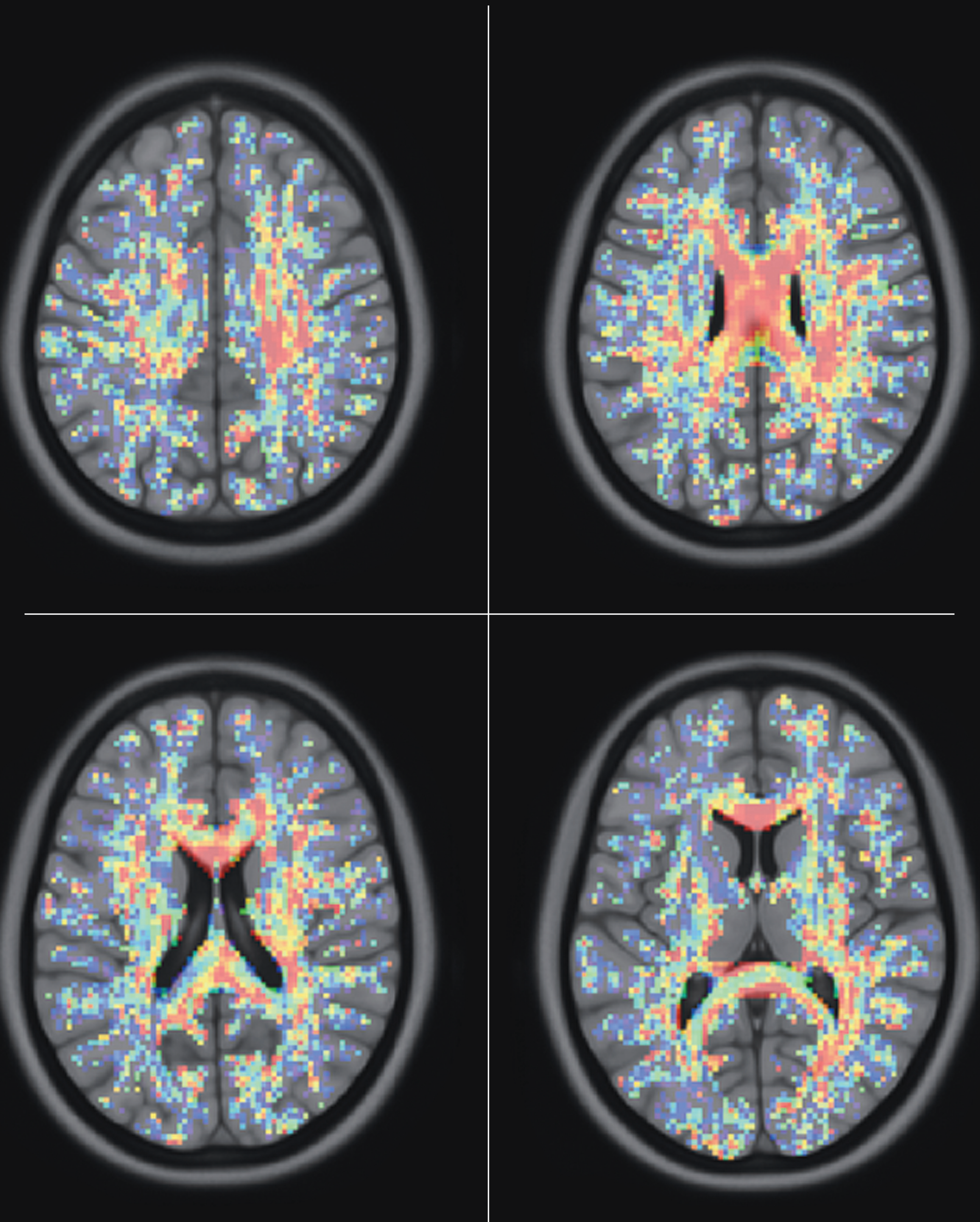

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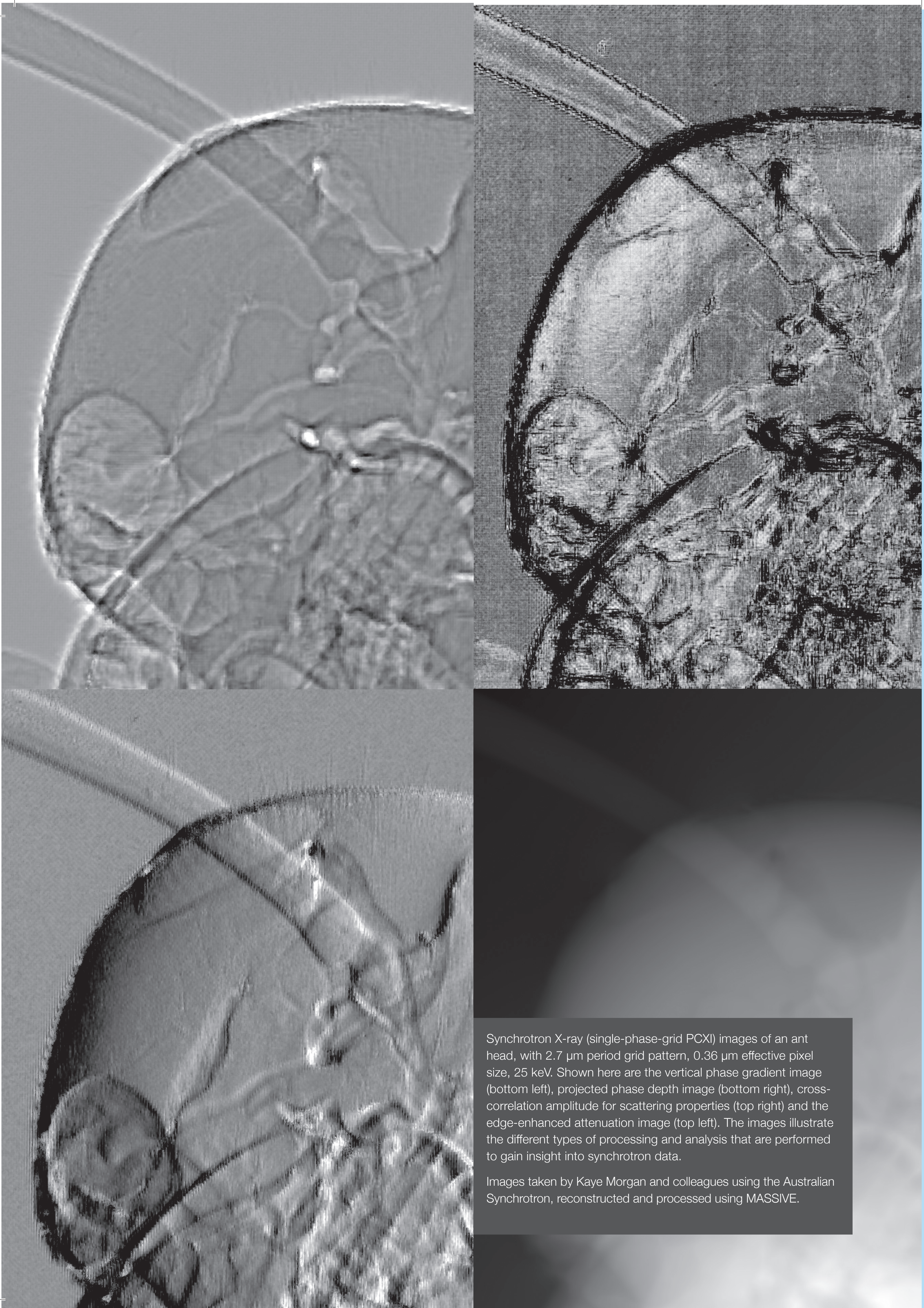

Synchrotron X-ray (single-phase-grid PCXI) images of an ant head, with 2.7 μm period grid pattern, 0.36 μm effective pixel size, 25 keV. Shown here are the vertical phase gradient image (bottom left), projected phase depth image (bottom right), cross-correlation amplitude for scattering properties (top right) and the edge-enhanced attenuation image (top left). The images illustrate the different types of processing and analysis that are performed to gain insight into synchrotron data.

Images taken by Kaye Morgan and colleagues using the Australian Synchrotron, reconstructed and processed using MASSIVE.

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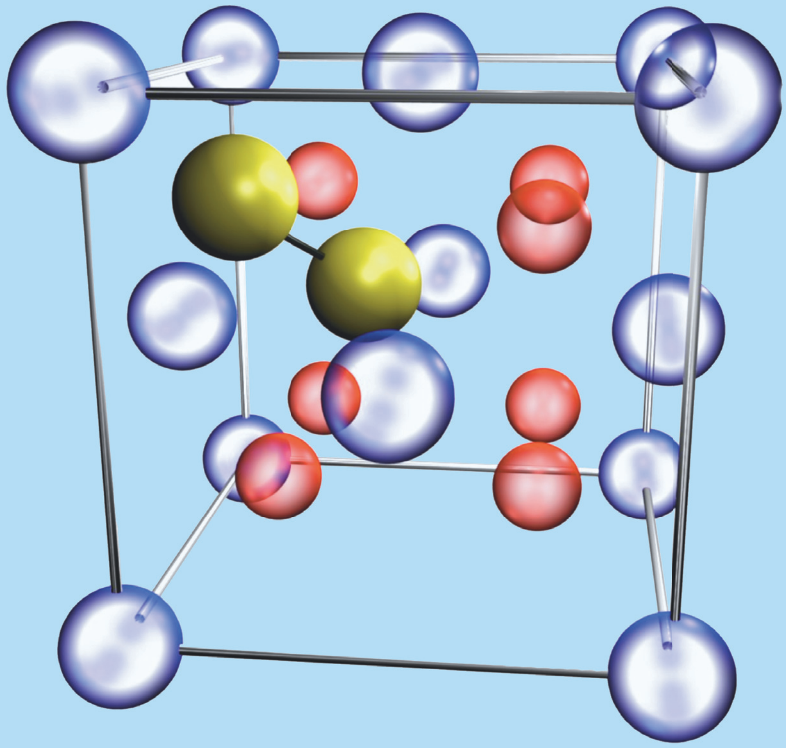

Modelling Novel Alloys

Researchers from the ANSTO Nuclear Materials Modelling and Characterisation program are using MASSIVE to simulate the fundamental structure-property relationships of nuclear materials.

Dr. Simon Middleburgh and his group examines materials before, during and after radiation damage processes using a range of experimental and atomistic modelling techniques. These simulations provide information to support development of new materials that could be used in advanced energy applications such as advanced fission and fusion systems as well as specialist materials for the high technology sector.

The group's work contributes to global research into radiation damage effects, whilst also improving the design of materials for use within nuclear environments, such as reactor pressure vessels, additives to fuel and waste-forms.

Using MASSIVE, the group is able to propose and test new materials that might be capable of accommodating transmutation products and crystal damage as part of radiation processes — and thus potentially useful as structural nuclear reactor materials, additives to nuclear reactor fuel or waste-forms. Using density functional theory and empirical atomic methods, Dr. Middleburgh is simulating the expected radiation tolerance and response to displacing irradiation in a number of ceramics.

The results of the simulations provide researchers with an indication of what ceramic recipe might form stable products as part of nuclear decay. These theoretical materials are then manufactured and their properties tested in real life by the dedicated scientists at ANSTO.

This high throughput simulation-based screening method has allowed Dr. Middleburgh and his team to increase their productivity and thus their publication of research articles. Indeed, in a recent report, Dr. Middleburgh noted "This resource (MASSIVE) is expected to continue to be used as the cornerstone of (their) research over the foreseeable future. Without it, the sheer number of published papers that have been accepted would not have been possible this year."

"We have found the resource immeasurably important to our research and we are so grateful for the expert running and maintenance of the resource. We have achieved a great deal in the short time and hope to achieve more in the following years with the same resource. We have nothing but praise for the facility and the people that run it"

> "This resource (MASSIVE) is expected to continue to be used as the cornerstone of (their) research over the foreseeable future. Without it, the sheer number of published papers that have been accepted would not have been possible this year."

Above — An outcome of one of the ANSTO defect simulations of a ceramic oxide (ThO_2) showing the position of a molecule of peroxide (2 oxygens shown in yellow), oxygen (red) and thorium (purple). In this example the ease of excess oxygen accommodation and migration indicated the oxide behaved differently to other fuel types, thus saving the researchers time and money on difficult experiments whilst improving future fuel safety.

