



Multi-modal Australian ScienceS Imaging
and Visualisation Environment

NCI Specialised Facility in Imaging and Visualisation

Paul McIntosh, Senior HPC Consultant



MASSIVE

AN HPC COLLABORATION TO UNDERPIN
SYNCHROTRON SCIENCE



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Monash University, Clayton, Australia

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Chris Hall, Anton Maksimenko, Santosh Panjekar, David
Paterson, Mark Tobin

Australian Synchrotron, Clayton, Australia

Chris Ryan, Darren Thompson

CSIRO, Clayton, Australia

DATA MANAGEMENT

SHARE

IMAGING
LOCUS

INSIGHT
Lens



ANALYSIS
Filters



CAPTURE
Light Source,
Samples



MASSIVE



HPC for Characterisation Specialised Facility for Imaging and Visualisation

Partners

Monash University
Australian Synchrotron
CSIRO

HPC

130 active projects
474 user accounts
100+ institutions across Australia

Instrument Integration

Integrating with key Australian
Instrument Facilities.

Affiliate Partners

ARC Centre of Excellence in
Integrative Brain Function
ARC Centre of Excellence in
Advanced Molecular Imaging

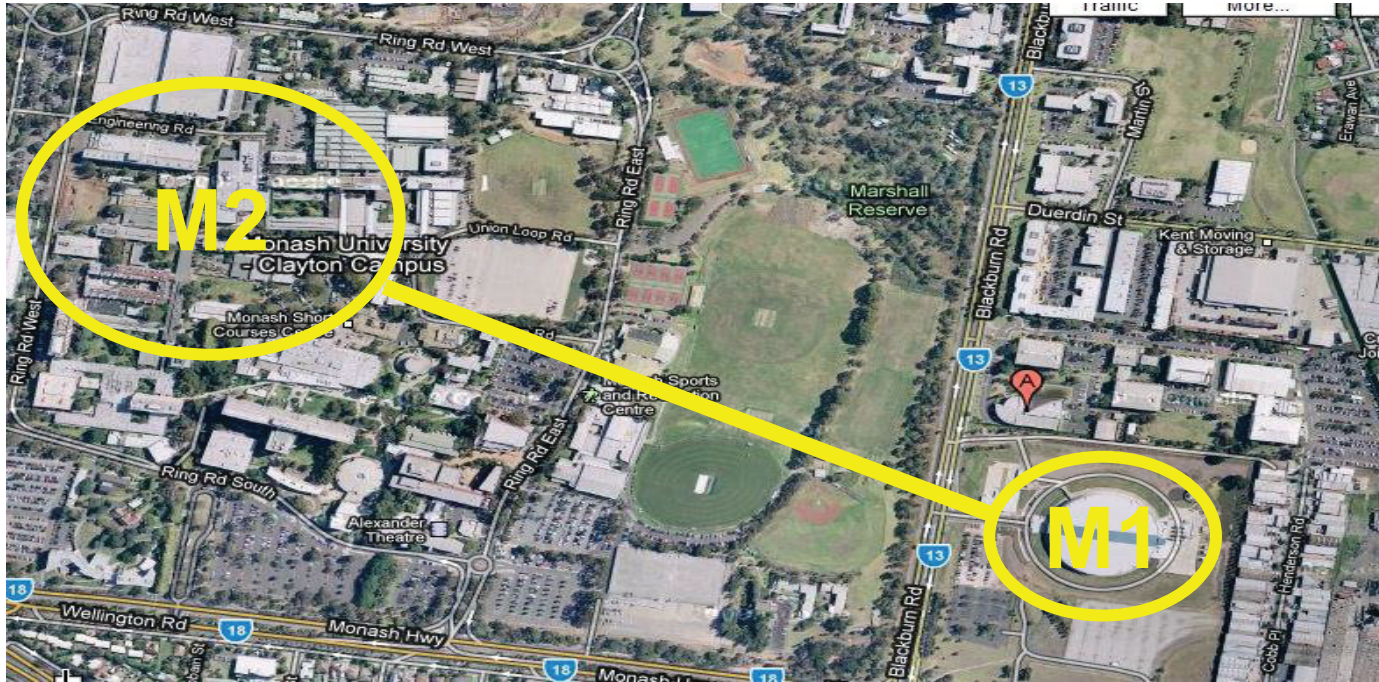
Interactive Vis

200+ users

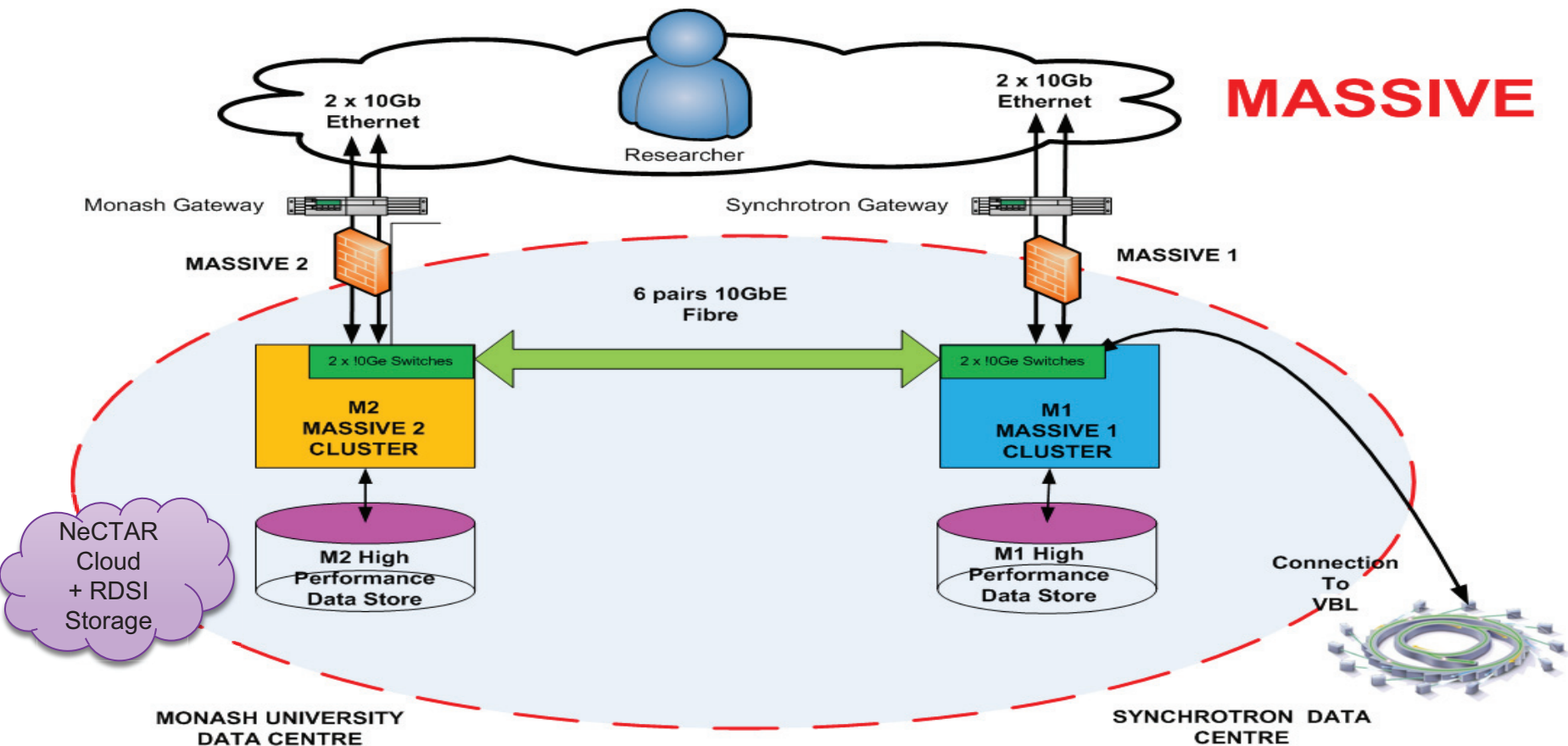
166 merit allocated projects
725 users

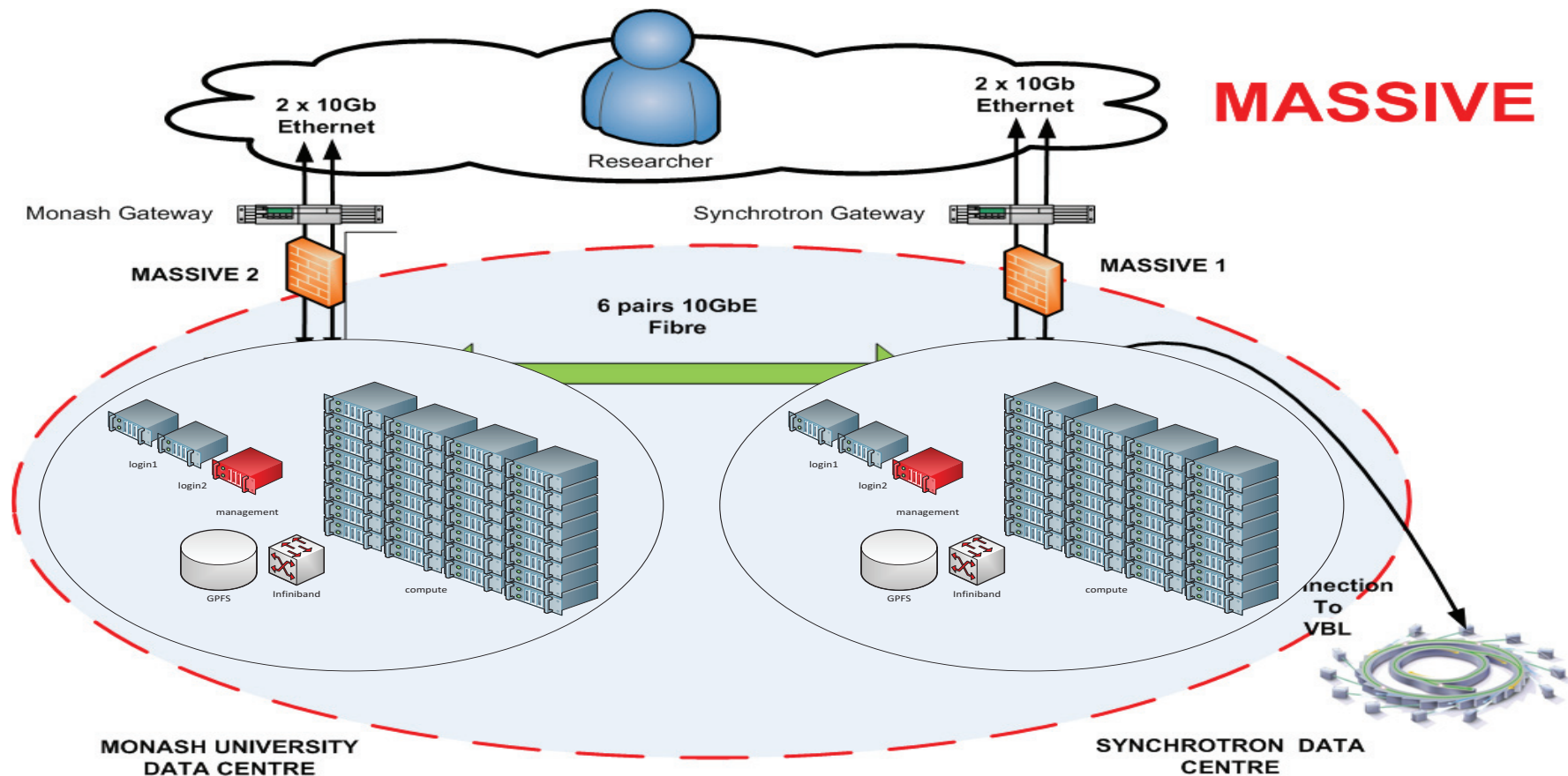
**Large cohort of long
tail researchers**

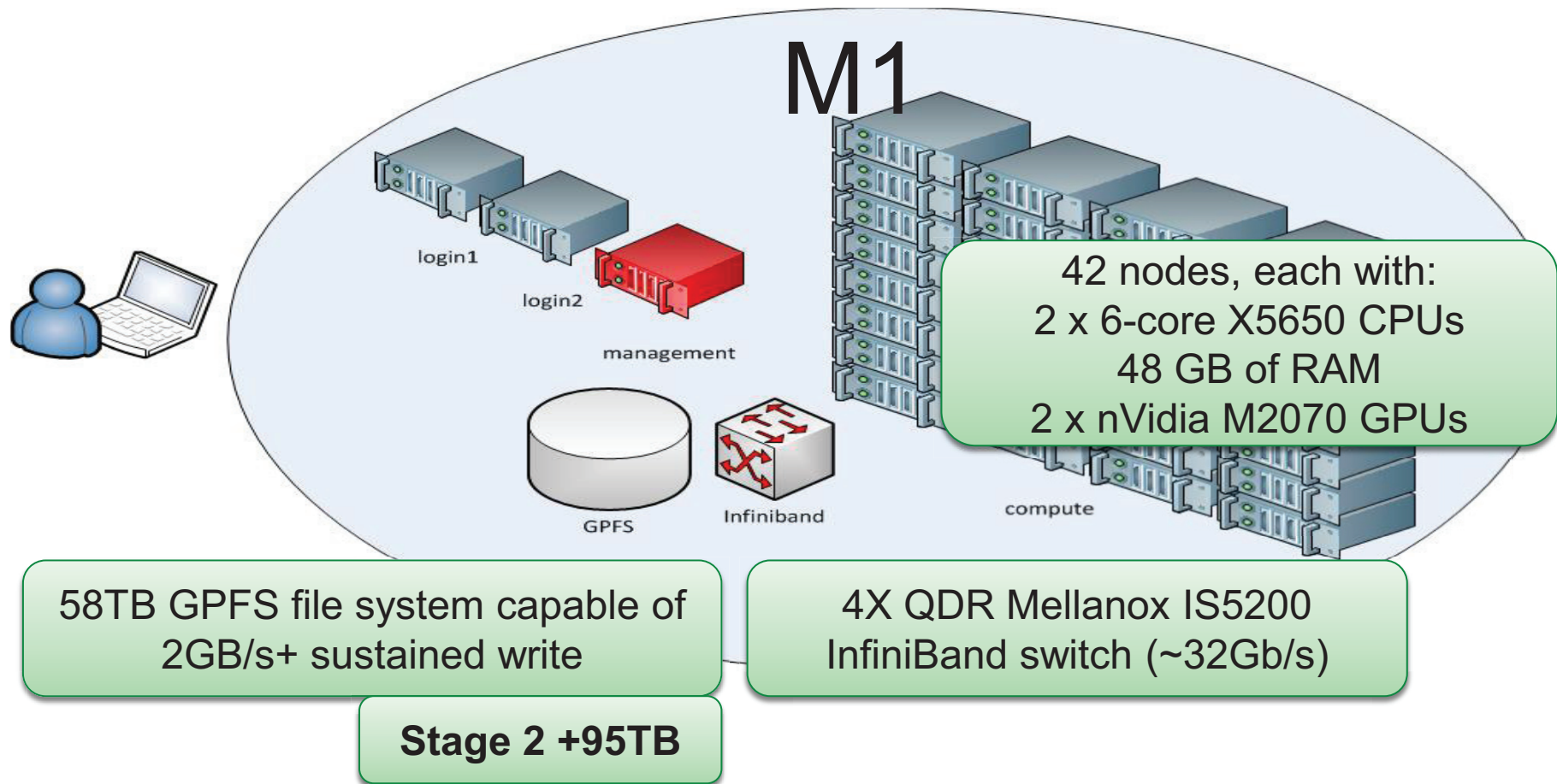
MASSIVE

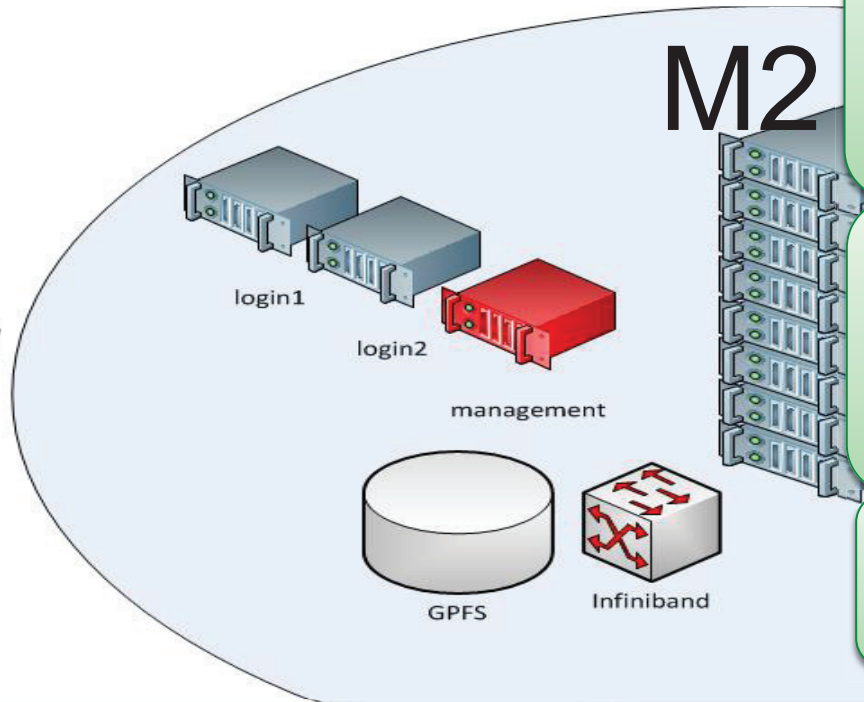


Source: Google Maps









M2

Stage 2:

+ 56 64GB RAM nodes
+20 128GB RAM nodes
+86 NVIDIA Tesla K20's
+20 Intel Xeon Phi's

32 compute nodes:
2 x 6-core X5650 CPUs
48 GB of RAM
2 x nVidia M2070 GPUs

10 Vis nodes:
192 GB RAM
2 x nVidia M2070Q

250TB GPFS file system capable of
3GB/s+ sustained write

4X QDR Mellanox IS5200
InfiniBand switch (~32Gb/s)

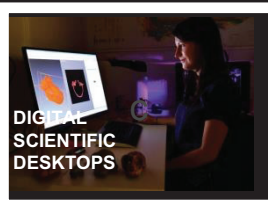
Stage 2 +100TB

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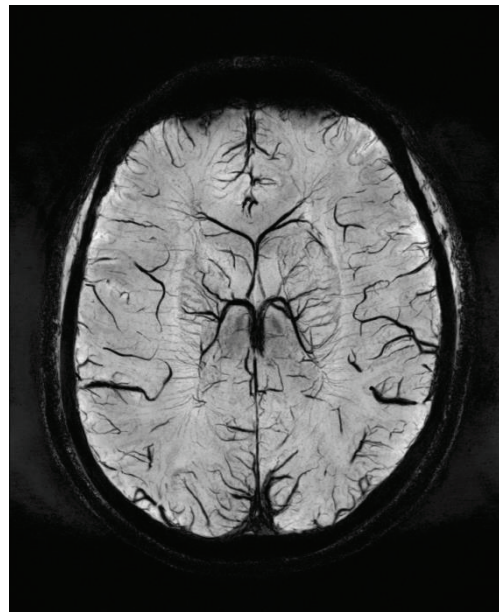
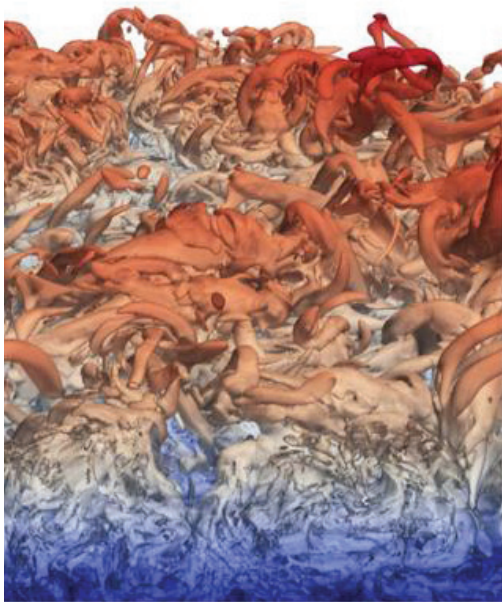


CAPTURE
Light Source,
Samples

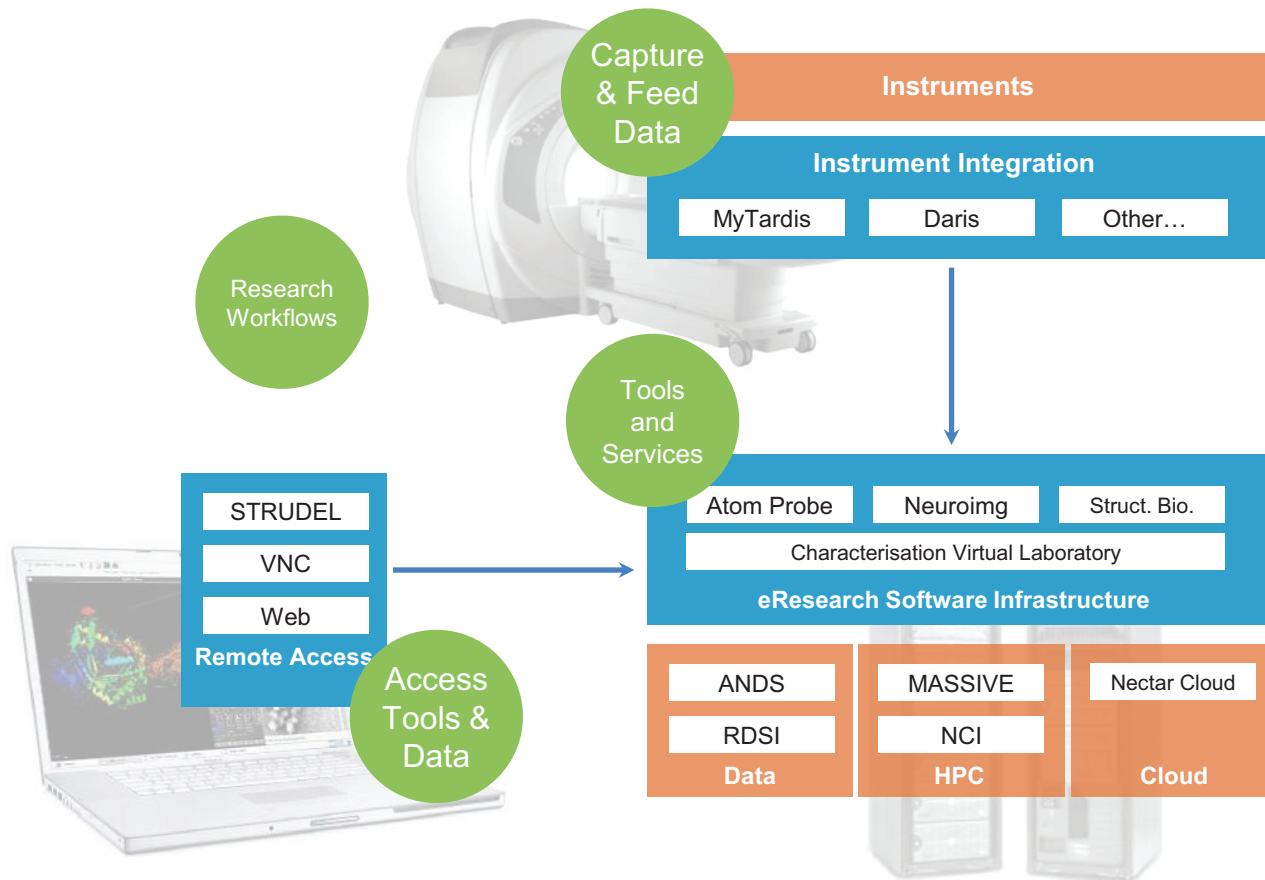


3D+ Analysis and Vis

Often “in-experiment”



Accelerate the long tail...



Strudel



Strudel

File Edit Identity Help

Site:

Username:

Project:

Hours:

Nodes:

Show Advanced Options ☐

par/mc's MASSIVE desktop (m21101)

Trash Home System

 **MASSIVE**

ParaView 3.10.1 64-bit

File Edit View Sources Filters Tools Macros Help

RTData Volume

Pipeline Browser

builtin: Wavelet1

Object Inspector

Properties Display Information

Whole Extent: -10 -10 -10 10 10 10

Center: 0 0 0

Maximum: 255

X Freq: 60 Y Freq: 30 Z Freq: 40

X Mag: 10 Y Mag: 10 Z Mag: 5

Standard

Statistics Inspector

Name	Data Type	No. of Cells	No. of Points	Memory
Wavelet1	Image (Uniform R)	8000	9261	0.037

ParaView Debug Window - <Finished> - Blender Deb - <Finished> - ParaView 3.10.1 64-bit

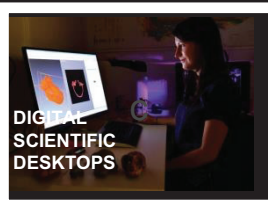
10:36

DATA MANAGEMENT

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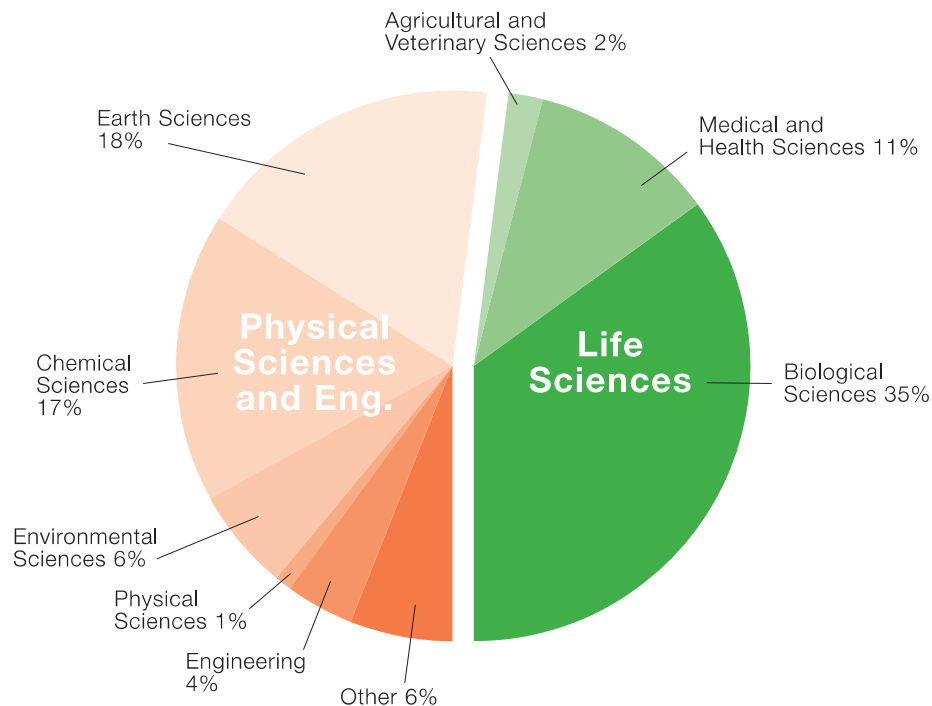


