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OF QUEENSLAND  
AUSTRALIA

CREATE CHANGE


# A journey towards end-to-end services for instrument based e-Science

David Abramson

Research Computing Centre

University of Queensland, Brisbane, Australia

# Wish I was there ....



David Abramson – Virtual Ride

07:24 on Monday, 21 June 2021

## Magugnano to Riva del Garda, Lake Garda

Add a description

Add private notes

With someone who didn't record? [Add Friends](#)

4 Rides on this route →

This Ride **26.8 km/h**

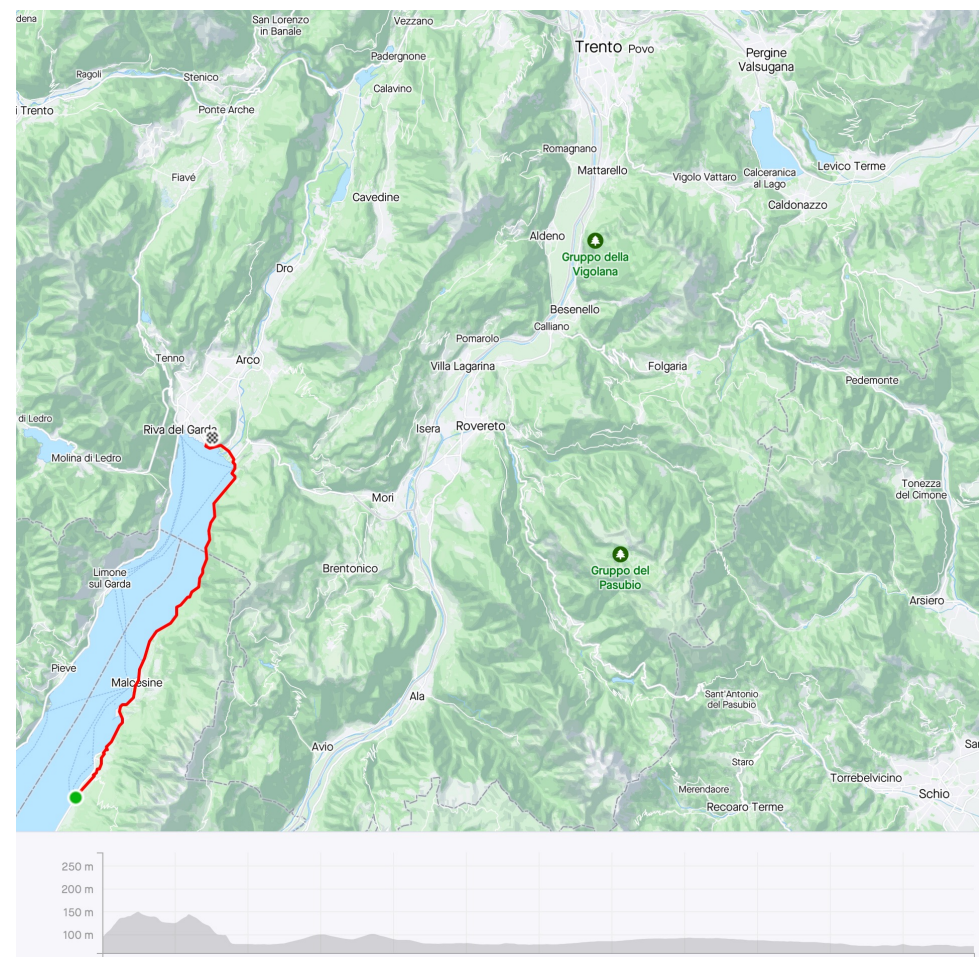
Trending Faster ▲

23.94 km	53:41	135 m	12
Distance	Moving Time	Elevation	Relative Effort
152 w	484 kJ	68	87%
Weighted Avg Power	Total Work	Training Load	Intensity

	Avg	Max
Speed	26.8km/h	60.5km/h
Heart Rate	102bpm	114bpm
Cadence	63	85
Power	150W	232W
Calories	483	
Elapsed Time	53:41	

Show Less

FulGaz Bike: Brisbane Domane



# Introduction

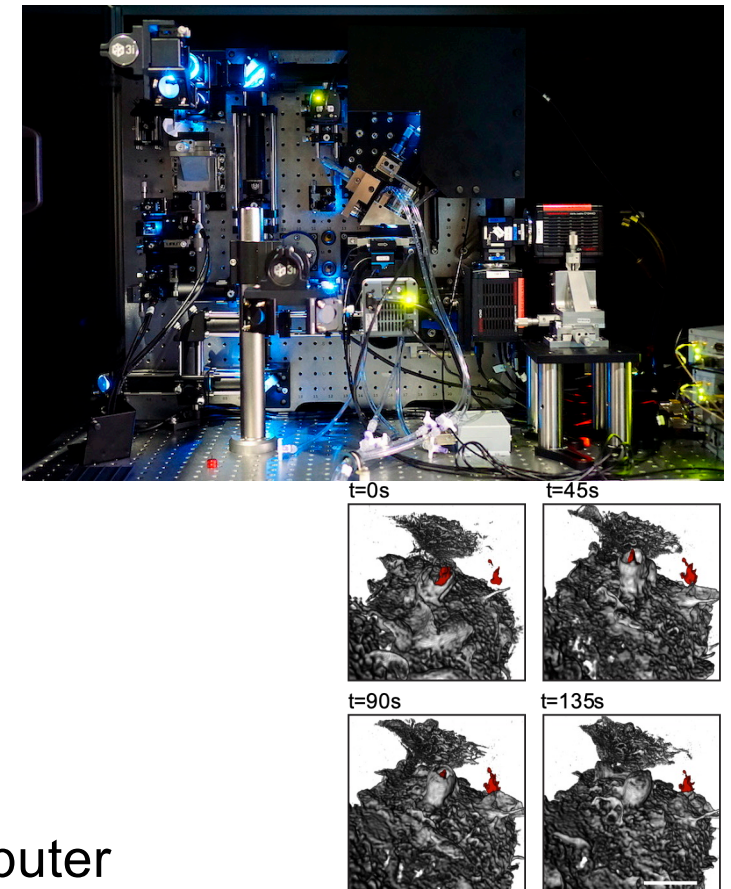
- Motivation
- Service Framework
- Implementation at UQ
- Case Studies
- Conclusions





“I just want the pretty picture, movie and graph, not how the pipes are connected, nor why I need some big computer to process it”.