Image provided by Dr Simon Middleburgh

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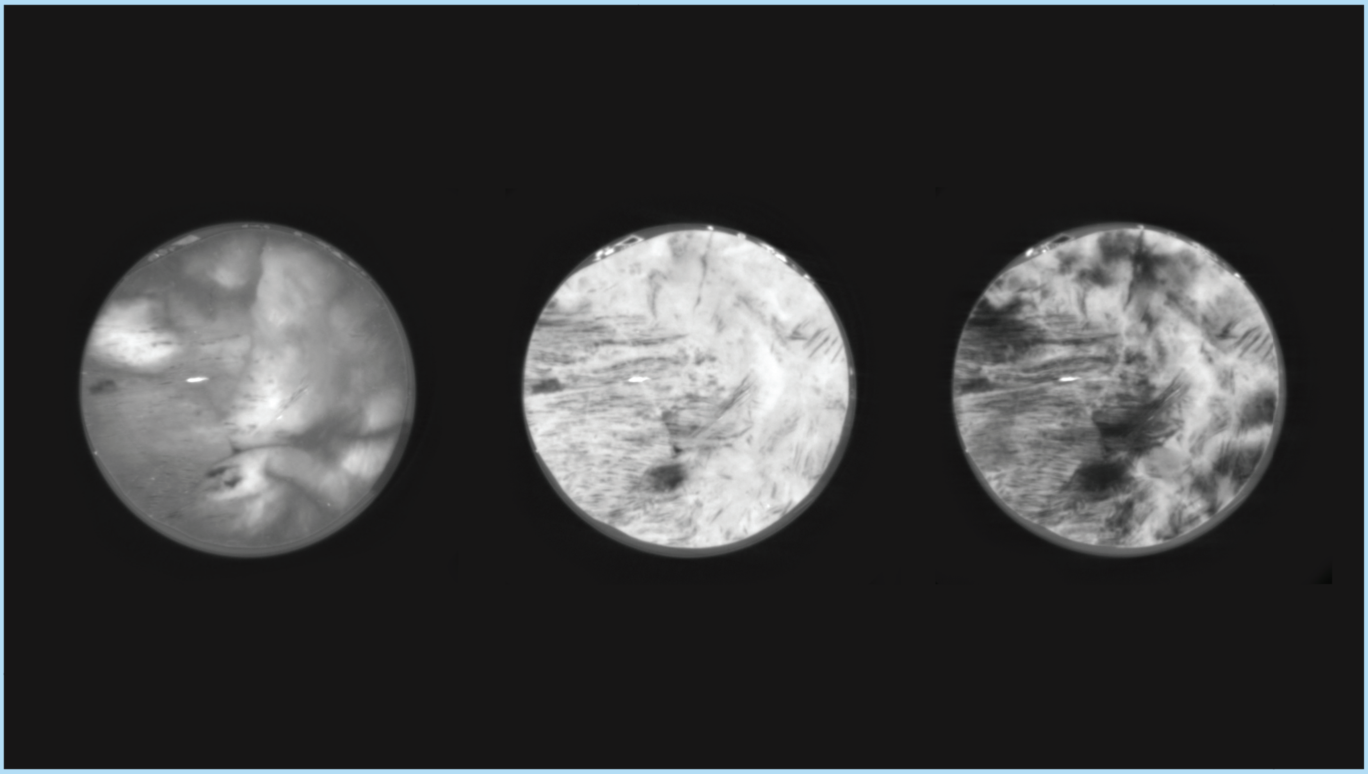

Imaging and Medical Beamline

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 at the molecular level in 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 has been a collaboration between Australian Synchrotron, Monash University, CSIRO and VeRSI / VPAC.

The capability will be broadly applicable to many research areas. There is already anticipation in the research community of the possibilities available to medicine, life sciences and geosciences. Two case studies below highlight the potential:

Mining Data to Find Oil and Gas

With increasing interest in carbon sequestration and coal-seam gas extraction, it is increasingly important to improve our understanding of gas exchange in coals. Recent experiments on the microstructure, porosity and fluid flow in porous rocks are showing how water and CO_2 can be used to drive oil and gas through reservoir rocks.

The capabilities of MASSIVE are allowing geologists to gain a greater understanding of fluid movement. Using Micro-CT, Dr Sherry Mayo and Ben Clennell (CSIRO) are able to visualise porosity of samples as small as three or four millimetres across. Coupling this with sophisticated data processing techniques, such as Data Constrained Modeling analysis and K-edge subtraction, they are able to determine the porosity, connectivity and composition of rock core samples.

High-speed tomography at the Australian Synchrotron has enabled time-resolved studies of gaseous exchange in different types of Australian coal.

Researchers believe this has enormous consequences for improving the outcomes of coal seam gas extraction and carbon sequestration.

Deeper insight has been gained by linking these techniques with the X-ray image processing capabilities of X-TRACT. X-TRACT gives researchers increased scope by providing higher resolution imagery, spatial reference, drift correction and multiple methods of amplitude/phase reconstruction.

This is possible due to the combination of X-TRACT software running on MASSIVE, allowing scientists to analyse large amounts of data in near real time. This makes dynamic studies of geomaterials much more practical, as a significant proportion of the data processing can be done during data capture.

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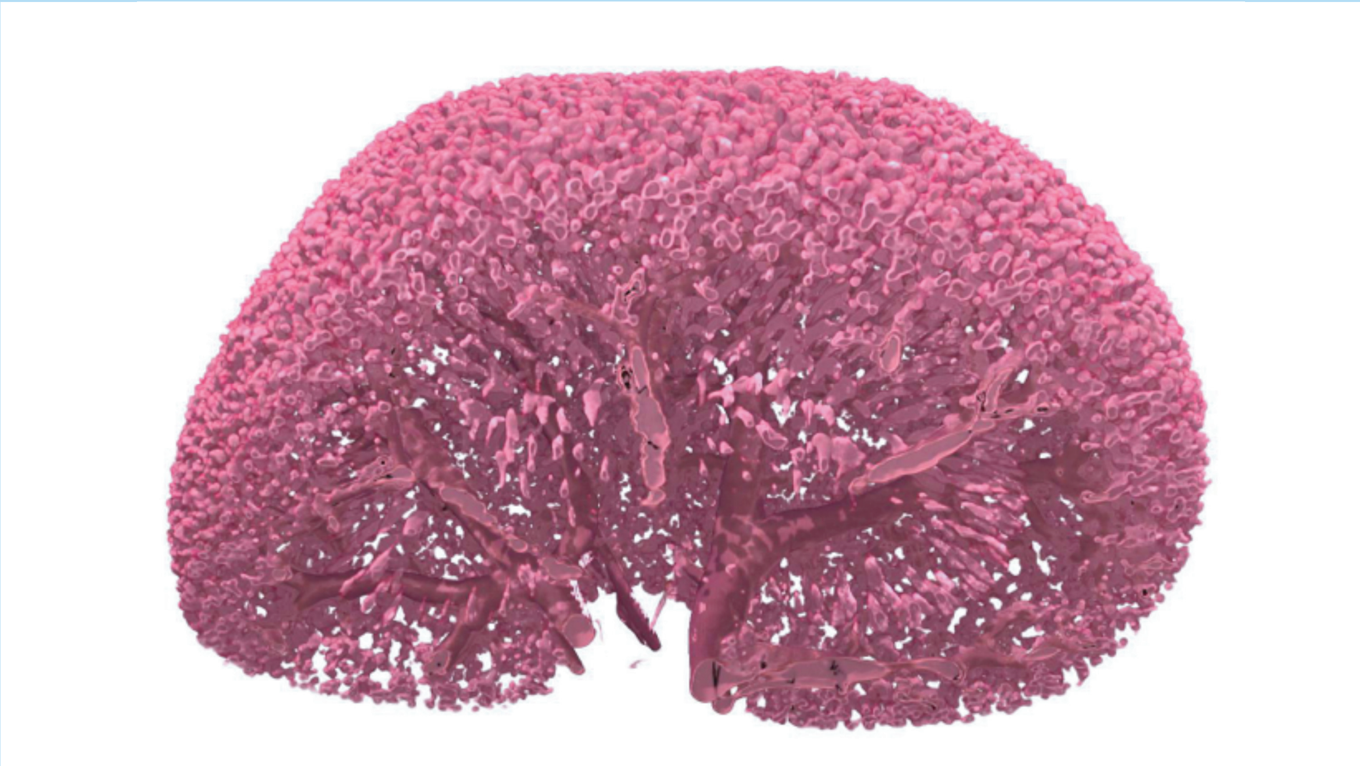

Chronic Kidney Disease

In 2012, Chronic Kidney Disease contributed to over 830,000 deaths, worldwide. In Australia, up to 2,000 Australians commence kidney replacement therapy each year. The disease causes the functional units of the kidney (nephrons) to change shape or size – becoming enlarged or obliterated by scar tissue.

Study of the disease is time consuming and expensive. The gold standard stereological method for quantification of nephron number and volume is unbiased stereology. Laborious and expensive, it requires the kidney to be sampled, embedded in resin and exhaustively sectioned before glomeruli are counted manually. Several days of work are needed to do this. Synchrotron X-ray Micro-CT offers a viable alternative.

Using the capabilities of MASSIVE, the Swiss Light Source and IMBL, Dr James Armitage (Deakin University), Prof John Bertram (Monash University), and Dr Karen Siu (Monash University and Australian Synchrotron), and other members of their team, aim to develop a faster, more efficient method to visualise and quantify nephrons. This will allow for faster, more cost effective detection of the disease.

The IMBL provides high-resolution, phase-contrast X-ray imaging of biomedical samples. MASSIVE's computational power allows the team to view the high-resolution 3D images within minutes of data capture. This has not been possible in Australia before.

These capabilities allow researchers to quickly establish whether a previous scan has successfully produced the desired data – before proceeding with the next step of the experiment.

A multidisciplinary solution

Studies like this are possible thanks to the contributions and expertise of multidisciplinary groups. By combining skillsets in high contrast imaging, highly specialised image processing expertise and software development capabilities, these teams are able to develop analytical tools which are producing higher resolution images and new imaging techniques to find the best possible stepping-stone towards deeper understanding.

Harnessing computing power for sophisticated imaging techniques is helping create 3D, high resolution imaging of otherwise invisible detail

Opposite — Xenon gas diffusing into the coal (first and second frame) and then being displaced by CO2 (last frame).

Above — Rendering of a kidney sample collected at the IMBL and processed and rendered on MASSIVE.

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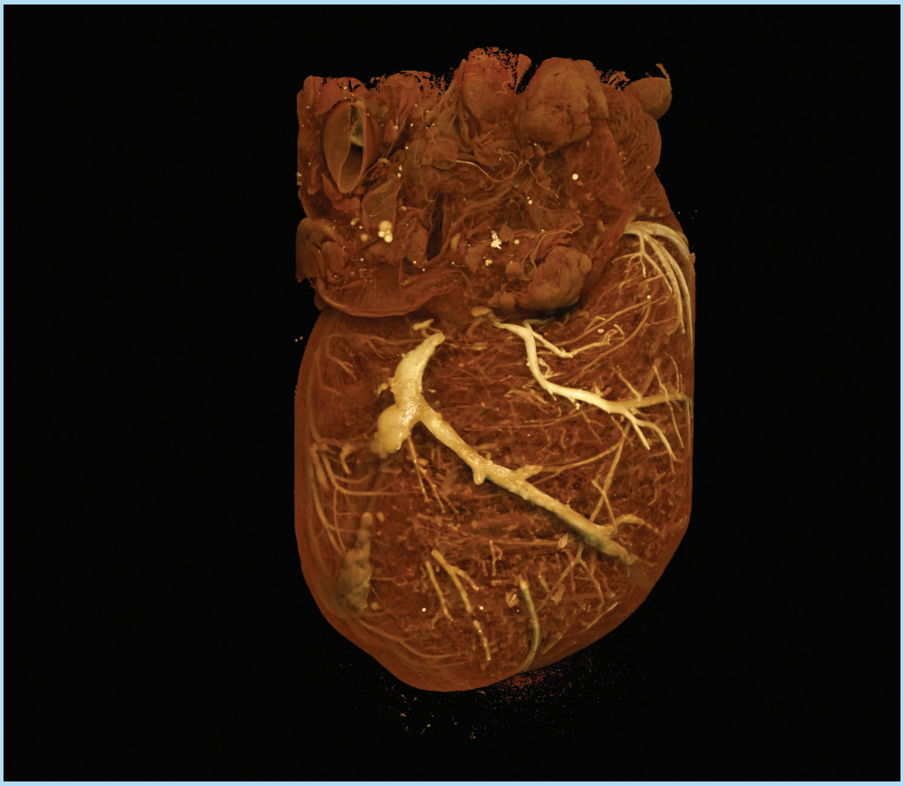

About X-TRACT

X-TRACT is an application for advanced processing of X-ray images and has been under active development at CSIRO for well over ten years. X-TRACT has been designed to fully leverage the processing capabilities of modern hardware. This increased capability boosts the performance of computationally intensive operations that utilise multiple processors, cores and GPUs.