ANALYSIS
Filters

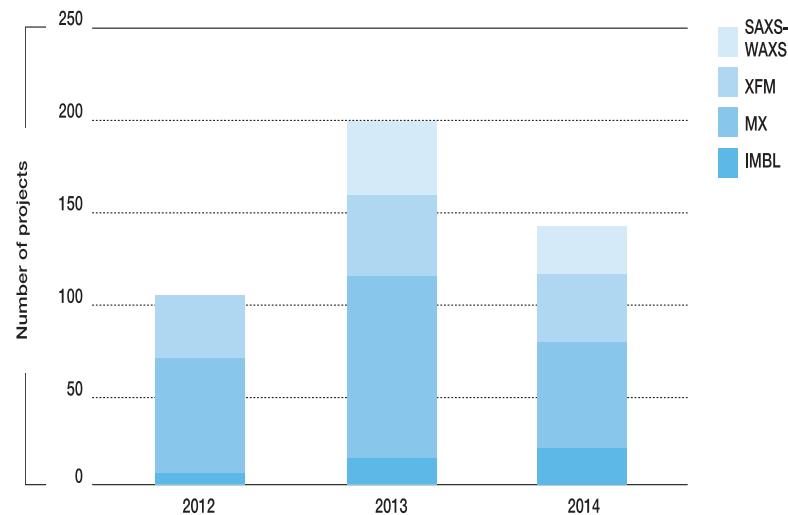


CAPTURE
Light Source,
Samples

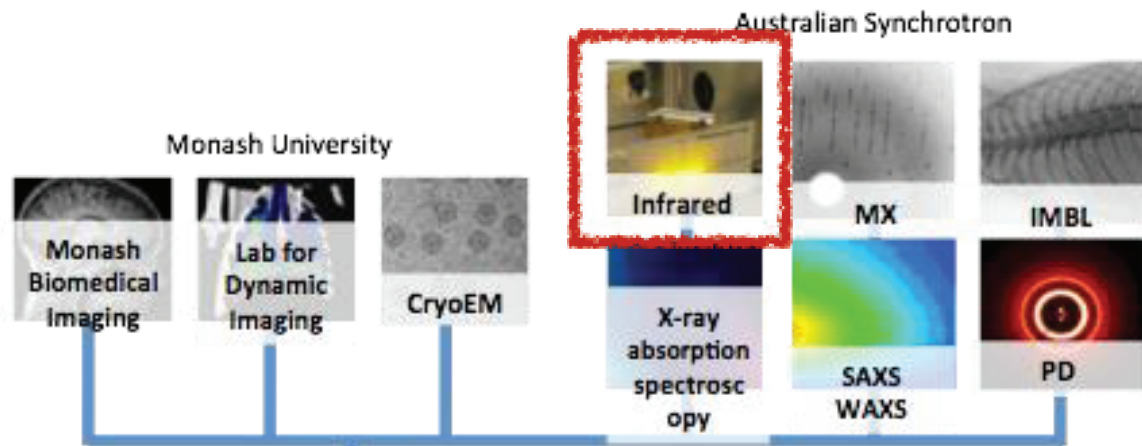




Research areas supported by the M1 and M2 computers during or shortly after beamtime.

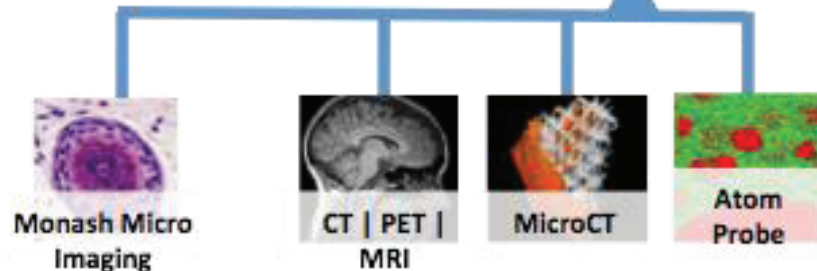


HPC usage by beamline 2012 to 2014 (MX1 and MX2 are shown combined).



Integration

Key Australian Instruments
Integrated with MASSIVE

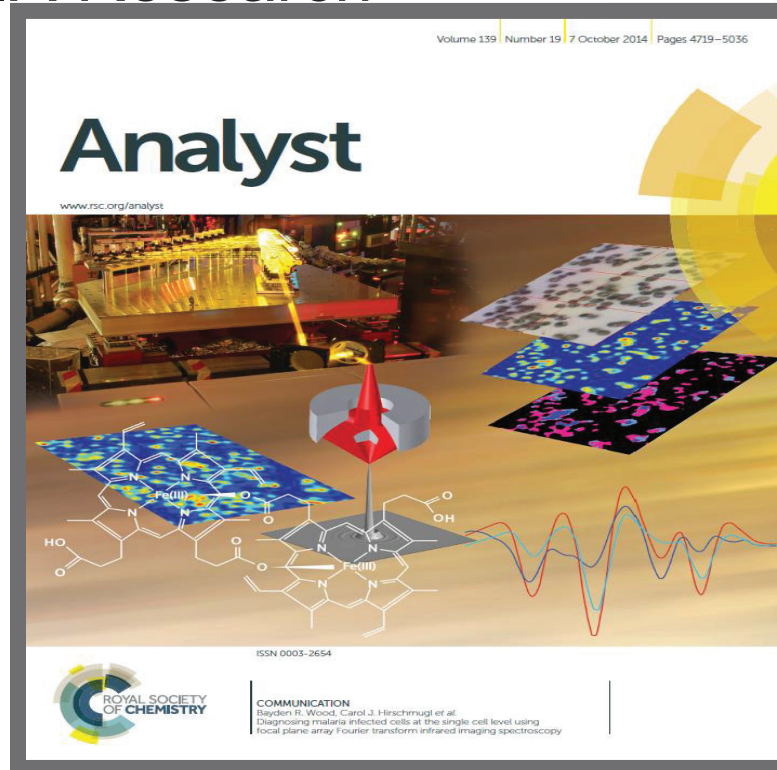
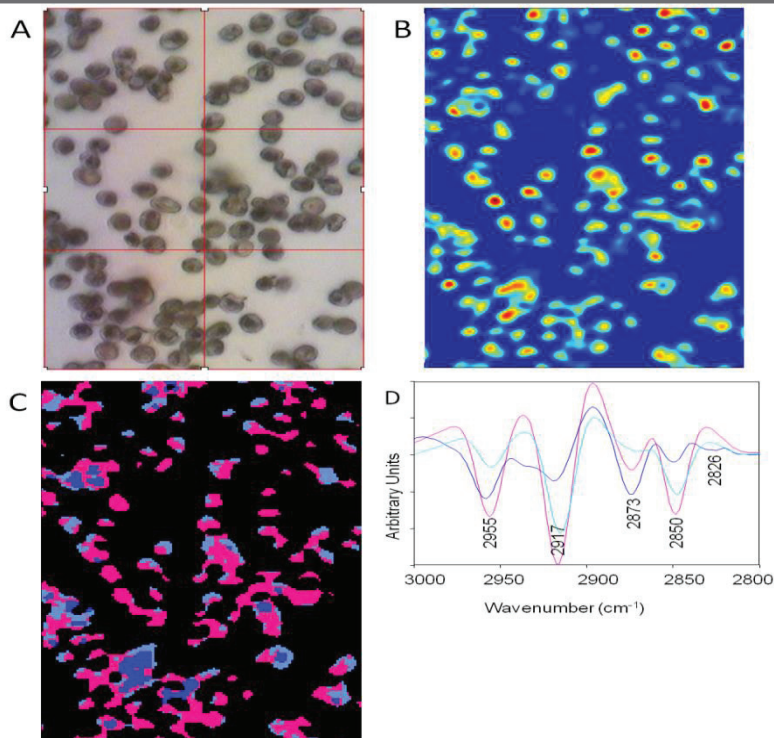


Australian Characterisation
Council

Infrared Microscopy Beamline



Synchrotron Infrared Microspectroscopy in MALARIA Research



RMieS – EMSC on MASSIVE



- How fast is it on MASSIVE?
- An FTIR image containing 62,500 spectra.
- Desktop PC 2.93 GHz Intel Core i7 CPU
16 GB RAM & Windows 7 Enterprise 64 bit
53 Hours .
- MASSIVE
42 minutes .