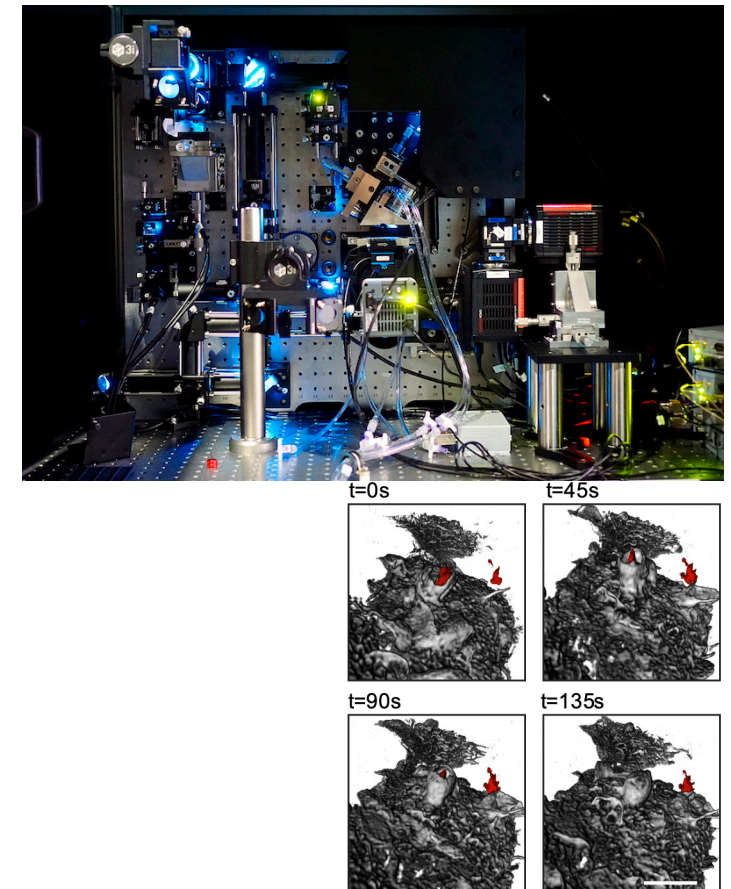
- Live-cell imaging optical microscope
  - Spatial resolution 512 x 2048 x 151 pixels,
  - Temporal resolution 60 volumes per minute
  - 5-10 TBytes per day!
- A researcher must contact the facility operator to book a time slot.
- Each 3 D volume must be pre-processed
  - multiple channel alignment,
  - transformations
  - deconvolution techniques to remove errors and imaging artifacts.
  - Need an advanced GPU based supercomputer.
- Images must be transferred to a campus supercomputer