The software provides a user-friendly graphical interface which makes it ideal for specialised CT and a broad suite of conventional image processing operations. In particular, there is extensive functionality for X-ray CT in both parallel and cone beam geometries, including multiple methods for reconstruction and X-ray phase retrieval as well as the simulation of phase-contrast imaging. A large number of operations such as FFT, filtering, algebraic, geometric, and pixel value operations are also provided.

About the Imaging and Medical Beamline

The Australian Synchrotron Imaging and Medical Beamline (IMBL)offers high-resolution, phase-contrast X-ray imaging of biomedical samples and a wide range of engineering materials.

Synchrotron X-ray imaging techniques are particularly suited to the study of living processes and will have benefits beyond the research findings. For instance, the capability for *in-vivo* imaging of small animals will enable longitudinal studies to be undertaken and may well reduce the number of animals used for biomedical research purposes. The X-ray imaging capability also provides opportunities for *in-situ* materials processes, such as alloy solidification and precipitation phenomena. As a result, the techniques have numerous biomedical, materials science and industrial applications, from research into the physics and biophysics of cancer therapy techniques to commercially valuable advances in medical, industrial and biomedical imaging technologies.

Opposite— Rat lung — Vascular cast of the left lung from a rat showing the 8-9 levels of branching of the arterial (blood) vessels down to the capillaries. Taken on IMBL at the Australian Synchrotron, the image represents two scans that are stitched together to achieve the image.

Above — Rat heart — Microfil™ filled vascular cast of a heart from an insulin resistant rat. Vessels appear white within the brown cardiac muscle. Taken on IMBL at the Australian Synchrotron, the image represents two scans that are stitched together to achieve the image.

Thanks to: James Pearson Monash University/IMBL, Mikiyasu Shirai and Hirotsugu Tschimochi National Cerebral & Cardiovascular Center, Japan and Daryl Schwenke, University of Otago, New Zealand.

CT reconstructions and renderings by Anton Maksimenko, Australian Synchrotron.

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07.

Training and Outreach

In 2013 MASSIVE offered 20 events. Highlights included hosting OzViz 2013, a range of Australian Synchrotron data analysis workshops and the first year of operation of the INCF Victoria, Australia node.

INCF

The Victorian Node of the International Neuroinformatics Coordinating Facility (INCF) was established in 2012 by Monash University and The University of Melbourne, through MASSIVE and VSLCI, respectively. This is the first year of node operations and the focus of activity has been on commencing operations, community building and securing future funding. In particular, in 2013 the INCF Victoria, Australia node:

- Officially launched with a workshop on 22 February 2013. The launch events included a keynote address from the Executive Director of the INCF (Professor Sean Hill) and a plenary address by Dr Allan Jones (CEO of the Allen Institute for Brain Research).
- Promoted the INCF through the establishment of a website (www.incf.org.au) and participation in the Australasian Cognitive Neuroscience Conference and the MASSIVE roadshows in Sydney and Perth.
- Sought funding to develop an Australia-wide INCF node through involvement with the successful ARC Centre of Excellence for Integrative Brain Function, that will see the Victorian INCF node nationalise in 2016.
- Supported collaboration between INCF researchers in Victoria (Monash University, Professor Rosa) and Poland (Nencki Institute, Professor Wojcik) to connect Monash's atlas of the marmoset brain with Nencki Institute's 3D Brain Atlas Reconstructor. This project was demonstrated at the 2013 Society for Neuroscience meeting and has facilitated free and accessible utilisation of the marmoset brain atlas.
- Engaged the broader INCF community to demonstrate the capabilities available in Australia such as MASSIVE and the CVL.
- Participated in the Neuroinformatics Congress, with four researchers presenting.
- Successfully bid to host the 2015 Neuroinformatics Congress in Australia.
- Contributed to INCF programs:
  - > Dr Simon Milton, University of Melbourne, has joined the Data Sharing Program.
  - > Prof Gary Egan, Monash University, is a member of the INCF Training Committee.
  - > Proposal to INCF Board to develop a Multiscale Connectomics program

Building on these successes, in 2014 the node will develop a web-based guide to neuroinformatics resources in Victoria (Australia), provide dedicated access to MASSIVE for INCF members, support the Centre for Integrative Brain Function and plan for the 2015 congress.

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Australian Synchrotron Data Processing and Analysis Workshops

Australian Synchrotron is a significant data producer and it is vital Australian Synchrotron users are aware of MASSIVE and its data processing capabilities. To help achieve this, MASSIVE has sponsored a set of Data Processing and Analysis Workshops.

The workshops run in 2013 were: 7th International Workshop on Infrared Microscopy and Spectroscopy with Accelerator Based Sources (WIRMS 7); NADIA Software Training Workshop for Beginners; and the Synchrotron, Accelerator and Neutron New User Symposium.

From the 10th to the 14th November 2013, the 7th WIRMS conference was hosted by the Australian Synchrotron. The conference was attended by staff and users from many of the synchrotron and free electron laser facilities around the world. The conference was also attended by a very large number of Australian IR beamline users and consequently the conference was a unique and ideal opportunity for showcasing MASSIVE and its data processing capabilities. Of particular note at this WIRMS conference were the rapid and novel developments of FTIR tomography and near field infrared imaging. These two emerging techniques generate enormous data sets and are precisely the type of experimental imaging for which MASSIVE is a good platform for handling the required image processing and reconstruction. The Biomedical and Biological WIRMS community was well represented over two dedicated sessions and included a presentation by Keith Bambery (AS) which provided an overview of the MASSIVE computing resource and on synchrotron IR spectrum signal correction and image processing using MASSIVE. Johanna Howes (UTS) presented her research into the photobiology of the Great Barrier Reef corals, work which was heavily reliant on MASSIVE for the synchrotron IR microspectroscopy data analysis.

OzViz 2013

From 9 to 10 Dec 2013, MASSIVE hosted the annual OzViz workshop and the Accelerated Computing Workshop (ACW) 2013. The workshop attracted more than 120 attendees from across Australia and a number of international institutions.

OzViz was first held in 2001, and is the premier annual workshop for visualisation practitioners, academics and researchers from across Australia and New Zealand. The workshop provides an opportunity for participants to present research outcomes, share innovative ideas, learn new techniques, publicise work and meet colleagues. It is a multidisciplinary event, with participants typically from a broad range of fields such as mathematics, geoscience, architecture, biology, medicine and astronomy presenting alongside computer graphics and visualisation experts.

OzViz is the premier annual workshop for visualisation practitioners, academics and researchers from across Australia and New Zealand.

Left— Launching the Victorian INCF Node. From left to right Professor Gary Egan (Director, Monash Biomedical Imaging), Professor Allan Jones (CEO, Allen Institute for Brain Research), Professor Sean Hill (Executive Director of the INCF), and Professor Paul Bonnington (Director, Monash eResearch Centre).

Above — Researchers experiencing a digital archeological reconstruction of Angkor by Dr Tom Chandler in the CAVE2™ facility at Monash University as part of OzViz 2013.

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Training Events

Title		Location	Date/s	Participants^
Introduction to HPC/Linux Course	MASSIVE team	Victorian Partnership for Advanced Computing (VPAC)	04/02/2013	9
Intermediate HPC/ Linux Course	MASSIVE team		05/02/2013	4
NADIA Software Training Workshop for Beginners	Australian Synchrotron	Education Lab, National Centre for Synchrotron Science (NCSS), Australian Synchrotron, 800 Blackburn Rd, Clayton VIC	11/07/2013	7
Introduction to HPC and Linux Course	MASSIVE team	Computer Lab G11, Building 60, Engineering Faculty, Monash University Clayton Campus VIC	18/07/2013	12
Intermediate HPC and Linux	MASSIVE team		19/07/2013	12
Avizo Training Day (Introduction)	Australian Synchrotron	Lecture Theatre E6, Building 60, Monash University Clayton Campus VIC	31/10/2013	7
7th International Workshop on Infrared Microscopy and Spectroscopy with Accelerator Based Sources (WIRMS)	Australian Synchrotron	Mantra Erskine Beach Resort, Mountjoy Parade, Lorne VIC	10/11/2013 – 14/11/2013	96
Avizo Training Day (Intermediate)	Vendor	Ground Floor Seminar Room (Rooms G29/G30), New Horizons (Building 82), Monash University Clayton Campus VIC	11/12/2013	11
OzViz 2013	Sponsored and MASSIVE team		09/12/2013 – 10/12/2013	122
Total			**Equivalent of approximately 12 days**	

Outreach Events

CSIRO Computational Sciences Workshop (two presentations)	MASSIVE team	Melbourne	20/03/2013 – 21/03/2013	100+
Presentation and Demonstration at the International Neuroinformatics Coordinating Facility Nodes Meeting	MASSIVE team	Stockholm, Sweden	18/03/2013	30+
Presentation at IVEC	MASSIVE team	CSIRO, Western Australia	6/03/2013	~30
Presentation at the Centre for Microscopy, Characterisation and Analysis, UWA	MASSIVE team	University of Western Australia, Western Australia	7/03/2013	~10
Synchrotron, Accelerator and Neutron New User Symposium	Australian Synchrotron	Webster Theatre at the Veterinary Science Conference Centre University of Sydney, Camperdown, Sydney NSW	26/07/2013	130
Neuroinformatics 2013: INCF Congress	MASSIVE team (Poster presentation)	INCF Congress, Stockholm	28/07/2013	~30
MASSIVE Roadshow – University of Sydney at the Brain & Mind Research Institute	MASSIVE team (Presentation)	Level 5 Lecture Theatre, Brain & Mind Research Institute, 94 Mallett Street (M02F), Camperdown NSW	28/10/2013	12
MASSIVE and CVL demonstration at INCF booth at Society for Neuroscience Conference and online	Monash University	Society for Neuroscience Conference, San Diego	11/11/2013	~30
Victorian Platform Technologies Network (VPTN) Facilities Showcase	MASSIVE team (Presentation)	Swanston Room, Melbourne Town Hall, VIC	12/11/2013	140
Supercomputing (Australian HPC booth)	MASSIVE team	Supercomputing 2013, Denver Convention Centre	19/11/2013 – 21/11/2013	Hundreds
2013 Australian Synchrotron User Meeting	MASSIVE team (Exhibitor)	National Centre for Synchrotron Science (NCSS), Australian Synchrotron, 800 Blackburn Road, Clayton VIC	21/11/2013 – 22/11/2013	215

^Attendance if known, otherwise registrations

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08.

Usage and Users

Since its inception, MASSIVE has steadily grown the number of institutional users from 11 (2011) to 33 (2012) and 74 (2013). The organisations involved cover research institutes, hospitals, universities, private industry and government departments across Australia and internationally. In 2013, this equated to supporting over 150 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). Each partner or investor operates an access process to allocate its prorated MASSIVE time (jn line with minimum requirements set by MASSIVE).

The NCI allocates its share of resources to Australian researchers through the National Computational Merit Allocation Scheme (NCMAS), where research groups may apply for computational and associated data resources in October for use in the following year. Services and resources are allocated to projects of significant research merit conducted by researchers at Australian publicly funded research organisations.

Applications to the NCMAS are assessed by an expert panel of researchers, based on the:

- Quality of the research (taking into account its significance, impact and innovation) and the standing of the research team and its leadership;
- Appropriateness of the resources for the task;
- Reasonableness of the resources requested;
- Track record of applicants in using NCI resources allocated previously.