ABOUT US

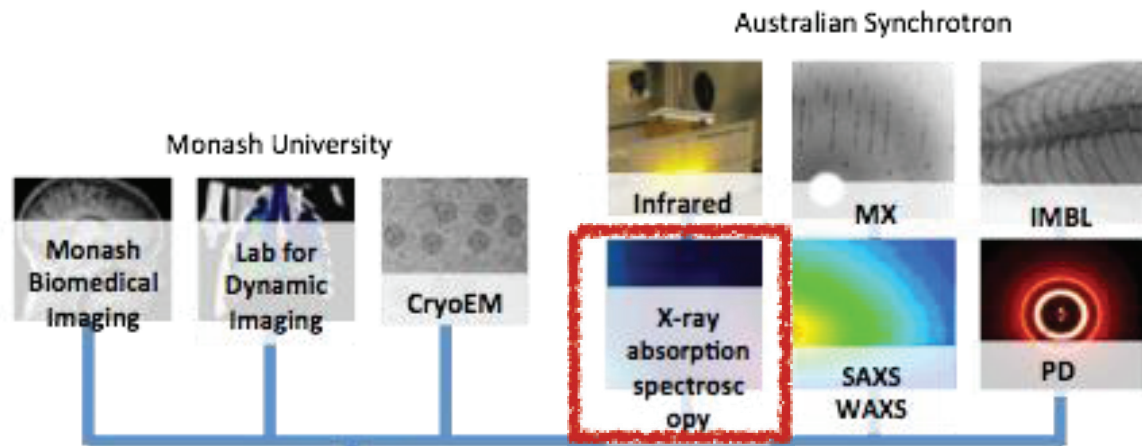
You are here: [Home](#)

IR workshop is MASSIVE-ly useful

[highlights](#) [IR](#) [IR1](#) [highlights-IR1](#)

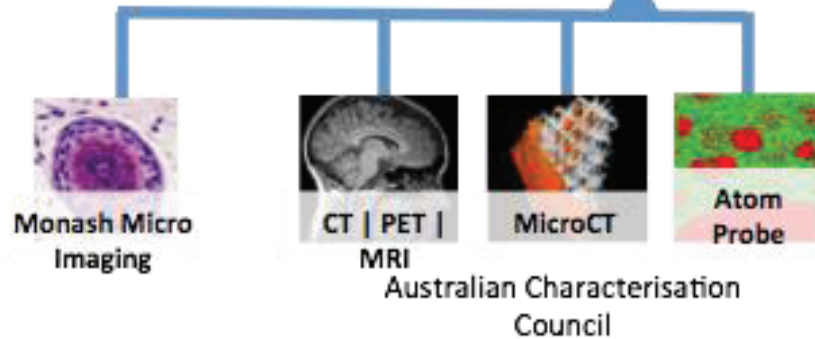
More than 40 researchers and potential new users of synchrotron infrared analysis workshop at the AS in June 2012.

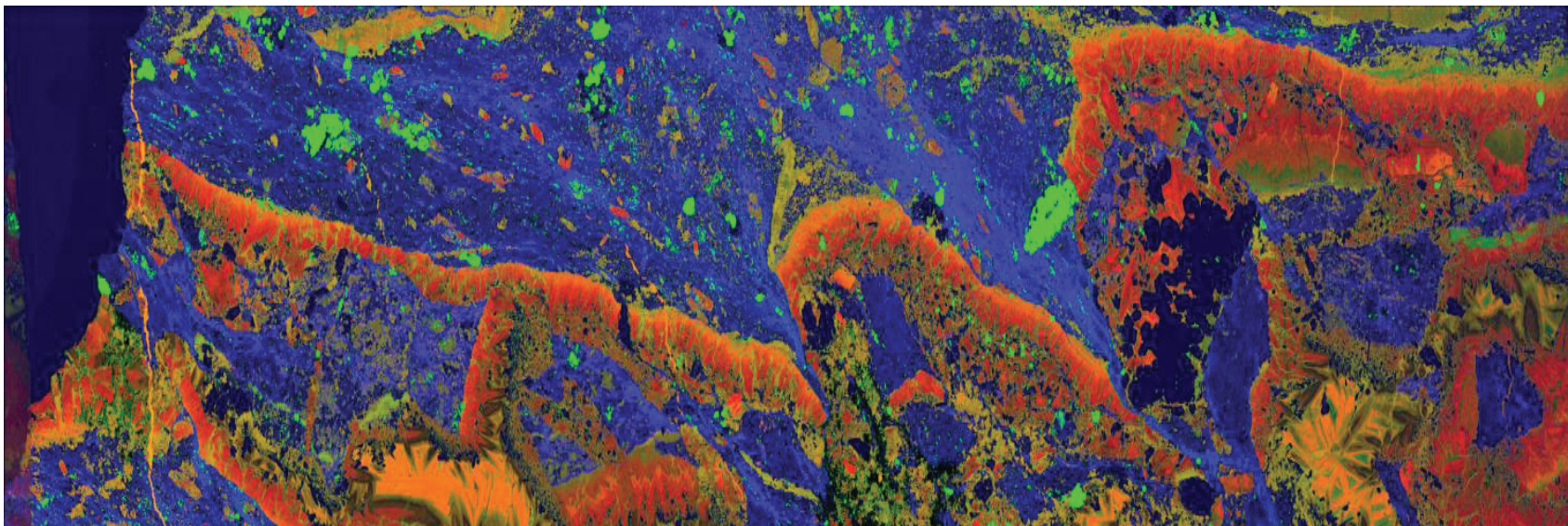




Integration

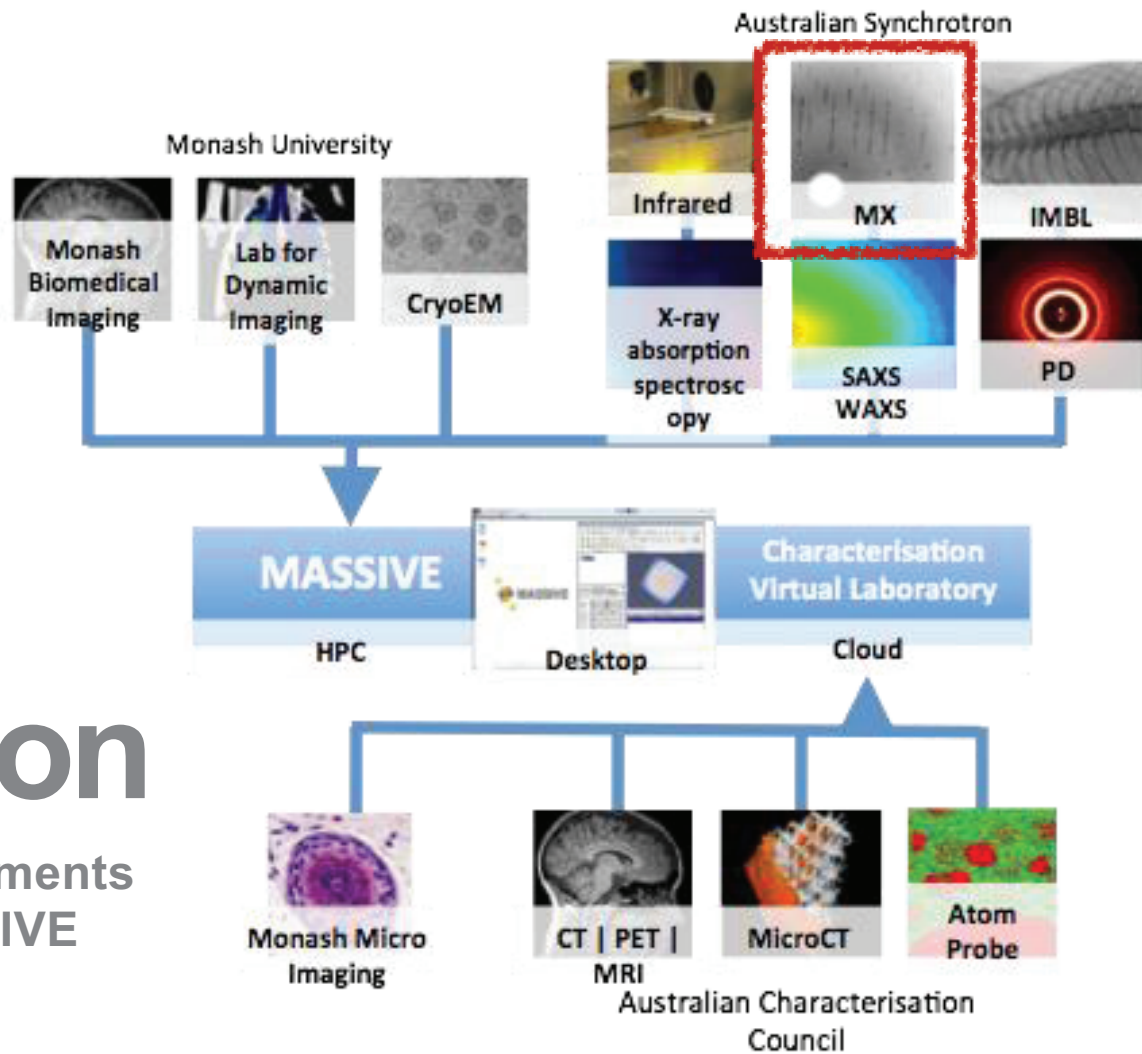
Key Australian Instruments
Integrated with MASSIVE