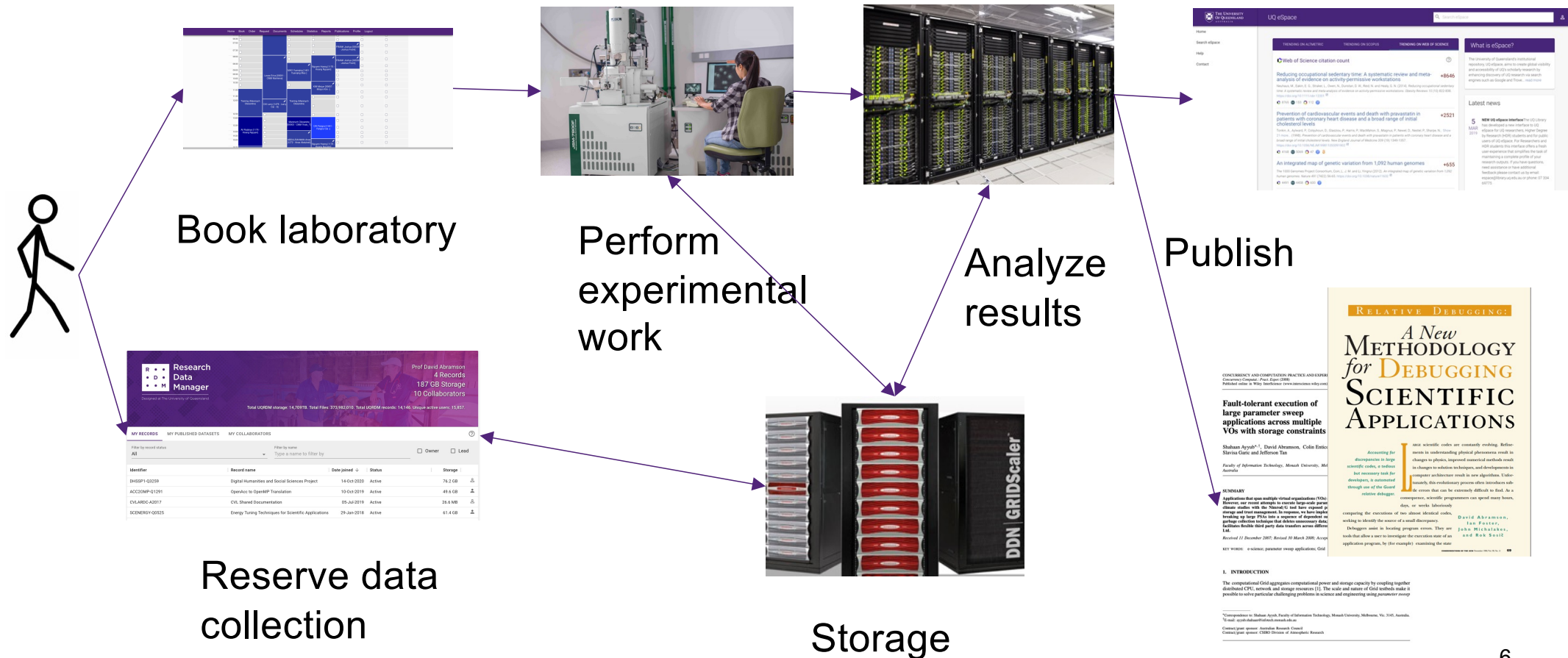


“I just want the pretty picture, movie and graph, not how the pipes are connected, nor why I need some big computer to process it”.

- Biologists, must master the software tools to
  - transfer the data across the university network
  - submit jobs using a queue-based scheduling mechanism
  - visualise and analyse on a range of computers from high powered desktops to a research cloud
- Primary, secondary, and associated processing meta-data, is stored for archive on scalable hierarchical storage system
- Instrument and experimental meta-data
  - might be recorded along with the images or
  - may be ingested into an image repository for subsequent sharing and archive or
  - Stored on local desktop or external disk drives.



# Instrument Researcher Workflow





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# Service Framework



## Service Framework

- Booking an instrument and associated laboratory.
- Automatic provisioning of sufficient storage capacity for the scale of the experiments.
- The removal of explicit data movement steps and the knowledge of the various storage subsystems.
- Processing data on advanced computational platforms without complex manual configuration.
- Automatic archiving and sharing of both primary and secondary data sets.
- Automatic capture of instrument and experiment meta-data.



## Booking an instrument and associated laboratory

- *We envisage a system that*
  - allows researchers to book time on an instrument
  - required e-infrastructure to be simultaneously scheduled and managed.
- For example
  - if a user needs to pre-process data sets on the fly, they also require access to processing software on the correct computational platforms.
  - This allows the data flows to be optimised so it moves seamlessly between workflow steps.



## Automatic provisioning of sufficient storage capacity for the scale of the experiments

- *We envisage* a scheme in which storage is allocated as a side effect of documenting a project.
- Storage for imaging data and the description of the research project become linked, and provisioning (and ultimate removal) can be automated.





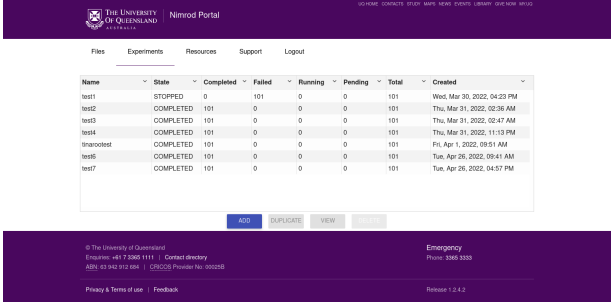
## The removal of explicit data movement steps and the knowledge of the various storage subsystems

- *We envisage* a system that transports data between computers transparently, arranging for the right data to appear at the right time, and for only one archival copy of the data to be retained.



# Processing data on advanced computational platforms without complex manual configuration

- We envisage a range of Web portals, or Science Gateways
  - mask the underlying complexity of the computational platforms.
  - gateways provide simple point and click style interfaces and take on the task of submitting jobs to supercomputers transparently
  - We also envisage a Science Gateway that delivers a desktop experience, thus users familiar with graphical desktop software can use it as though it were installed on their local machine.
  - This dramatically simplifies software deployment and license management, a historically difficult task for centralised software support teams on distributed infrastructure.



The screenshot shows the 'Nimrod Portal' interface. It features a navigation bar with links for Files, Experiments, Resources, Support, and Logout. Below this is a table displaying job execution details. The table has columns for Name, State, Completed, Failed, Running, Pending, Total, and Created. The data rows show various jobs (test1, test2, test3, test4, test5, test6, test7) with their respective states and completion counts. At the bottom of the table are buttons for 'Add', 'Configure', 'View', and 'Refresh'. The footer contains copyright information for The University of Queensland, contact details, and a release version of 1.0.4.2.

Name	State	Completed	Failed	Running	Pending	Total	Created
test1	STOPPED	0	101	0	0	101	Wed, Mar 30, 2022, 04:23 PM
test2	COMPLETED	101	0	0	0	101	Thu, Mar 31, 2022, 02:30 AM
test3	COMPLETED	101	0	0	0	101	Thu, Mar 31, 2022, 02:47 AM
test4	COMPLETED	101	0	0	0	101	Thu, Mar 31, 2022, 11:13 PM
test5	COMPLETED	101	0	0	0	101	Fri, Apr 1, 2022, 09:51 AM
test6	COMPLETED	101	0	0	0	101	Tue, Apr 26, 2022, 09:41 AM
test7	COMPLETED	101	0	0	0	101	Tue, Apr 26, 2022, 04:57 PM

## Automatic archiving and sharing of both primary and secondary data sets

- *We envisage an e-infrastructure* and associated services that manages the data life-cycle automatically.
- Takes care of moving data from working storage, which is often fast and expensive, to cheaper long-term storage systems





## Automatic capture of instrument and experiment meta-data.

- *We envisage* a storage architecture that supports both managed and unmanaged data sets simultaneously in the same e-infrastructure.
- The solution allows previously unmanaged collections to be *upgraded* to managed ones on demand.
  - significant benefit as users transition from unmanaged to managed data collections and simplifies the transition to better data management techniques
  - F.A.I.R. is a journey that takes time.