Institutions

Researchers from the following institutions used MASSIVE in 2013:

University

Australian National University
Curtin University
University of Otago
University of Queensland
University of Sydney
Deakin University
Monash University
University of Western Australia
La Trobe University
University of Wollongong
Massey University
University of Adelaide
RMIT
University of Melbourne
University of New South Wales
University of Newcastle
University of South Australia
University of Hawaii at Manoa
James Cook University
Queensland University of Technology
Swinburne University
Universidad Politécnica de Madrid
Universität Heidelberg
Universität Leipzig
University of Amsterdam
University of California San Diego
University of Illinois Chicago
University of Manchester
University of Technology Sydney
Victoria University
Flinders University
University of Tasmania
University of Waikato
Dartmouth College
Griffith University
University of Sunshine Coast
Nanyang Tech University
University of Auckland
University of Canterbury
Victoria University of Wellington
University of Sassari

Research Institute

ANSTO
Australian Synchrotron
IVEC
CSIRO
Baker IDI
Bionics Institute
Brain Research Institute
Garvan Institute of Medical Research
Institute of Nuclear Physics, Polish Academy of Sciences
Neuroscience Research Australia
QIMR Berghofer Medical Research Institute
Russian Academy of Sciences
Synchrotron Light Research Institute
VERSI
Victorian Partnership for Advanced Computing
Burnet Institute
Centenary Institute
Ludwig Institute
Monash Institute of Medical Research
RIKEN Yokohama Institute
St Vincent's Institute
The Florey Institute of Neuroscience and Mental Health
Victor Chang Cardiac Research Institute
Walter and Eliza Hall Institute of Medical Research
AgResearch Ltd
Callaghan Innovation

Medical

Eastern Health
Alfred Health
Melbourne Health
Women's and Children's Hospital, Adelaide
The William Buckland Radiotherapy Centre

Industry

IBM
Australian Red Cross Blood Service

Government

Ames Laboratory
Department of Primary Industries
Museum Victoria
State Library New South Wales

Key
Instrument
Linux
Linux and Instrument

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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.

CSIRO, Monash University and VPAC make allocations internally. These allocations are made in consultation with the MASSIVE Coordinator and the MASSIVE team to ensure that the requirements of any potential allocation can be met.

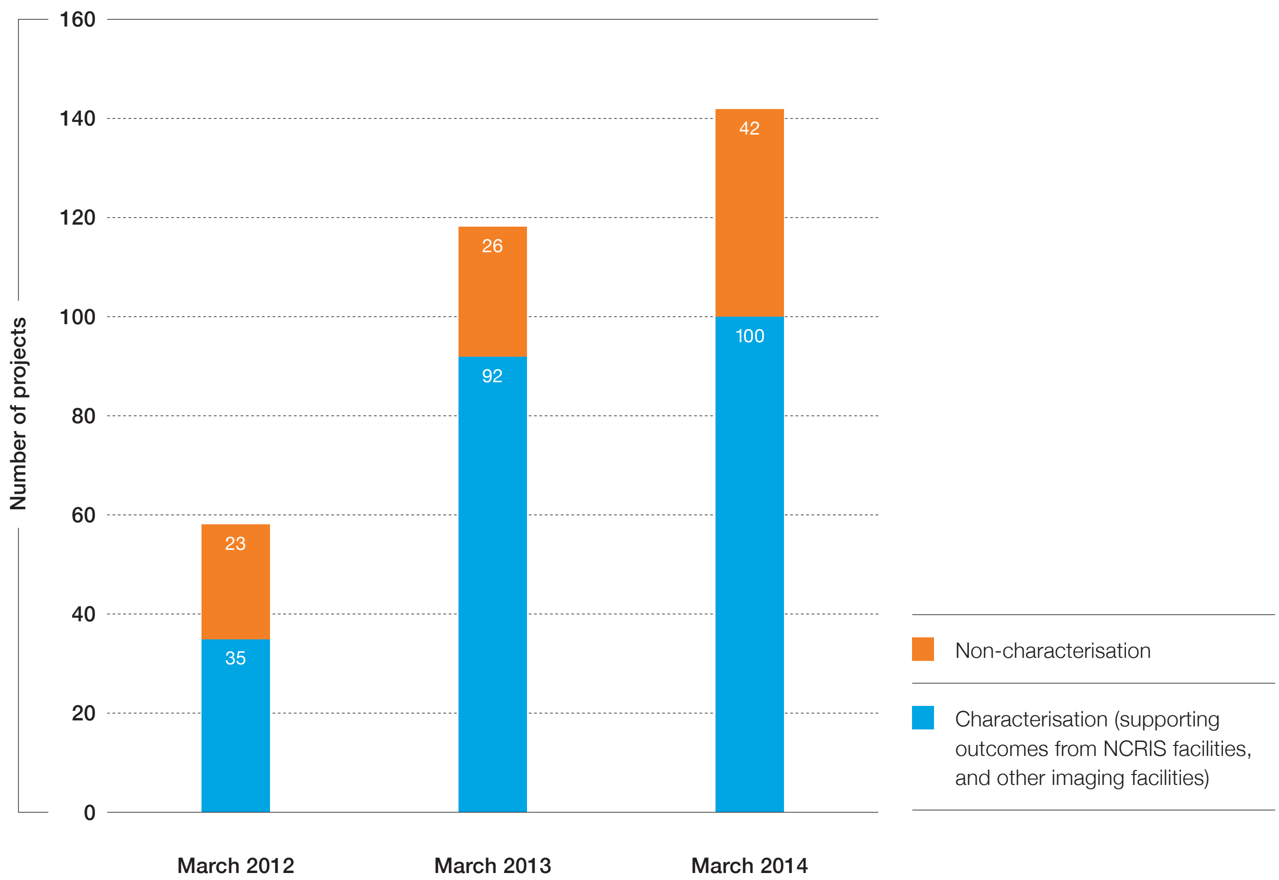
A proportion of MASSIVE computational time is reserved for discretionary use by the Coordinator on behalf of the Steering Committee. This share is intended to allow the project to allocate CPU time in a strategic manner, to assist new users, to introduce potential investors, and to support allocations outside the usual MASs. This share is 10% of the whole facility. The resource share allocation for 2013 was unchanged compared to 2012.

How MASSIVE is being used

In 2013, approximately 70% of projects on MASSIVE were focused on processing, analysis or visualisation of characterisation data (e.g. data produced by National Collaborative Research Infrastructure Strategy (NCRIS) Characterisation facilities, or other imaging instrumentation).

Note: These data do not include the Australian Synchrotron merit allocation projects that are assigned time on MASSIVE as part of beamline time.

MASSIVE Projects that Support the Characterisation Community.



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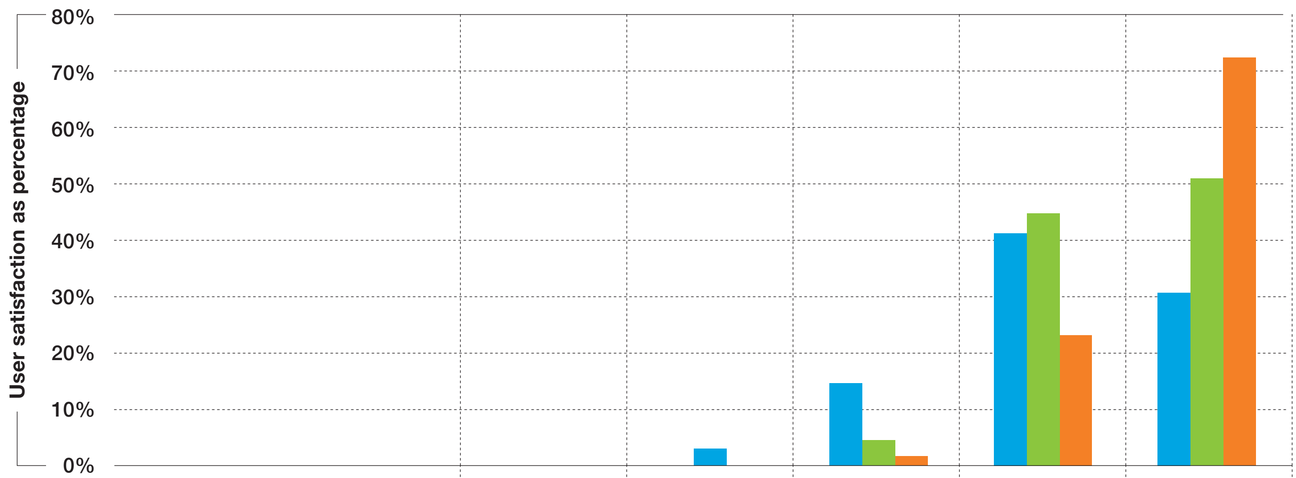
User Satisfaction

MASSIVE conducts an annual survey to monitor user satisfaction with facilities and support. In 2013, nearly 70 users responded to our survey and feedback was very positive with the majority of respondents indicating they were either satisfied or very satisfied with the facility (see figure below)

These positive responses are consistent with our 2012 user survey. However, it is clear there is room for improvement of the User Guide, given a number (2 of 68, 3%) of respondents indicated some dissatisfaction with it. In response to this survey result, we have initiated a review of the user manual.

User Satisfaction with MASSIVE



Question	Very Dissatisfied	Dissatisfied	Neither satisfied nor dissatisfied	Satisfied	Very satisfied
(orange) Please rate how satisfied you were with MASSIVE user support and consulting. For example, this includes support requests through help@massive.org.au or any further assistance and interaction with the MASSIVE team.	0	0	1	16	50
(blue) Please rate how satisfied you were with the MASSIVE User Guide (www.massive.org.au/userguide).	0	2	10	28	21
(green) Please rate how satisfied you were with the MASSIVE facility in general.	0	0	3	30	34

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Allocation of MASSIVE Share Across Partners and Investors

Partner or Investor	Allocation (%)
Australian Synchrotron	24.7
CSIRO	15.6
Monash	19.1
NCI	12.8
VPAC	12.8
Discretionary share	10
System management and testing	5
Total	**100**

MASSIVE Usage Data for 2013 (in system units)

		Projects (as of 12/02/2014)	Jan-Jun 2013	Jul-Dec 2013	Totals 2013
Total Available			**9,741,120**	**9,741,120**	**19,482,240**
Dynamically Scheduled	Monash	64	830,445	1,378,193	2,208,638
	VPAC	14	383,624	247,007	630,631
	NCI	17	597,278	623,937	1,221,215
	Synchrotron	23	536,898	1,319,711	1,856,609
	CSIRO	7	69,361	104,441	173,802
	Discretionary	17	601,341	933,544	1,534,885
	Total	**142**	**3,018,947**	**4,606,833**	**7,625,780**
	MOSP (System Testing & Maintenance)	6	76,266	121,167	197,433
Statically Reserved	CT Reserved	10 nodes	525,600	525,600	1,051,200
	Vis Reserved	10 Q1/2 23 Q3/4 nodes	525,600	1,208,880	1,734,480
Total Used			**4,146,413**	**6,462,480**	**10,608,893**
Unused			**5,594,707**	**3,278,640**	**8,873,347**
Percentage Unused #			**57.43%**	**33.66%**	**45.55%**

MASSIVE supports a large proportion of near realtime use (interactive desktop and instrument processing) and therefore aims for usage of approximately 70-80% of CPU time available – allowing space on the system for near realtime projects to access CPU time when needed. Jan-Jun 2013 saw a significant increase in available CPU time with the commissioning of stage-2 hardware and therefore had higher than normal unused capacity.

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09.
Governance

MASSIVE is governed by a Steering Committee, which is advised by two Science Advisory Committees, one representing the synchrotron science community and the other representing the imaging and visualisation community.

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. In 2013, the Coordinating Institution was Monash University. The Collaboration Agreement, signed by all Partner Organisations, sets out a number of roles, including the MASSIVE Coordinator. The Coordinator conducts the work of the Steering Committee as it relates to MASSIVE, including direction and management, and is a non-voting ex-officio member of the Steering Committee.

To support activities of a technical nature (e.g. purchase and installation of infrastructure), the Steering Committee has created the MASSIVE Technical Working Group (MTWG), on which all the partner organisations are represented. In 2013, the major role of the MTWG was to oversee the stage 2 upgrade.

The CVL has a separate Steering Committee and governance arrangements. Monash University undertakes a large portion of it's role in the CVL through MASSIVE, and Wojtek James Goscinski is the manager of the CVL.

Steering Committee

Meeting four times per year, the MASSIVE Steering Committee is responsible for overall governance of MASSIVE. It comprises a representative from each of the partner organisations: the Australian Synchrotron, CSIRO, Monash University and VPAC.

Other members of the committee include an independent Chair, the MASSIVE Coordinator and optionally others with skills considered necessary for the effective direction setting of MASSIVE. The Steering Committee is provided with advice from the two Science Advisory Committees.