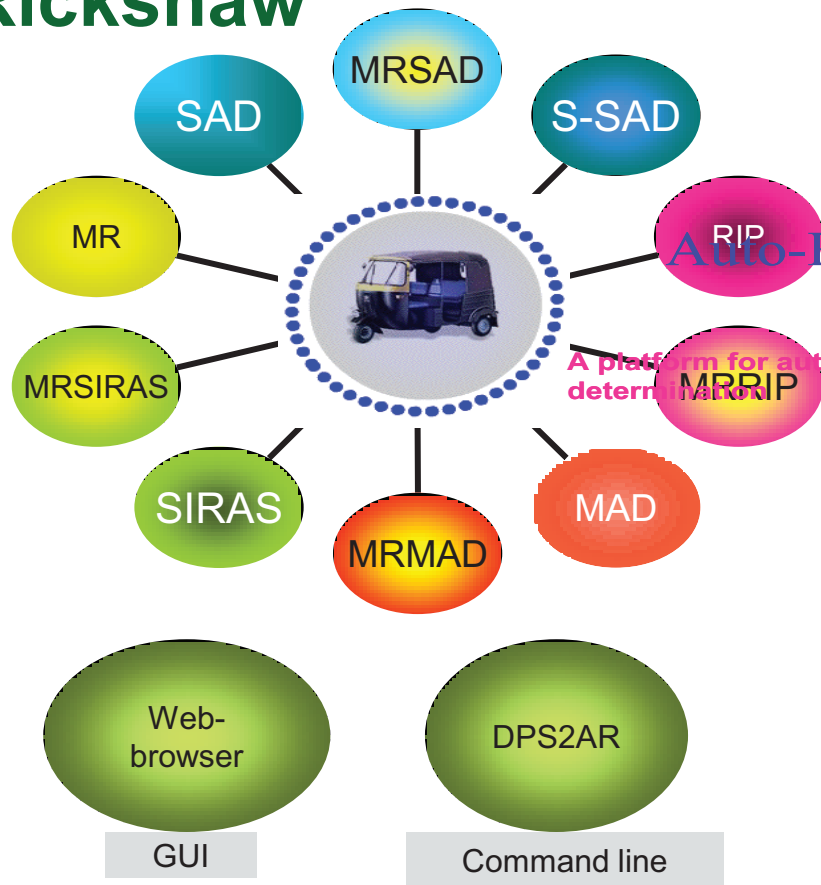
GeoPIXE@XFM workshop
<https://events.synchrotron.org.au/event/17/>



Integration

Key Australian Instruments
Integrated with MASSIVE

Overview of Auto-Rickshaw



Version
Beamline Advanced

Quick
Longer



AR server (open to world)
<http://www.embl-hamburg.de/Auto-Rickshaw>

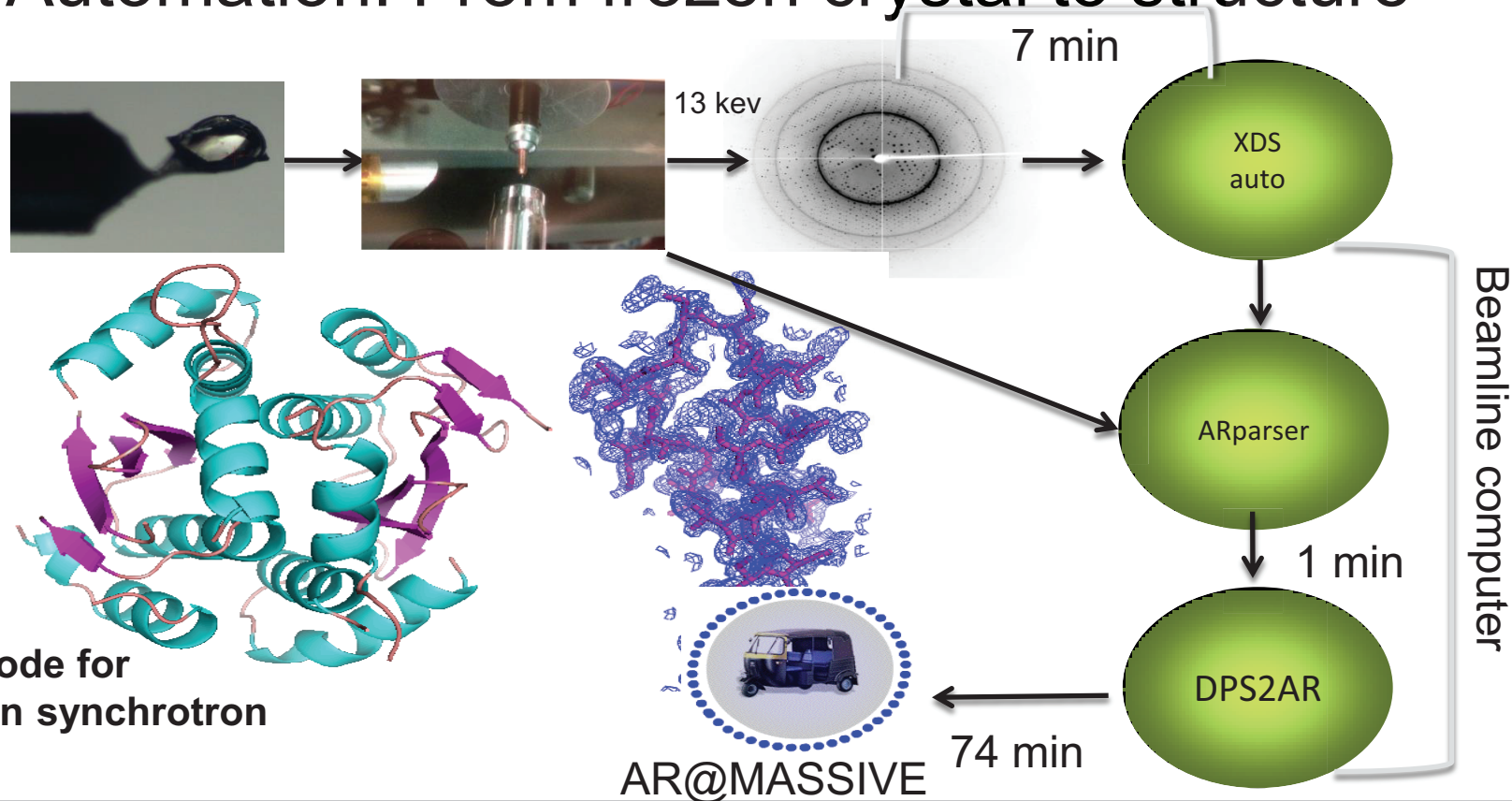
AR server @ MASSIVE
Open to Academic users from
Australian Synchrotron beamlines

Necessary Input required

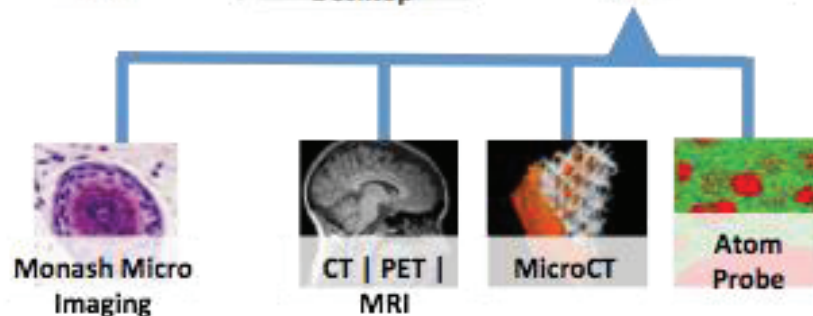
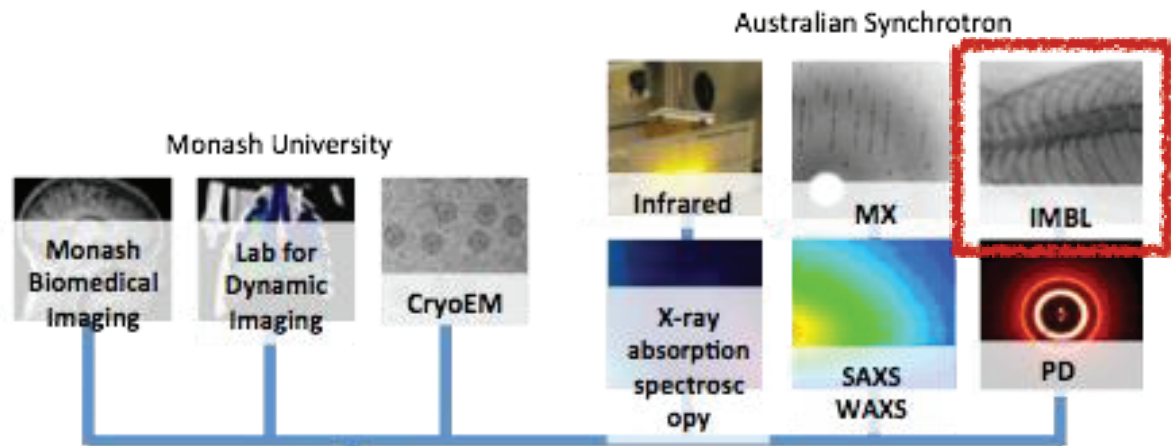
- No. of residues per monomer
- No. of expected heavy atom sites per monomer
- No. of monomers per a.u.
- Space group
- X-ray data
- Sequence file (optional)
- Model file PDB-format (optional)
- Email address