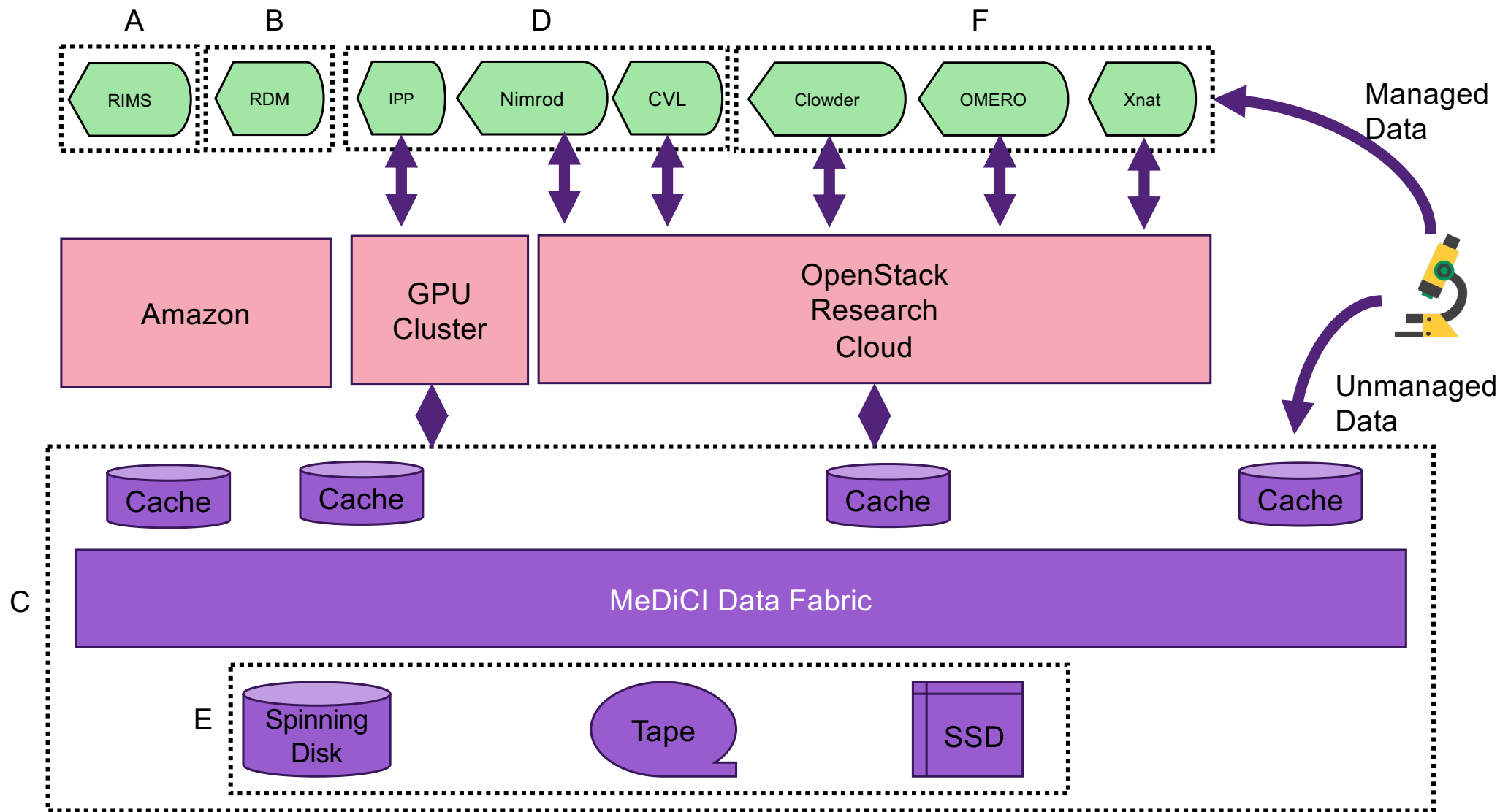




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# Implementation @ UQ



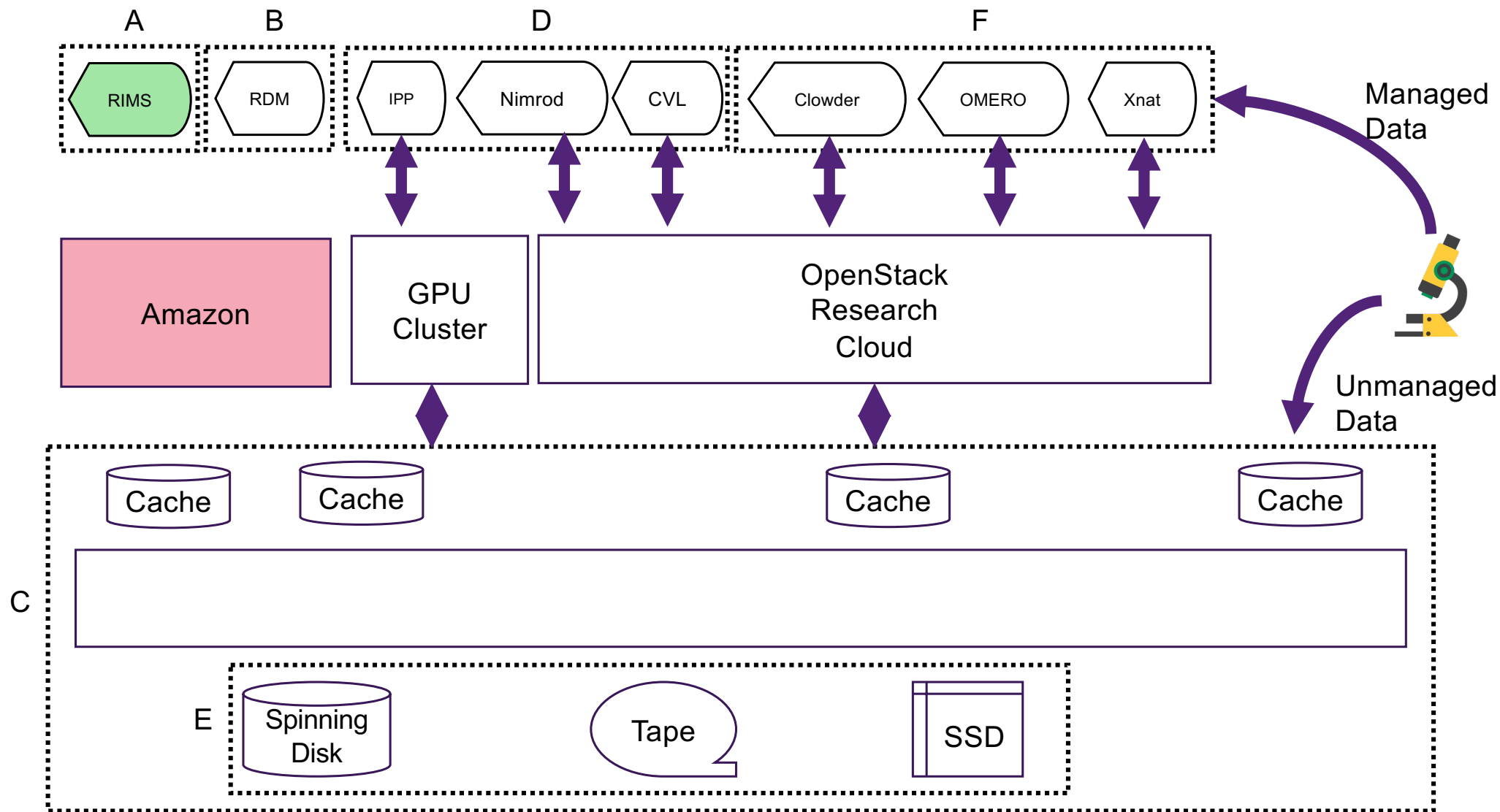




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# Booking an instrument and associated laboratory