In 2013, the MASSIVE Steering Committee comprised:

Dr Robert Hobbs,
Chair
Dr Ann Borda,
VPAC
Professor Paul Bonnington,
Monash University
Professor Andrew Peele,
Australian Synchrotron
Dr Alfred Uhlherr,
CSIRO
Dr Wojtek James Goscinski,
MASSIVE Coordinator (ex officio)

In 2013 the MASSIVE Steering Committee met on:

5th March
9th May
15th August
14th November

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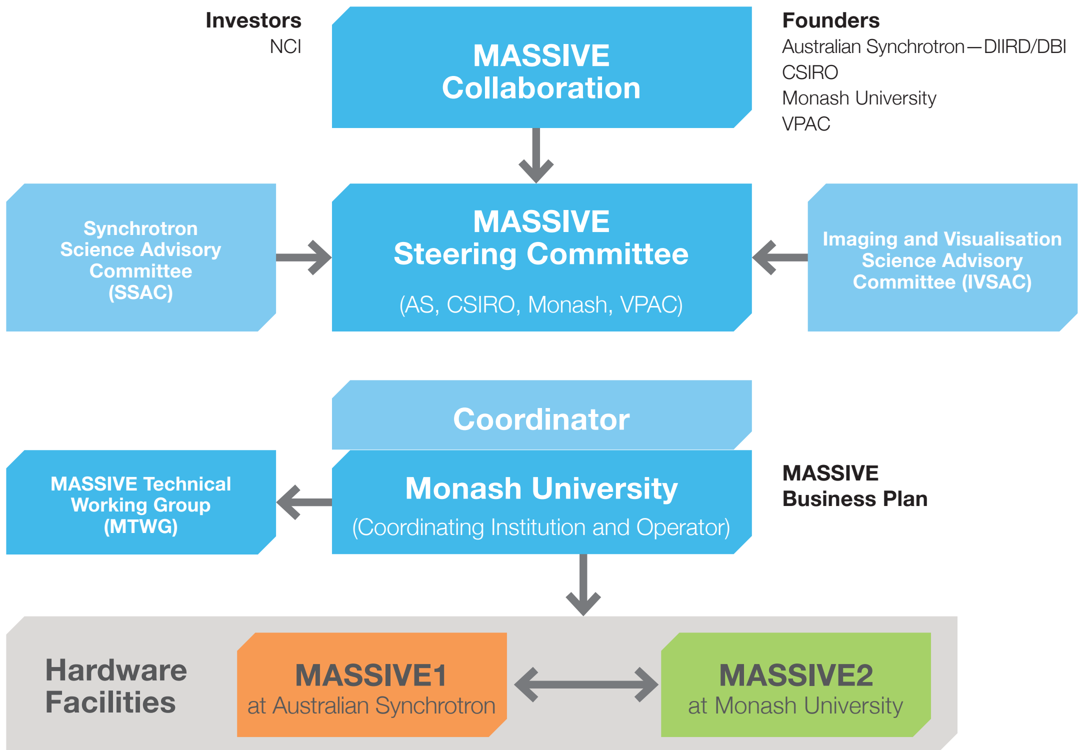
MASSIVE Governance Structure in 2013



Science Advisory Committees

Two Science Advisory Committees (SAC) provide user feedback and advice to the MASSIVE Steering Committee.

Synchrotron Scientific Advisory Committee

The Synchrotron Scientific Advisory Committee (SSAC) represents the views of Synchrotron users. As such, it includes representatives from relevant beamline user groups with MASSIVE access. SSAC members are appointed by the Australian Synchrotron and is formed as a sub-session of the IMBL Beamline Advisory Committee (BAP)

Imaging and Visualisation Scientific 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).

Chaired by Professor Gary Egan (Monash University), the Imaging and Visualisation Advisory Committee has seven members:

Dr Andreas Fouras,
Monash University
Dr Christopher Fluke,
Swinburne University (from April 2013)
Dr Pascal Vallotton
(CSIRO) (to April 2013)
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)

In 2013, the IVSAC met twice (April, August), with a third meeting (December) cancelled due to unforeseen circumstances. Throughout 2013, the committee has provided advice and support on:

- The Victorian node of the INCF;
- The development of the CVL and the way it interacts with successful NeCTAR Tools proposals;
- CT reconstruction for the IMBL;
- MASSIVE's training and outreach program; and
- MASSIVE's role in supporting strategic areas, including neuroimaging and synchrotron science.

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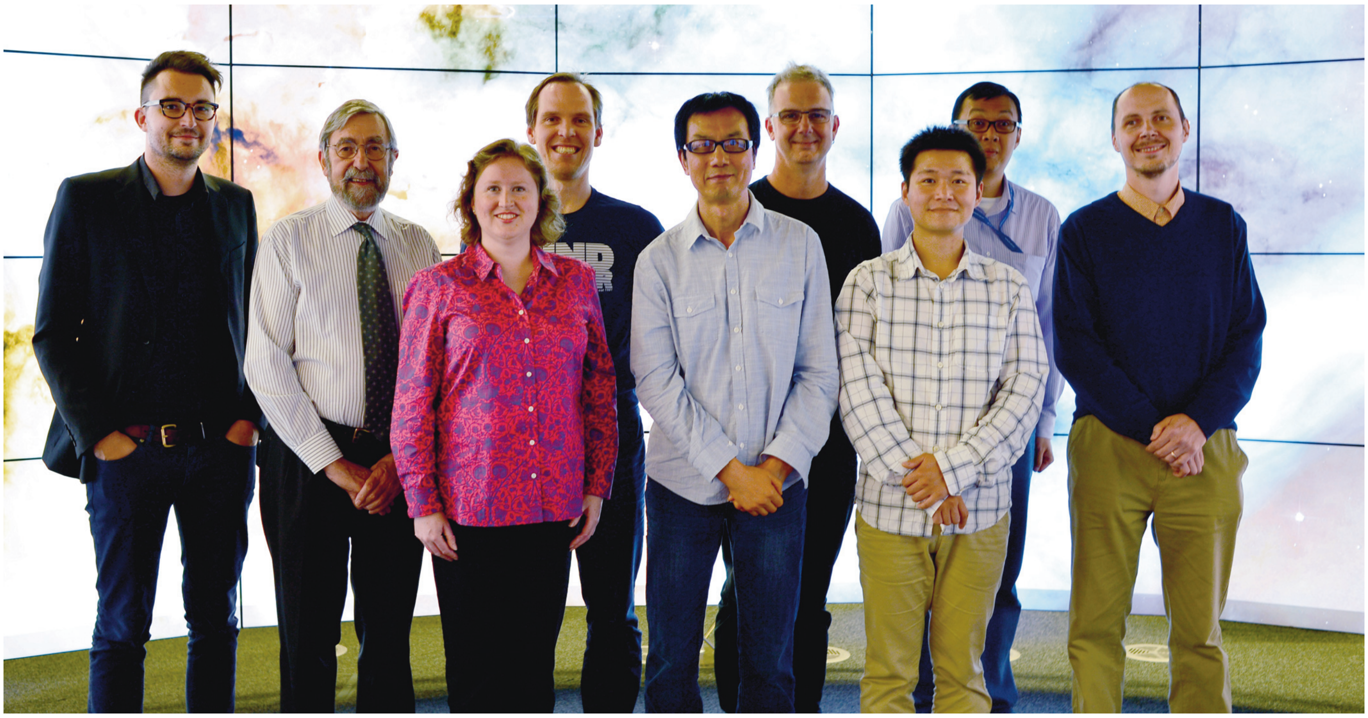
10.

Team and Operations

The MASSIVE team has grown in 2013, matching the growth in our capacity and increase in demand for services. The transition of operations to Monash University has allowed an increased investment in talented staff.

In early 2014, the MASSIVE team consists of the following staff.



From left to right:
Wojtek James Goscinski PhD – MASSIVE Coordinator
Robert Hobbs PhD – Chair, MASSIVE Steering Committee
Wendy Mason PhD – eResearch Engagement Specialist
Chris Hines PhD – Senior HPC Consultant
Jupiter Hu – Software Specialist (CVL)
Paul McIntosh PhD – Technical Manager and Senior HPC Consultant
Kai Xi PhD – HPC Consultant
Damien Leong – Senior HPC Consultant
Laszlo Kun – HPC Consultant

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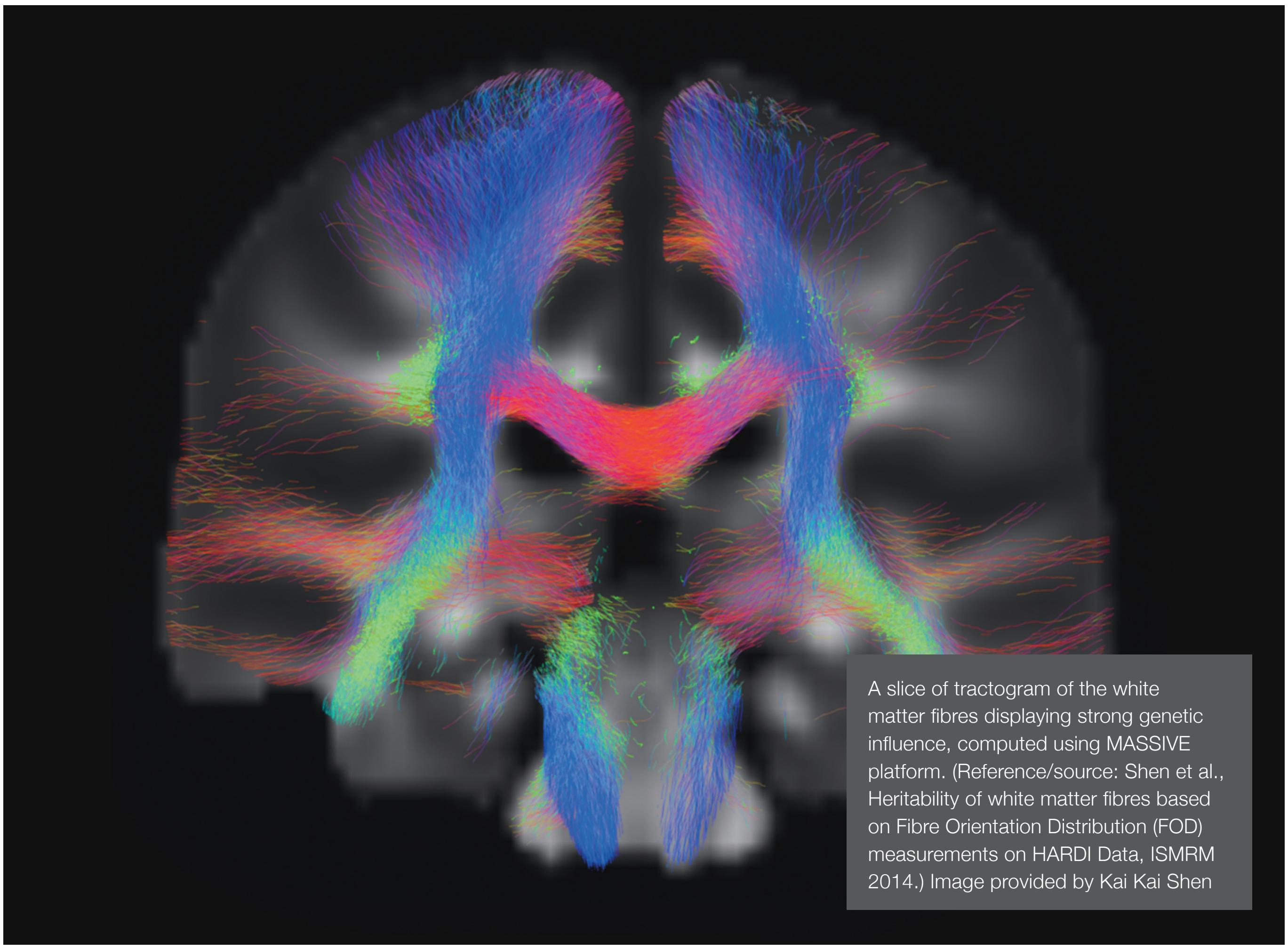
Transition of Operations

In early 2013, MASSIVE operations transitioned from VPAC to Monash University. This strategic change has had a number of positive impacts in 2013:

- The MASSIVE project made savings by leveraging Monash-led national IT research infrastructure projects.
- Savings made under this transition have been reinvested back into increased staffing for the project, such as:
  - > Moving to a more dedicated staff model; and
  - > Creating a new HPC Integration role that has strengthened and increased the scope of the MASSIVE Instrument Integration Program as well as supporting mutually beneficial projects, including the CVL and other NeCTAR-funded projects.
  - > Aligning MASSIVE with the strategic research directions of the MASSIVE partners. For example, providing flexible support to the operation of, and improvements to, the IMBL CT reconstruction service, and increasing the scope of the Instrument Integration Program in general.

These changes allow MASSIVE to provide a higher level of service to existing projects and provide flexible service to strategic activities, which is important to secure future funding beyond 2014.



A slice of tractogram of the white matter fibres displaying strong genetic influence, computed using MASSIVE platform. (Reference/source: Shen et al., Heritability of white matter fibres based on Fibre Orientation Distribution (FOD) measurements on HARDI Data, ISMRM 2014.) Image provided by Kai Kai Shen

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11.