Automation: From frozen crystal to structure



Total number of residues in asu 400 Total number of heavy atoms in asu 3
Space group P212121 Phasing method SAD Max resolution: 1.5 (No sequence input)
Output from Auto-Rickshaw [a partially refined model (R-factor/Rfree): 0.369 / 0.401]

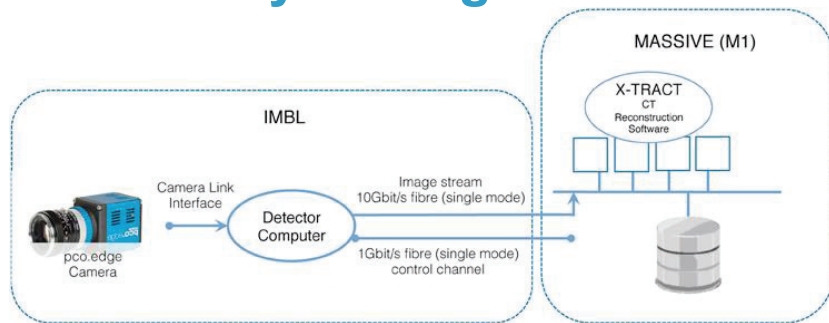


Integration

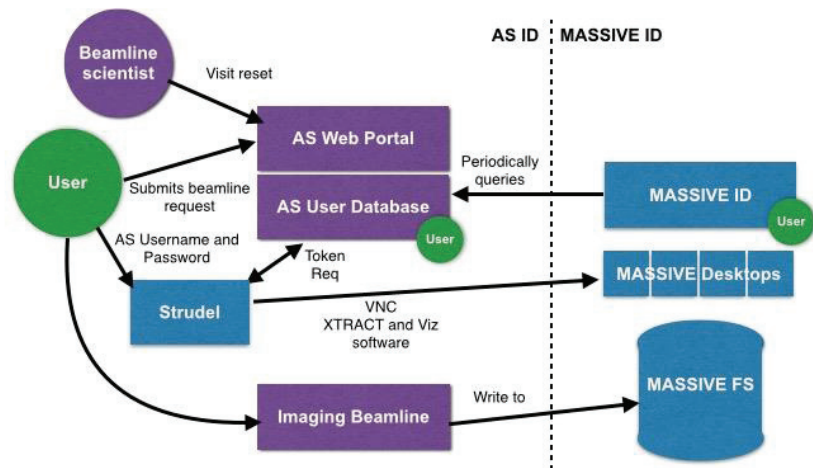
Key Australian Instruments
Integrated with MASSIVE