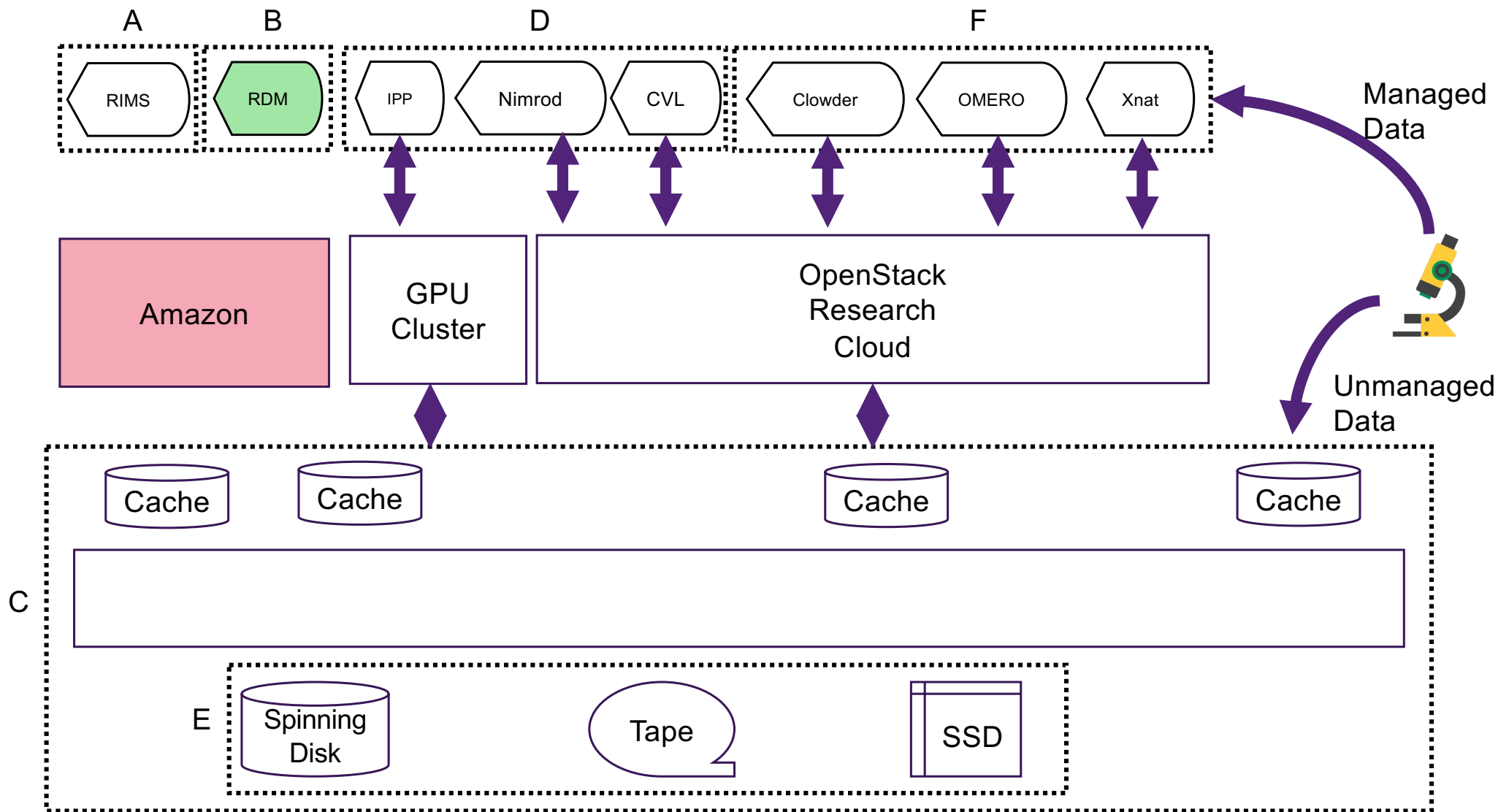


- | <a href="#">Home</a> <a href="#">Book</a> <a href="#">Order</a> <a href="#">Request</a> <a href="#">Documents</a> <a href="#">Schedules</a> <a href="#">Statistics</a> <a href="#">Reports</a> <a href="#">Publications</a> <a href="#">Profile</a> <a href="#">Logout</a>                       |  |  |  |   |  |  |  |
|--|--|--|--|---|--|--|--|
| Systems available for booking  |  |  |  |   |  |  |  |
| <b>ELECTRON BEAM LITHOGRAPHY</b> <ul style="list-style-type: none"> <li>• BEAMER HOTDESK (L106A)</li> <li>• CLEANROOM ( METROLOGY) (L114)</li> <li>• CLEANROOM (CHEMICAL) (L114)</li> <li>• EBPO REMOTE PC (L106A)</li> <li>• EBPOS150 (L117)</li> <li>• RAITH E-LINE PLUS SEM (L116)</li> </ul> |  | <b>FIB</b> <ul style="list-style-type: none"> <li>• AIBN FIB NX5000 (AIBN L1 R121)</li> <li>• AIBN FIB SCIOS (AIBN L1 R115)</li> </ul>                               |  | <b>FORKLIFT</b> <ul style="list-style-type: none"> <li>• FORKLIFT (SCIENCE LOADING DOCK)</li> </ul>   |  |  |  |
| <b>FREEZE FRACTURE/DEHYDRATION</b> <ul style="list-style-type: none"> <li>• AIBN CPD (112)</li> <li>• AIBN LEICA AFS 2 (PEBBLES) (112)</li> </ul>  |  | <b>IMAGE PROCESSING</b> <ul style="list-style-type: none"> <li>• 2D/3D SEGMENTATION &amp; PARTICLE PICKING (AIBN L1)</li> <li>• AIBN VR WORKSTATION (117)</li> </ul> |  | <b>LIGHT MICROSCOPES</b> <ul style="list-style-type: none"> <li>• AIBN OPTICAL OLYMPUS BX61 (117)</li> <li>• HAWKEN OLYMPUS DSX-1000 (1103)</li> <li>• LEICA LMD LASER DISSECTION LIGHT MICROSC (GM)</li> </ul> |  |  |  |