MASSIVE3

Monash University and the MASSIVE partners are committed to MASSIVE3 — the next generation of the MASSIVE project. This 4½-year project will be run in two stages with a projected budget of approximately $10M.

- **July 2014 – December 2015:** During this time, MASSIVE will continue running as an extension of the combined MASSIVE1 and MASSIVE2 projects. MASSIVE will extend the capabilities developed under the CVL, provide support to key partnered ARC Centres of Excellence and develop relationships with key international projects.
- **January 2016 onward:** MASSIVE will undertake a new program of work that will include major investment in a new HPC system and development of new capabilities, including a new Instrument Integration Program. Under this plan, MASSIVE aims to be a significant Australian participant in key international collaborations, such as the €1B Human Brain Project to provide an Australian-based HPC centre of activity for this ambitious computational project.

These strategies and opportunities are designed to support Australia's Strategic Research Priorities (June 2013).

The MASSIVE agenda for 2014 and beyond, covers four key areas.

Instrument Integration

MASSIVE is underpinning the capabilities of a number of characterisation instruments, including beamlines. This integration has strongly increased the research capability and capacity of these instruments. Each integration requires individual solutions based on the equipment-facility combinations in place and MASSIVE will build on our experiences to integrate activities into other characterisation instruments such as new synchrotron beamlines, biomedical imaging (through NIF and the Victorian Biomedical Imaging Capability), electron microscopy and other key Australian flagship instruments. Additionally, there is an opportunity to extend services to clinical studies, leveraging Monash University ISO 27K accreditation for secure data management.

Characterisation Infrastructure

MASSIVE has been actively building software infrastructure for the Australian characterisation community. The capability developed, including desktops on the cloud, will be extended to a wider range of users in 2014. In addition, MASSIVE will extend the CVL to more easily allow users to access data through data management systems, and national long term data storage infrastructure and collections. This work will be essential to the design of a new HPC system in 2015, which will have a hybrid cloud and HPC architecture, allowing researchers the flexibility of a cloud environment and the power of an HPC capability.

Big Brain Initiatives

Through key initiatives, including membership of the INCF, development of a remote desktop environment, and integration of key MRI and CT instruments, MASSIVE has developed a large cohort of users in neuroinformatics (over 25 projects). Our support in the neurosciences will continue in 2014 and onward in particular this includes participation in the ARC Centre for Integrative Brain Function (www.cibf.edu.au). Beyond 2015, MASSIVE aims to be a contributor to significant international neuroscience collaborations, including the €1B Human Brain Project.

Molecular Modelling

Molecular modelling, for materials and life sciences, is a major activity of MASSIVE (~20% of all projects include some form of molecular modelling). This community is well versed in the use of HPC for research. As such, we see further opportunities to engage with this research area and develop services and support particularly suited to this specialised community. In particular, characterisation facilities, such as ANSTO and AMMRF, are increasingly applying molecular modelling to support traditional characterisation techniques. This is particularly true at ANSTO where simulation of nuclear materials is often easier than physical experiments.

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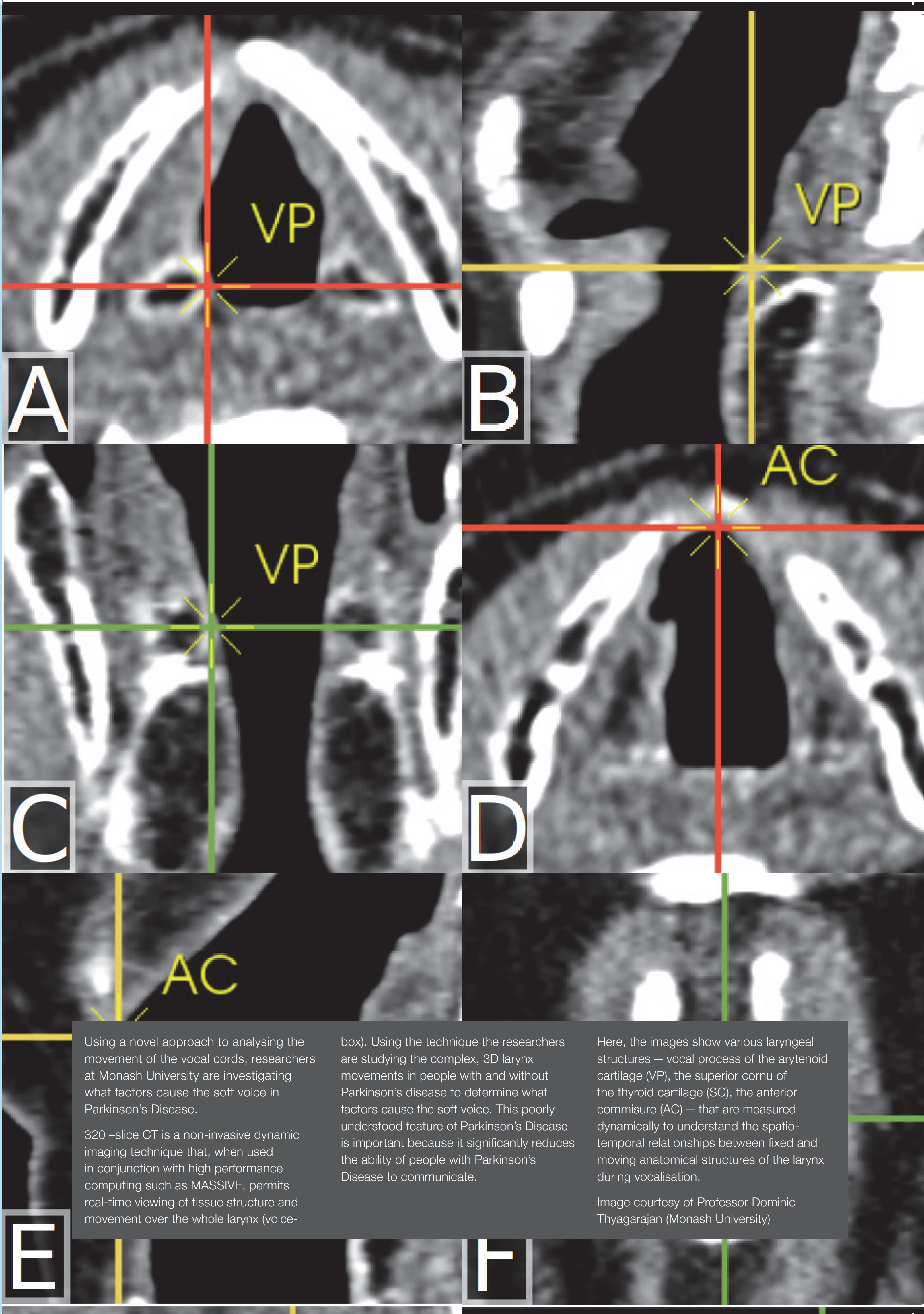

Using a novel approach to analysing the movement of the vocal cords, researchers at Monash University are investigating what factors cause the soft voice in Parkinson's Disease.

320 –slice CT is a non-invasive dynamic imaging technique that, when used in conjunction with high performance computing such as MASSIVE, permits real-time viewing of tissue structure and movement over the whole larynx (voice-box). Using the technique the researchers are studying the complex, 3D larynx movements in people with and without Parkinson's disease to determine what factors cause the soft voice. This poorly understood feature of Parkinson's Disease is important because it significantly reduces the ability of people with Parkinson's Disease to communicate.

Here, the images show various laryngeal structures — vocal process of the arytenoid cartilage (VP), the superior cornu of the thyroid cartilage (SC), the anterior commisure (AC) — that are measured dynamically to understand the spatio-temporal relationships between fixed and moving anatomical structures of the larynx during vocalisation.

Image courtesy of Professor Dominic Thyagarajan (Monash University)

12.
Projects

The following is a list of projects on MASSIVE at 31st December 2013. Both 2013 and 2014 NCMAS projects are included. Merit allocation projects that use MASSIVE through beamline access at Australian Synchrotron are not listed.

Project Title	Chief Investigator(s)	
3D EEG imaging	Dr Yakov Nesterets, CSIRO	Partner Share
3D Visualisation and Registration of Embryonic Animal Development	Dr Kieran Short, Monash University	Partner Share
A functional magnetic resonance imaging (fMRI) study addressing cognitive function in individuals with Friedreich Ataxia	Prof Nellie Georgiou-Karistianis, Monash University	Partner Share
A new, high spatial-resolution, dataset on internet use in Australia.	Dr Simon Angus, Monash University	Partner Share
ACAS-CLIC Collaboration	Dr Mark Boland, Australian Synchrotron	Partner Share
Accelerator Physics	Mr Kent Wootton, Australian Synchrotron	Partner Share
ADS	A/Prof Alex Fornito, Monash University Mr Chao Suo, Monash University Prof Murat Yucel, Monash University	Partner Share
Advanced Modelling of Biological Fluid	Dr Pauline Assemat, Monash University	Partner Share
An investigation of ageing brain structure in health and disease	Dr Marnie Shaw, Australian National University Dr Nicolas Cherbuin, Australian National University	NCMAS for 2014
An investigation of the effects of intranasal oxytocin on socio-emotional brain regions in Huntington's disease	Dr Govinda Poudel, Monash University Dr Izelle Labuschagne, Monash University	Partner Share
An MD study of radiation effects in candidate structural materials for demanding engineering applications	Dr Roman Voskoboynikov, ANSTO	Partner Share
Analysis of Brain MR images for the study of Alzheimer's disease	Dr Pierrick Bourgeat, CSIRO	Partner Share
Analysis of longitudinal structural MRI for TasCOG and CDOT studies	Dr Richard Beare, Monash University	NCMAS for 2014
Anatomical Image Processing and Biomechanical Modelling	Mr Christopher Walmsley, Monash University Dr Colin McHenry, Monash University Michelle Quayle, Monash University	Partner Share
Application of GPUs to Large-Scale Atomistic MD Simulation of Poliovirus.	Dr Andrew Hung, RMIT	Partner Share
ASPREE Image Pilot Study	Dr Parnesh Raniga, CSIRO & Monash University	NCMAS for 2013
Atomistic simulations for physical and electronic properties of nanomaterials	Dr Nikhil Medhekar, Monash University	NCMAS for 2013
Australian Synchrotron Scientific Programming Group	Dr Ulrich Felzmann, Australian Synchrotron	Partner Share