Australian Characterisation
Council

Hardware Layer Integration

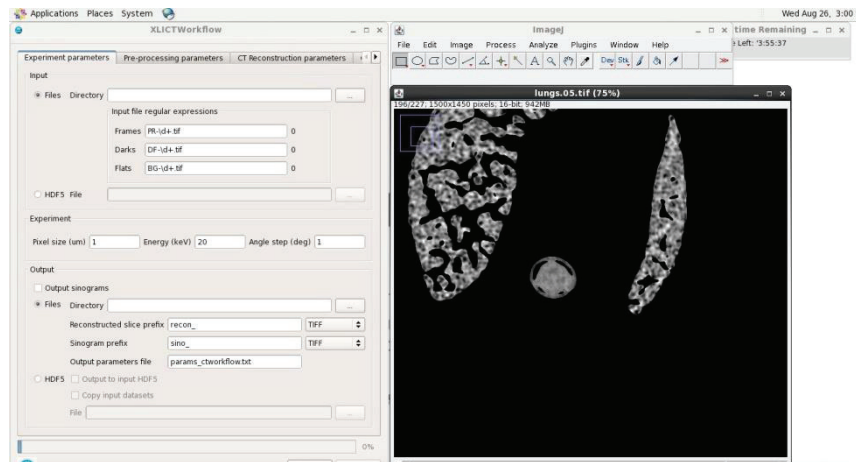


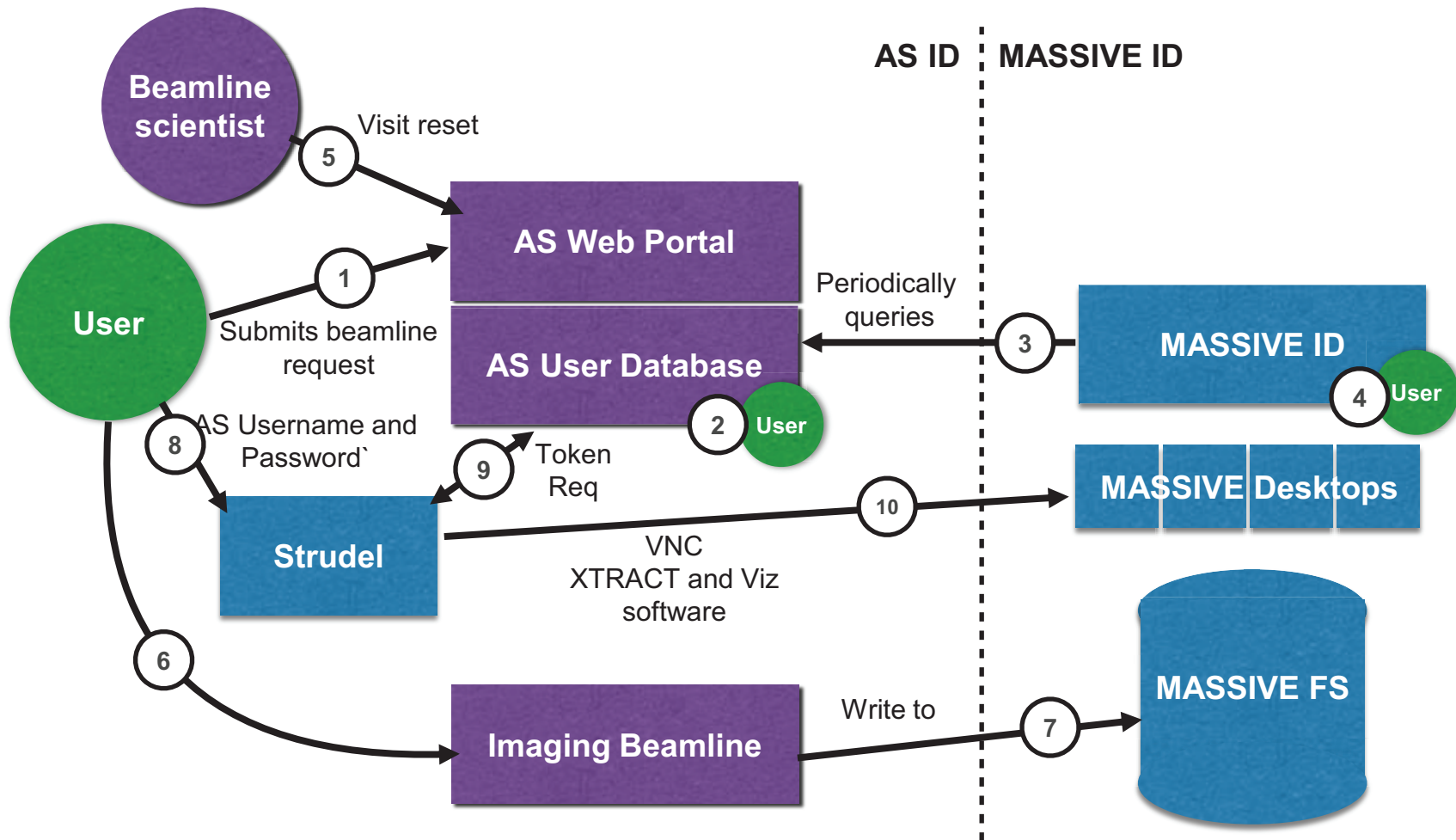
Systems View

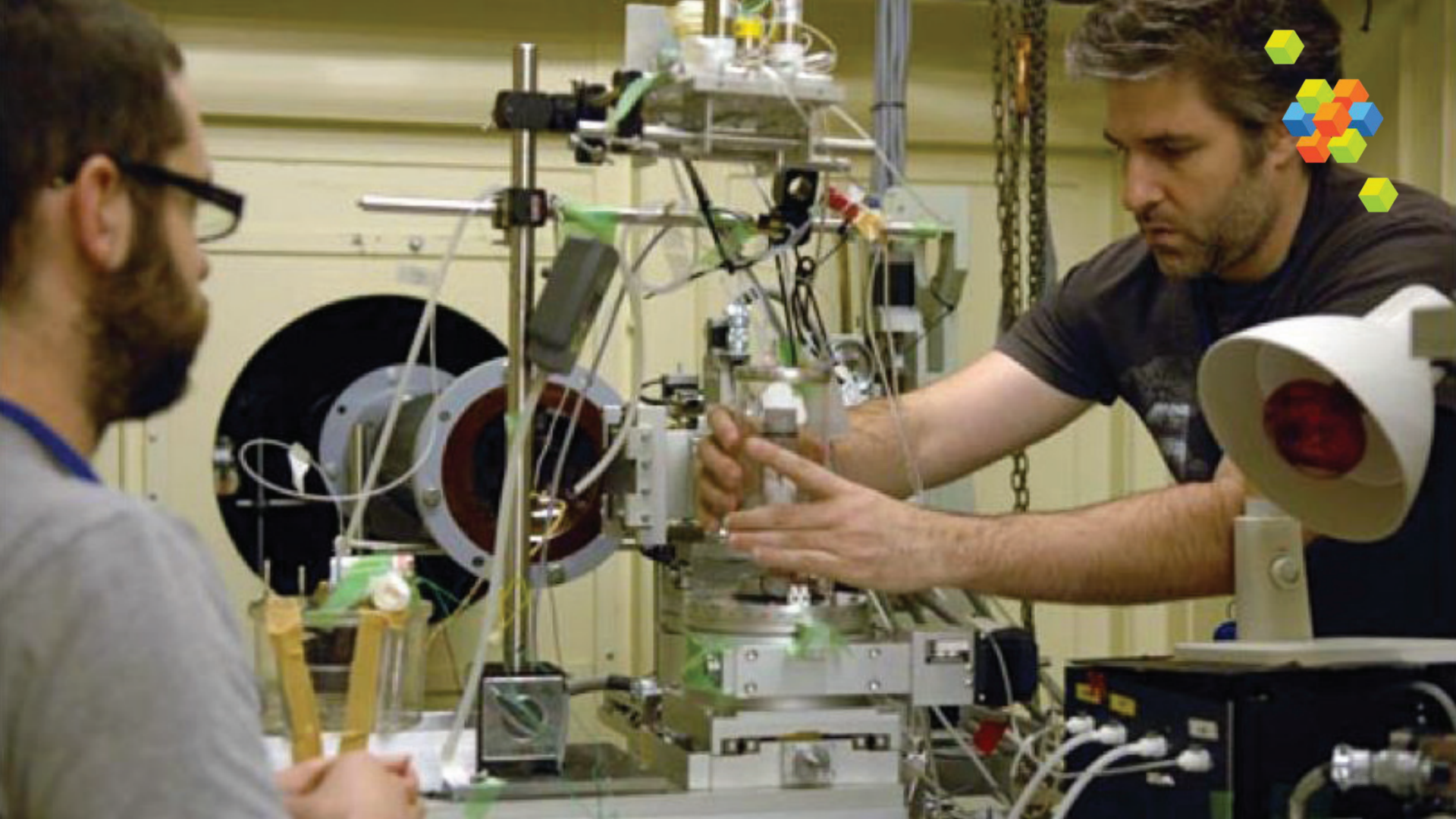


User view

Remote Desktop with Australian Synch credentials

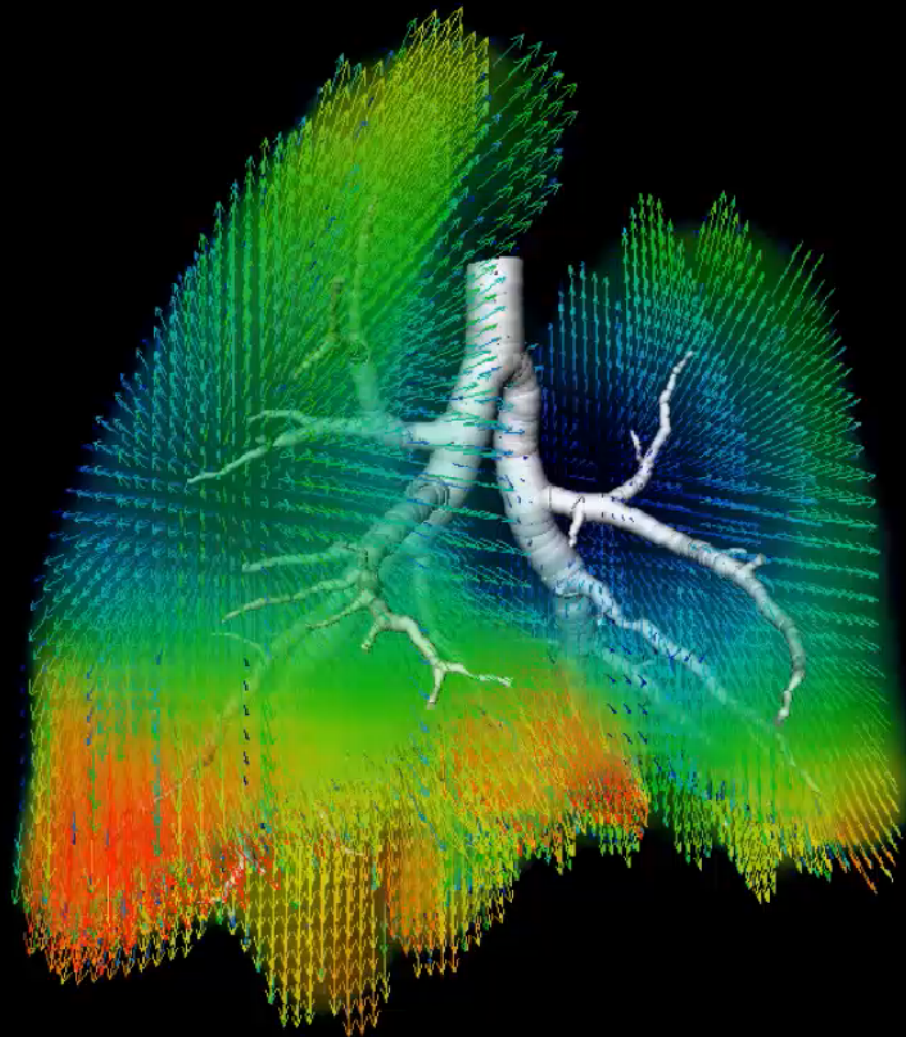












Outcomes

Increasingly large cohort of long tail researchers with big data problems opportunities

Automated or semi-automated processing from the instrument

Capturing new HPC and long tail researchers (10s of new users per beamline per week)

Desktop interactive access

e.g Psychology, wet lab biomed

Desktop users progressing to batch access for big processing

Institutions

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

University	Research Institute	Medical
Australian National University	ANSTO	Alfred Health
Curtin University	Australian Synchrotron	Eastern Health
Deakin University	CSIRO	GGZ inGeest
James Cook University	Garvan Institute of Medical Research	Melbourne Health
La Trobe University	Baker IDI	IRCCS Burlo Garofolo Hospital
Massey University	Bionics Institute	Peter Mac
Monash University	Brain Research Institute de Bascule	QLD Health
Queensland University of Technology	Indian Institute of Astrophysics	Royal Adelaide Hospital
RMIT	Institute of Nuclear Physics, Polish Academy of Sciences	The William Buckland Radiotherapy Centre
Southern Cross University	Neuroscience Research Australia	Women's and Children's Hospital, Adelaide
University of Adelaide	QIMR Berghofer	Industry
University of Hawaii at Manoa	QIMR Berghofer Medical Research Institute	IBM
University of Melbourne	Russian Academy of Sciences	4DX
University of New South Wales	Synchrotron Light Research Institute	Australian Red Cross Blood Service
University of Newcastle	VERSI	AgResearch Ltd
University of Otago	Victorian Partnership for Advanced Computing	Carrick Gold Ltd
University of Queensland		GNS Science
University of South Australia		Government
University of Sydney		Ames Laboratory
University of Technology Sydney		IVEC
University of Wollongong		Department of Primary Industries
Western Australia		Museum Victoria
		State Library New South Wales
		Western Australian Museum
		DSTO
		NGV (National Gallery Vic)
		Synchrotron SOLEIL
		SA Museum
		Natural History Museum, UK

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