| <b>MASS PHOTOMETRY</b>   |  | <b>MASS SPEC IMAGING</b>   |  | <b>NOVEL IMAGING</b>  |  |  |  |

	Home	Book	Order	Request	Documents	Schedules	Statistics	Reports	Publications	Profile	Logout	
06:30	<input type="checkbox"/>					<input type="checkbox"/>	<input type="checkbox"/>		<input type="checkbox"/>			<input type="checkbox"/>
07:00	<input type="checkbox"/>					<input type="checkbox"/>	<input type="checkbox"/>		FRANK Joshua [00639 - Joshua Frank]	<input type="checkbox"/>		<input type="checkbox"/>
07:30	<input type="checkbox"/>					<input type="checkbox"/>	<input type="checkbox"/>			<input type="checkbox"/>		<input type="checkbox"/>
08:00	<input type="checkbox"/>					<input type="checkbox"/>			FRANK Joshua [00639 - Joshua Frank]	<input type="checkbox"/>		<input type="checkbox"/>
08:30	<input type="checkbox"/>									<input type="checkbox"/>		<input type="checkbox"/>
09:00	<input type="checkbox"/>									<input type="checkbox"/>		<input type="checkbox"/>
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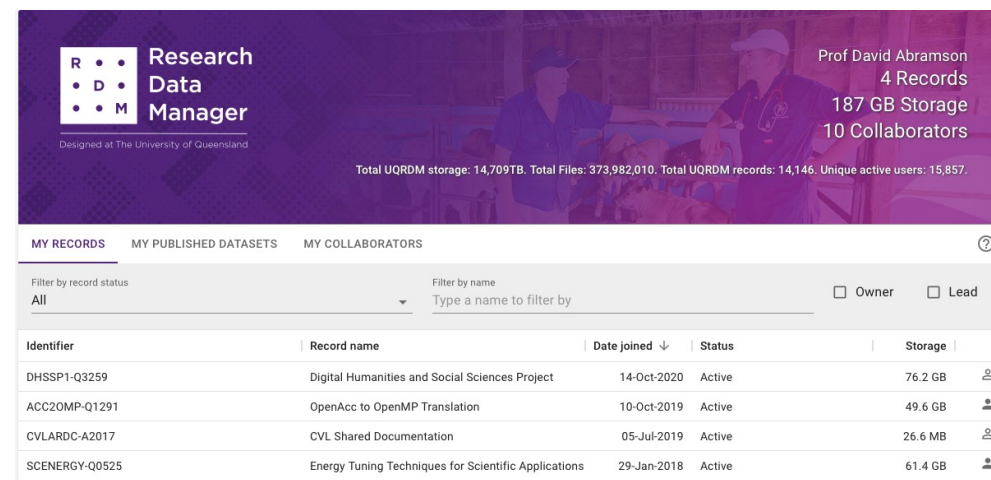
# Automatic provisioning of sufficient storage capacity for the scale of the experiments





# Research Data Manager (RDM)

- Integrated data management system covering the entire research data lifecycle.
- Seamless provisioning of easily accessible, secure and sharable data storage in real-time
- Enables publication of datasets into UQ eSpace.