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Project Title	Chief Investigator(s)	
Automation, processing and visualisation of large multi-dimensional micro-imaging datasets generated at Monash Micro Imaging	Mr Keith Schulze, Monash University	Partner Share
Beryllium intermetallics for fusion applications	Dr Simon Middleburgh, ANSTO	Discretionary
Biological Neuronal Network Simulation	Dr Aaron Harwood, University of Melbourne	Partner Share
Brain similarity study	Dr David Barnes, Monash University	Partner Share
CF PCXI	Dr Kaye Morgan, Monash University Dr Martin Donnelley, Monash University	Partner Share
Characterising Interatomic Bonds by Quantitative Electron Diffraction	Dr Philip Nakashima, Monash University	Partner Share
Coherent Diffraction Imaging	Dr Grant van Riessen, La Trobe University	Partner Share
Computational approaches towards the neuronal basis of consciousness	A/Prof Naotsugu Tsuchiya, Monash University	NCMAS for 2014
Computational Mesoscale Physics, Probing Complex and Hierarchical Material Structure	A/Prof Adrian Sheppard, Australian National University	NCMAS for 2014
Computer Fluid Dynamic and Dynamic Finite Element Simulation	Dr Mahnaz Jahedi, CSIRO	Partner Share
Connectome mapping	A/Prof Alex Fornito, Monash University Dr Ben Fulcher, Monash University Mr Chao Suo, Monash University Prof Murat Yucel, Monash University	Partner Share
Counting nephrons in the kidney via micro-CT	Dr James Armitage, Deakin University	Partner Share
Coupled Lattice Monte Carlo — Finite Element (LMC-FE) Multiscale Modelling of Composites	Prof George Franks, University of Melbourne	Partner Share
Cross-channel analysis of multi-channel elecrtophysiological data in space, time and frequency	Mr Dror Cohen, Monash University Mr Jochem van Kempen, University of Amsterdam A/Prof Naotsugu Tsuchiya, Monash University	Partner Share
CSIRO ASC Support	Dr Robert Bell, CSIRO	Partner Share
CUDA enabled learning classifier systems	Dr Michael Kirley, University of Melbourne	Partner Share
CVL Energy Materials (X-Ray)	A/Prof Adrian Sheppard, Australian National University Mr Stuart Hungerford, Australian National University	Discretionary
Data Constrained Modelling : Cluster-enabled nonlinear optimisation	Dr Fiona Chen, CSIRO	Partner Share
Decoding of perceptual decisions from combined fMRI and EEG signals	Dr Carsten Murawski, University of Melbourne	Partner Share
Decoding perceptual decisions from simultaneously recorded EEG and fMRI data	Dr Carsten Murawski, University of Melbourne	Partner Share
Depth Resolution In X-ray Fluorescence Microscopy (DXFM)	Dr Matthew Dimmock, Australian Synchrotron	Partner Share
Descriptive complexity of Protein Structures	Dr Arun Konagurthu, Monash University	Partner Share
Determining protein structures using transmission electron microscopy	Dr Geoffrey Kwai Wai Kong, Walter and Eliza Hall Institute of Medical Research	Discretionary
Development of New Thermoelectric Materials Based on the Defect Pyrochlore Structure	Dr Elvis Shoko, ANSTO	Partner Share
DFT studies of ionic transport and magnetic properties of inorganic materials	Dr Gordon Kearley, ANSTO, Dr Max Avdeev, ANSTO	Partner Share
Direct simulation Monte-Carlo for ultracold spinor gases	Mr Chris Watkins, Monash University Dr Lincoln Turner, Monash University	Partner Share
Dopamine	A/Prof Alex Fornito, Monash University Mr Chao Suo, Monash University Prof Murat Yucel, Monash University	Partner Share
Dynamic computed tomography of lungs in motion	Dr Andreas Fouras, Monash University	NCMAS for 2014
Electromagnetic Structure of Matter	Dr Waseem Kamleh, University of Adelaide	Discretionary
Electromagnetic Structure of Matter	Prof Derek Leinweber, University of Adelaide Dr Waseem Kamleh, University of Adelaide	NCMAS for 2014
Electronic and thermal properties of 2D transition metal dichalcogenides	Dr Nikhil Medhekar, Monash University	Partner Share
Electronic properties of hybrid solar cells: a test-case for the Bioscience Data Platform	Prof Salvy Russo, RMIT	Discretionary
Electronic Structural Modelling and CPMD Simulation for Molecules of Special Interest	Prof Feng Wang, Swinburne University	NCMAS for 2013

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Project Title	Chief Investigator(s)	
Evolutionary influence and phylogenetic constraints on morphology	Prof Scott Keogh, Australian National University	Discretionary
Exhaustive Search for 3-way Genomic Interactions Associated with Disease	Mr Qiao Wang, University of Melbourne	NCMAS for 2014
Exploring structure-property correlations in advanced materials: Nexus between computational simulation and atomic resolution microscopy	Ms Anna Ceguerra, University of Sydney Prof Simon Ringer, University of Sydney Dr Xiangyuan Cui, University of Sydney	NCMAS for 2013
Fast fibre tractography for magnetic resonance diffusion images	Dr David Barnes, Monash University	Partner Share
Feature selection for network anomaly detection	Prof Zahir Tari, RMIT	Partner Share
fMRI study of motor clumsiness in children	Dr Saman Kashuk, Monash University	Partner Share
Genetic and environmental influences on brain structure and function	A/Prof Alex Fornito, Monash University Mr Chao Suo, Monash University Prof Murat Yucel, Monash University	Partner Share
Genetics of brain structure and function	Dr Katie McMahon, University of Queensland	NCMAS for 2014
Geodynamics Modelling	Dr Fabio Capitanio, Monash University	Partner Share
GeoPIXE software AS users access	Dr Chris Ryan, Australian Synchrotron	Partner Share
GPlates	Mr John Cannon, University of Sydney	Discretionary
Graphene Electromechanical Actuation: Origins, Optimization, and Applications	Dr Zhe Liu, Monash University	Partner Share
Gravitational Waves from Turbulent Neutron Stars	A/Prof Andrew Melatos, University of Melbourne	NCMAS for 2014
High Entropy Alloys for Advanced Nuclear Applications	Dr Simon Middleburgh, ANSTO	Discretionary
High-resolution electron microscopy studies of protein structures	Dr Geoffrey Kwai Wai Kong	NCMAS for 2013
Identification and characterization of the pacemaker in the uni- and mutli-calyceal kidney	Dr Richard Lang, Monash University	NCMAS for 2014
Image reconstruction and simulation on the Xeon Phi	Dr William Ryder, University of Sydney	Discretionary
ImageHD	Dr Govinda Poudel, Monash University	Partner Share
Imaging and Medical Beamline	Mr Andreas Moll, Australian Synchrotron, Dr Ulrich Felzmann, Australian Synchrotron	Partner Share
IMBL Test Access	Dr Anton Maksimenko, Australian Synchrotron, Dr Christopher Hall, Australian Synchrotron	Partner Share
Implications of the Higgs boson discovery	Dr Csaba Balazs, Monash University	Partner Share
Improved skull thickness estimation for the reconstruction of 3D EEG brain images	Dr David Barnes, Monash University	Partner Share
Interfacing microscopic and macroscopic imaging	A/Prof Martin Lackmann, Monash University	Partner Share
Investigating neural mechanism of problem gambling and obsessive-compulsive disorder using MRI	A/Prof Alex Fornito, Monash University Mr Chao Suo, Monash University Ms Leah Braganza, Monash University Prof Murat Yucel, Monash University	Partner Share
Investigations into the sturtcure and function of the pacemakers driving pyleoureteric peristalsis	Dr Richard Lang, Monash University	Partner Share
Investigations of transitional and turbulent shear flows using direct numerical simulations (DNS), large eddy simulations (LES) and 3D Image Velcoimetry	Prof Julio Soria, , Monash University Mr Omid Amili, Monash University	NCMAS for 2014
Large scale 3D reconstruction for electron imaging	Dr Jing Fu, Monash University	Partner Share
Large scale registration of 2D and 3D brain histological data	Prof Marcello Rosa, Monash University Mr Tristan Chaplin, Monash University	Partner Share
Magnetic Properties of Tc Oxides and Tc Metal	Dr Eugenia Kuo	Discretionary
MBI testing and development (MOSP support)	Dr David Barnes, Monash University	Partner Share
Microstructural analysis in 3D	Prof Chris Davies, Monash University	Partner Share
Model-driven engineering of scientific software for graphical processing units	Dr David Barnes, Monash University	Partner Share
Modelling G protein-coupled receptors for drug discovery	Dr David Chalmers, Monash University	Partner Share
Modelling Nanoscale Materials	Dr Michelle Spencer, RMIT	Partner Share
Modelling the Subsurface Structure of Sunspots	Dr Hamed Moradi, Monash University	Partner Share
Molecular Dynamics Simultions on radiation damage of nuclear materials	Dr Meng Jun Qin, ANSTO	Discretionary
Molecular simulations of proteins	A/Prof Ashley Buckle, Monash University	Partner Share
Monash Biomedical Imaging Small Projects	Dr David Barnes, Monash University	Partner Share

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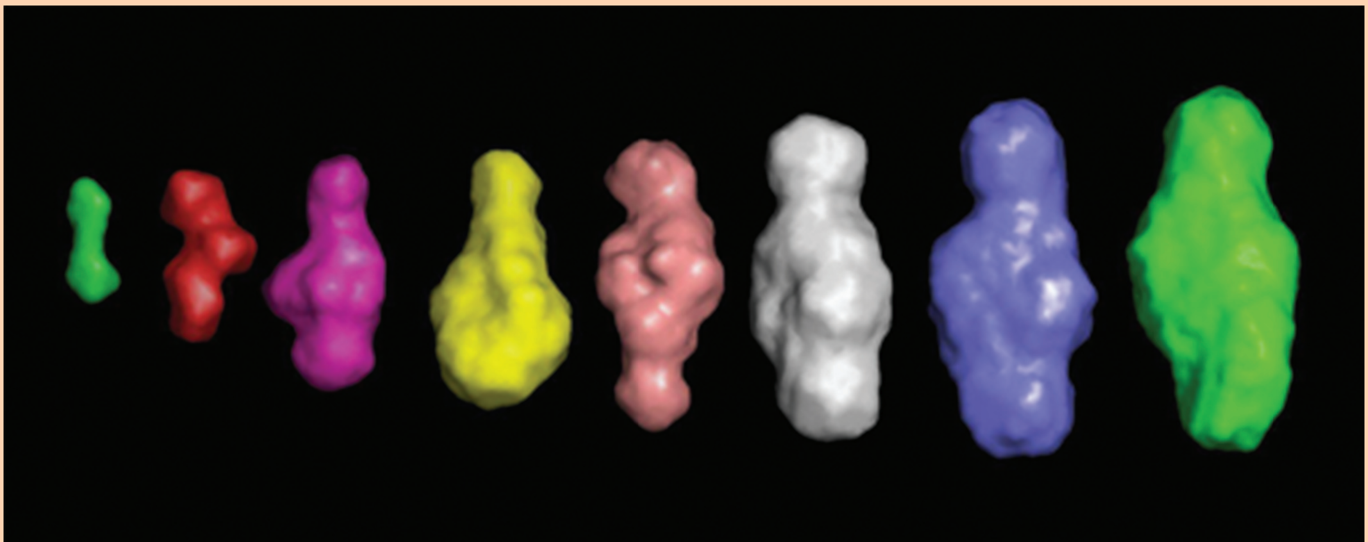
Project Title	Chief Investigator(s)	
Monash CAVE2 rendering and data organisation	Dr David Barnes, Monash University	Partner Share
Monte Carlo Calculations for Quality Assurance of Microbeam Radiation Therapy at the Australian Synchrotron	Dr Iwan Cornelius, University of Wollongong	NCMAS for 2014
Multimodal Kidney Image Analysis	Dr David Barnes, Monash University	Partner Share
MultiPET Reconstruction	Mr Christopher Bell, CSIRO	Partner Share
MX group access	Dr Tom Caradoc-Davies, Australian Synchrotron	Partner Share
Neural and physiological correlates of somatic contagion: A multidimensional model of empathy for pain	Dr Melita Giummarra, Monash University	Partner Share
Neuroanthropology	Dr Juan Dominguez, Monash University	Partner Share
Neuroimage biomarker for vulnerability to psychosis in young adults	A/Prof Alex Fornito, Monash University Mr Chao Suo, Monash University Prof Murat Yucel, Monash University	Partner Share
Neuroimaging after traumatic brain injury: What best relates to outcome?	Dr Jerome Maller, The Alfred	Partner Share
Next generation sequencing analysis (NGS) of mesothelioma samples	Dr Fernando Rossello, Monash University, Prof Neil Watkins, Monash Institute of Medical Research	Partner Share
Numerical modelling of solar photospheric magnetic activity	Dr Sergiy Shelyag, Monash University	Partner Share
Numerical search of better radiotherapy protocols using genetic algorithms	Dr Simon Angus, Monash University	Partner Share
Numerical study on the toughening mechanisms of 3D carbon nanotube reinforced composites	Dr Wenyi Yan, Monash University	Partner Share
OpenCL based, CFD solver with visualisation	Dr Tomasz Bednarz, CSIRO	Partner Share
Optimization of Calcium Cobaltates for High-Temperature Thermoelectric Conversion	Dr Elvis Shoko, ANSTO	NCMAS for 2013



Tannin structure has a significant effect on how wine tastes. A large number of highly purified synthetic tannins and wine tannins have been measured on the Australian Synchrotron Small Angle X-ray Scattering / Wide Angle X-ray Scattering (SAXS/WAXS) beamline. These studies have focused on the impact of ethanol, sugars and other significant wine components affect tannin structure of various vintages at molecular level. Dr Rachel Kilmister and Dr Peta Faulkner from the Grape and Wine Chemistry Group of the Department of Environment and Primary Industry (VIC) are studying wine tannins using synchrotron SAXS/WAXS and a range of laboratory techniques. As part of their research, they are visualising, in near real-time the molecular structure of the tannins impacted by ethanol, sugars and other wine components (image above). MASSIVE provides the near real-time primary data processing and basic analysis of data essential for researchers to run complex, fast moving experiments that produce vast amounts of data. The initial images of these tiny wine tannins in the figure were available within minutes of the samples going through the beamline. Scientific computing capabilities are proving indispensable to scientists in harnessing the full capability of one of the most powerful X-ray scattering beamlines worldwide.