**Research Data Manager**  
Designed at The University of Queensland

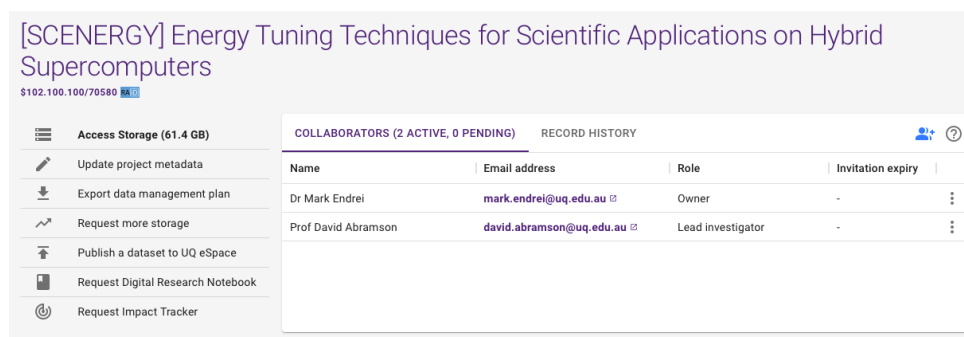
Prof David Abramson  
4 Records  
187 GB Storage  
10 Collaborators

Total UQRDM storage: 14,709TB. Total Files: 373,982,010. Total UQRDM records: 14,146. Unique active users: 15,857.

MY RECORDS | MY PUBLISHED DATASETS | MY COLLABORATORS

Filter by record status: All | Filter by name: Type a name to filter by | ☐ Owner ☐ Lead

Identifier	Record name	Date joined ↓	Status	Storage
DHSSP1-Q3259	Digital Humanities and Social Sciences Project	14-Oct-2020	Active	76.2 GB
ACC20MP-Q1291	OpenAcc to OpenMP Translation	10-Oct-2019	Active	49.6 GB
CVLARDC-A2017	CVL Shared Documentation	05-Jul-2019	Active	26.6 MB
SCENERGY-Q0525	Energy Tuning Techniques for Scientific Applications	29-Jan-2018	Active	61.4 GB

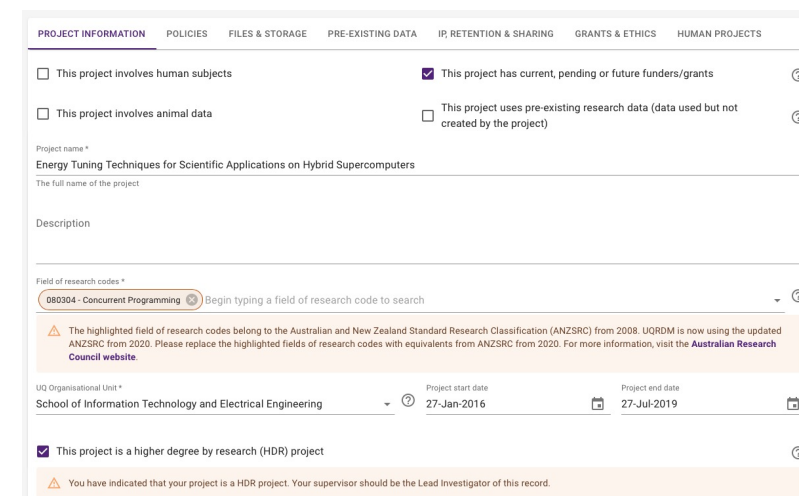


[SCENERGY] Energy Tuning Techniques for Scientific Applications on Hybrid Supercomputers  
\$102,100,100/70580

Access Storage (61.4 GB)  
Update project metadata  
Export data management plan  
Request more storage  
Publish a dataset to UQ eSpace  
Request Digital Research Notebook  
Request Impact Tracker

COLLABORATORS (2 ACTIVE, 0 PENDING) | RECORD HISTORY

Name	Email address	Role	Invitation expiry
Dr Mark Endrei	mark.endrei@uq.edu.au	Owner	-
Prof David Abramson	david.abramson@uq.edu.au	Lead investigator	-



PROJECT INFORMATION | POLICIES | FILES & STORAGE | PRE-EXISTING DATA | IP RETENTION & SHARING | GRANTS & ETHICS | HUMAN PROJECTS

☐ This project involves human subjects ☒ This project has current, pending or future funders/grants

☐ This project involves animal data ☐ This project uses pre-existing research data (data used but not created by the project)

Project name \*  
Energy Tuning Techniques for Scientific Applications on Hybrid Supercomputers

The full name of the project

Description

Field of research codes \*  
080304 - Concurrent Programming

The highlighted field of research codes belong to the Australian and New Zealand Standard Research Classification (ANZSRC) from 2008. UQRDM is now using the updated ANZSRC from 2020. Please replace the highlighted fields of research codes with equivalents from ANZSRC from 2020. For more information, visit the [Australian Research Council website](#).

UQ Organisational Unit \*  
School of Information Technology and Electrical Engineering