Image provided by Rachel Kilmister and Peta Faulkner

Project Title	Chief Investigator(s)	
Parameter Estimation of Stochastic Volatility Models using Particle Filtering	Prof Kenneth Lindsay, Queensland University of Technology	Discretionary
PXD_Bkg	Mr Andreas Moll, Australian Synchrotron	Partner Share
Quantifying the effects of partially coherent X-rays in coherent diffractive imaging	Mr Giang Tran, La Trobe University	Partner Share
Quantum Simulation of Condensed Matter for Direct Comparison to Soft X-Ray Synchrotron Experiments	Dr Bruce Cowie, Dr Kane O'Donnell, Australian Synchrotron	Partner Share
Radiation effects in advanced oxides, carbides and nitrides for high temperature applications	Dr Simon Middleburgh, ANSTO	Discretionary
Recontruction of 3D mice aortic arches with atherosclerotic plaques	Dr Pauline Assemat, Monash University	Partner Share
Regression on GPU	A/Prof Gleb Beliakov, Deakin University	Partner Share
Resonant Mie Scatter Correction for FTIR Microspectroscopy — IR Beamline Users	Dr Danielle Martin, Australian Synchrotron, Dr Keith Bambery, Australian Synchrotron, Dr Ljiljana Puskar, Australian Synchrotron, Dr Mark Tobin, Australian Synchrotron,	Partner Share
Resonant Mie Scattering Multiplicative Signal Correction for FTIR Micro-Spectroscopy	Dr Keith Bambery, Australian Synchrotron	Partner Share
SAXSWAXS autoprocessing pipeline	Dr Stephen Mudie, Australian Synchrotron	Partner Share
Segmentation and characterisation of electron backscatter diffraction images	Dr Richard Beare, Monash University	Partner Share
Simulations and visualisation of star and planet formation	Dr Daniel Price, Monash University	Partner Share
Single projection and tomographic x-ray imaging with the Australian Synchrotron's Imaging and Medical Beamline	Mr Jeremy Brown, Monash University	Partner Share
Sorting Acceleration in GPU	Dr Gang Li, Deakin University	Partner Share
STARImaging	Dr Richard Beare, Monash University	Partner Share
Statistics of Magnetised Supersonic Turbulence in the Interstellar Medium	Dr Daniel Price, Mr Terrence Tricco	NCMAS for 2013
Stellar Evolution and Nucleosynthesis	Dr Simon Campbell, Monash University	Partner Share
Structure, dynamics and interactions of malaria surface proteins as vaccine candidates and drug targets	Dr David Chalmers, Monash University	NCMAS for 2014
Studies of self-avoiding walks and related models of polymers	Dr Nathan Clisby, University of Melbourne	Partner Share
Supersymmetry at the Large Hadron Collider	Dr Csaba Balazs, Monash University	Partner Share
Synchrotron Cretaceous Mammals	Dr Alistair Evans, Monash University	Partner Share
Tandem Maia-Geopixe real-time fluorescence analysis	Dr 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	Dr Catherine Willmott, Monash University	Partner Share
The Characterisation Virtual Laboratory Test and Development	Dr Paul McIntosh, Monash University	Discretionary
The comparative physiology of oxygen delivery to the kidney	A/Prof Roger Evans, Monash University	Partner Share
The effect of cannabis on hippocampal morphometry and volume	Mr Chao Suo, Monash University Prof Murat Yucel, Monash University Dr Valentina Lorenzetti, Monash University	Partner Share
The Industrial Ecology Virtual Laboratory	Dr Arne Geschke, University of Sydney, Dr Tim Baynes, CSIRO	Partner Share
The Most Powerful Magnetic Fields in the Universe	A/Prof Andrew Melatos, University of Melbourne	Partner Share
Thermoelastic properties of hydrated sulphates	Dr Helen Brand, Australian Synchrotron	Partner Share
Three-dimensional (3D) Cellular Imaging and Visualization with Computational Tomography	Dr Shan Shan Kou, University of Melbourne	Partner Share
Thrombus Reconstruction	Dr Josie Carberry, Monash University	
Total Anatomical Modelling and Biomechanical analysis — Using High Performance Computing to realistically simulate human form and movement	Dr Colin McHenry, Monash University	NCMAS for 2014
Towards dynamic tectonic reconstructions	Prof Dietmar Muller, University of Sydney Dr Leonardo Quevedo, University of Sydney Dr Nicolas Flament, University of Sydney	NCMAS for 2014
Towards large-scale calculations of ionic liquids	Dr Ekaterina Pas, Monash University	Partner Share
Towards realistic verbal interactions between people and computers — a probabilistic approach	Prof Ingrid Zukerman, Monash University	Partner Share

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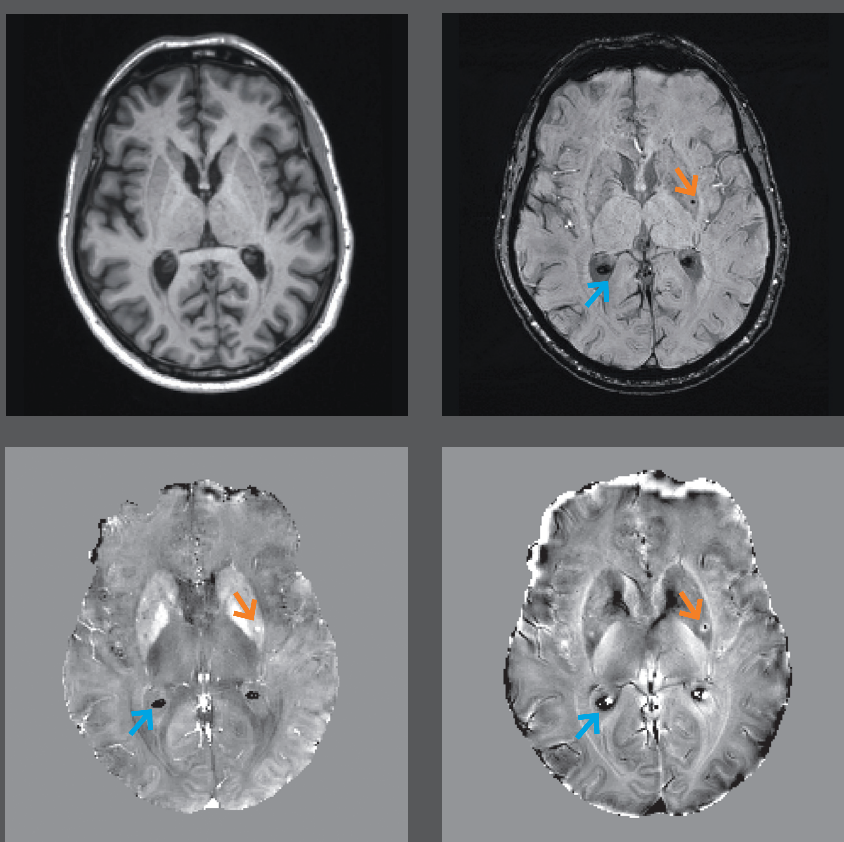
Project Title	Chief Investigator(s)	
Trials for Monash Clinical & Imaging Neuroscience	A/Prof Alex Fornito, Monash University Mr Chao Suo, Monash University Prof Murat Yucel, Monash University	Partner Share
Understanding the assembly of high electron affinity molecular acceptors on surfaces	Dr Chris Pakes, La Trobe University	Partner Share
Unsupervised clustering of high-content screen data	Prof Christophe Marcelle, Monash University Dr Juan Nunez-Iglesias, Monash University	Partner Share
Using GPUs to explore the genetic architecture of complex traits	Dr Joseph Powell, University of Queensland	Discretionary
Visualisation Evaluation	Dr Paul McIntosh, Monash University, Dr Tomasz Bednarz, CSIRO	Partner Share
Visualising Culture by Revealed Preferences Harvested from Internet Search	Dr Simon Angus, Monash University	Partner Share
Visualization of the Radiation Dose Deposition in Synchrotron X-ray Microbeam Radiation Therapy	Dr Iwan Cornelius, University of Wollongong Dr Michael Lerch, University of Wollongong	Discretionary
Vocal cord movements in Parkinson's disease	Prof Dominic Thyagarajan, Monash University	Partner Share
VPAC Member Support	Mr Craig West, VPAC	Partner Share
What is normal brain ageing? An investigation of changes in brain structure and cognition in mid-life	Dr Nicolas Cherbuin, Australian National University	Discretionary
X-ray Phase Imaging	Mr Aidan Carroll, La Trobe University, Prof Andrew Peele, Australian Synchrotron	Partner Share
XFM: Cosmochemistry with XFM	Dr Kathryn Dyl, CSIRO Dr Lenneke Jong, Australian Synchrotron, Dr Martin de Jonge, Australian Synchrotron, Prof Phil Bland, Curtin University	Partner Share



Axial slices from brain MRI of a subject who has both cerebral microbleeds (green arrow) and benign calcifications (blue arrow). The standard structural image (top left), does not show the microbleed and the calcifications are inconspicuous. A susceptibility weighted (SWI) scan, (top right), is sensitive to magnetic susceptibility changes and clearly shows the microbleed and the calcifications as dark regions. Magnetic susceptibility, the degree of magnetisation in response to an applied field, changes in brain tissue in the presence of metal (iron in the case of hemorrhages and calcium in calcifications). However the SWI cannot distinguish between microbleeds, which have positive susceptibility, and calcifications, which have negative susceptibility. A quantitative susceptibility map (QSM), (bottom left), can distinguish between microbleeds and calcifications. The generation of a QSM image requires a large amount of compute power (in this case provided through MASSIVE) in order to process and fit the MRI phase images (bottom right).

Images: Parnesh Raniga (CSIRO and Monash University)

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13.

Financial Statement

Income			Total at 31/12/2013	Total Budget
		Australian Synchrotron	-	-
		CSIRO	1,200,000	1,200,000
		DIIRD	1,450,000	1,450,000
		Monash	900,000	900,000
		NCI	1,200,000	1,200,000
		VPAC	800,000	800,000
		Other Transfers	119,970	119,970
		TOTAL Income	**5,669,970**	**5,669,970**

Expenditure				
	Machine Specific			
		Hardware Procurement	2,576,355	2,576,355
		Non-tender equip	17,681	22,681
		Facilities	150,736	201,111
		Software licenses	164,244	203,551
		SUBTOTAL	**2,909,016**	**3,003,698**
	Facility Specific		-	
		Establishment	118,846	118,846
		Training and outreach	230,764	255,864
		SUBTOTAL	**349,610**	**374,710**
	Massive			
		Management and Operations	1,973,529	2,480,297
		Steering Committee	27,363	34,363
		Establishment	18,745	18,745
		SUBTOTAL	**2,019,636**	**2,533,405**
	TOTALS			
		TOTAL Expenditure	**5,278,262**	**5,911,812**
		Interest	**246,646**	**246,536**

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14.

Abbreviations

AMMRF	Australian Microscopy and Microanalysis Research Facility
ANSTO	Australian Nuclear Science and Technology Organisation
ARC	Australian Research Council
ASHCo	Australian Synchrotron Holding Company
BAP	Beamline Advisory Committee
CPU	Central Processing Unit
CSIRO	Commonwealth Science and Industrial Research Organisation
CT	Computed Tomography
CVL	Characterisation Virtual Laboratory
DaRIS	Distributed and Reflective Informatics System
DSDBI	Department of State Development, Business and Innovation
GB	Gigabyte
GPU	Graphical Processing Units
HPC	High performance computing
IMBL	Imaging and Medical Beamline (at the Australian Synchrotron)
INCF	International Neuroinformatics Coordinating Facility
IR	Infrared
IVSAC	Imaging and Visualisation Scientific Advisory Committee
MAS	Merit Allocation Scheme
MASSIVE	Multi-modal Australian ScienceS Imaging and Visualisation Environment
MOSP	MASSIVE Operations Service Provider
MTWG	MASSIVE Technical Working Group
NCI	National Computational Infrastructure
NCMAS	National Computational Merit Allocation Scheme
NCRIS	National Collaborative Research Infrastructure Scheme
NeCTAR	National eResearch Collaboration Tools and Resources
NIF	National Imaging Facility
OECD	Organisation for Economic Co-operation and Development
PET/CT	Positron Emission Tomography / Computed Tomography
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
SLA	Service Level Agreement
SSAC	Synchrotron Scientific Advisory Committee
STRUDEL	The ScienTific Remote DEsktop Launcher
SU	System Units
SXRF	Synchrotron X-ray Fluorescence
TB	Terabyte
VeRSI	Victorian eResearch Strategic Initiative
VLSCI	Victorian Life Sciences Computational Initiative
VPAC	Victorian Partnership for Advanced Computing
XFM	X-ray Fluorescence Microscopy

- NCMAS National Computational Merit Allocation Scheme
- RDSI Research Data Storage Infrastructure

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