Project start date  
27-Jan-2016

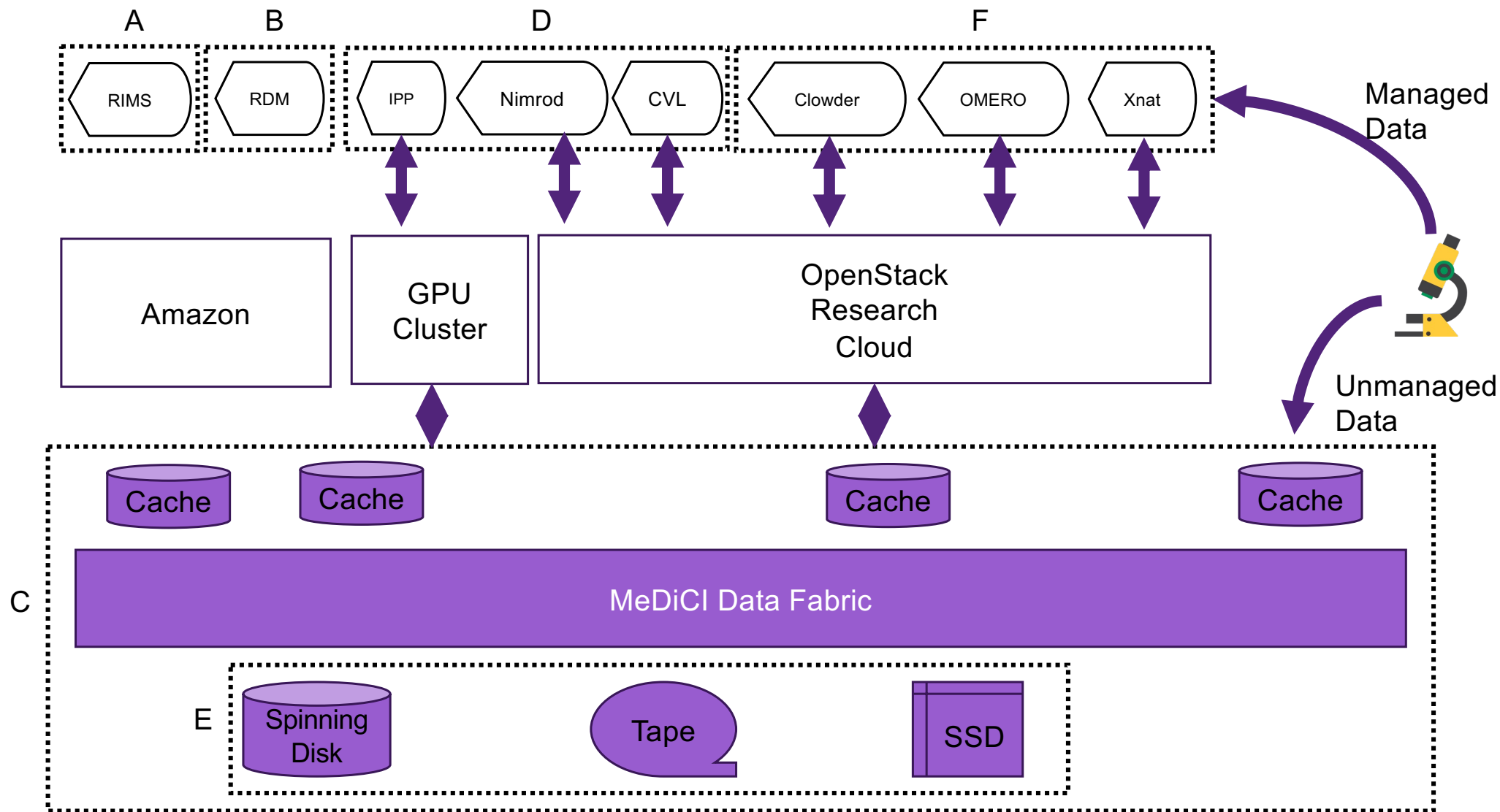
Project end date  
27-Jul-2019

☒ This project is a higher degree by research (HDR) project

You have indicated that your project is a HDR project. Your supervisor should be the Lead Investigator of this record.



The removal of explicit data movement steps and the knowledge of the various storage subsystems





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# MeDiCI

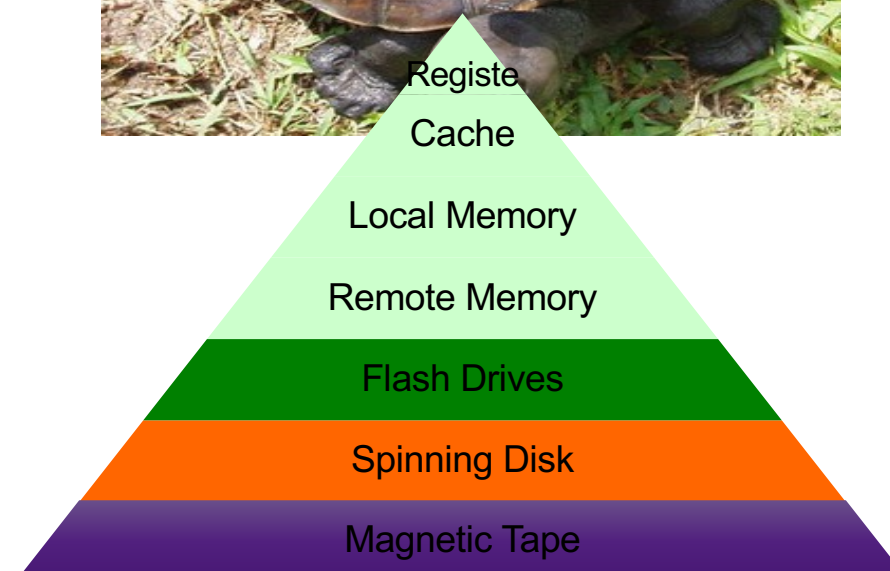
## Turtles Caches all the way down

“a jocular expression of the infinite regress problem in cosmology posed by the "unmoved mover" paradox.

The metaphor in the anecdote represents a popular notion of the theory that Earth is actually flat and is supported on the back of a World Turtle, which itself is propped up by a chain of larger and larger turtles.

Questioning what the final turtle might be standing on, the anecdote humorously concludes that it is turtles all the way down””

[https://en.m.wikipedia.org/wiki/Turtles\\_all\\_the\\_way\\_down](https://en.m.wikipedia.org/wiki/Turtles_all_the_way_down)

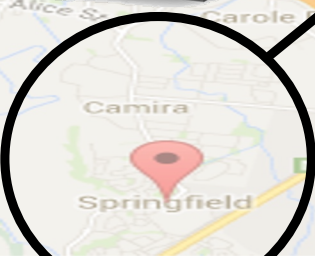




# UQ Landscape: An inconvenient truth



30 kms



## MeDiCI

- Centralising research data storage and computation
- Distributed data is further from both the instruments that generate it, some of the computers that process it, and the researchers that interpret it.
- Existing mechanisms manually move data
- MeDiCI solves this by

Augmenting the existing infrastructure,

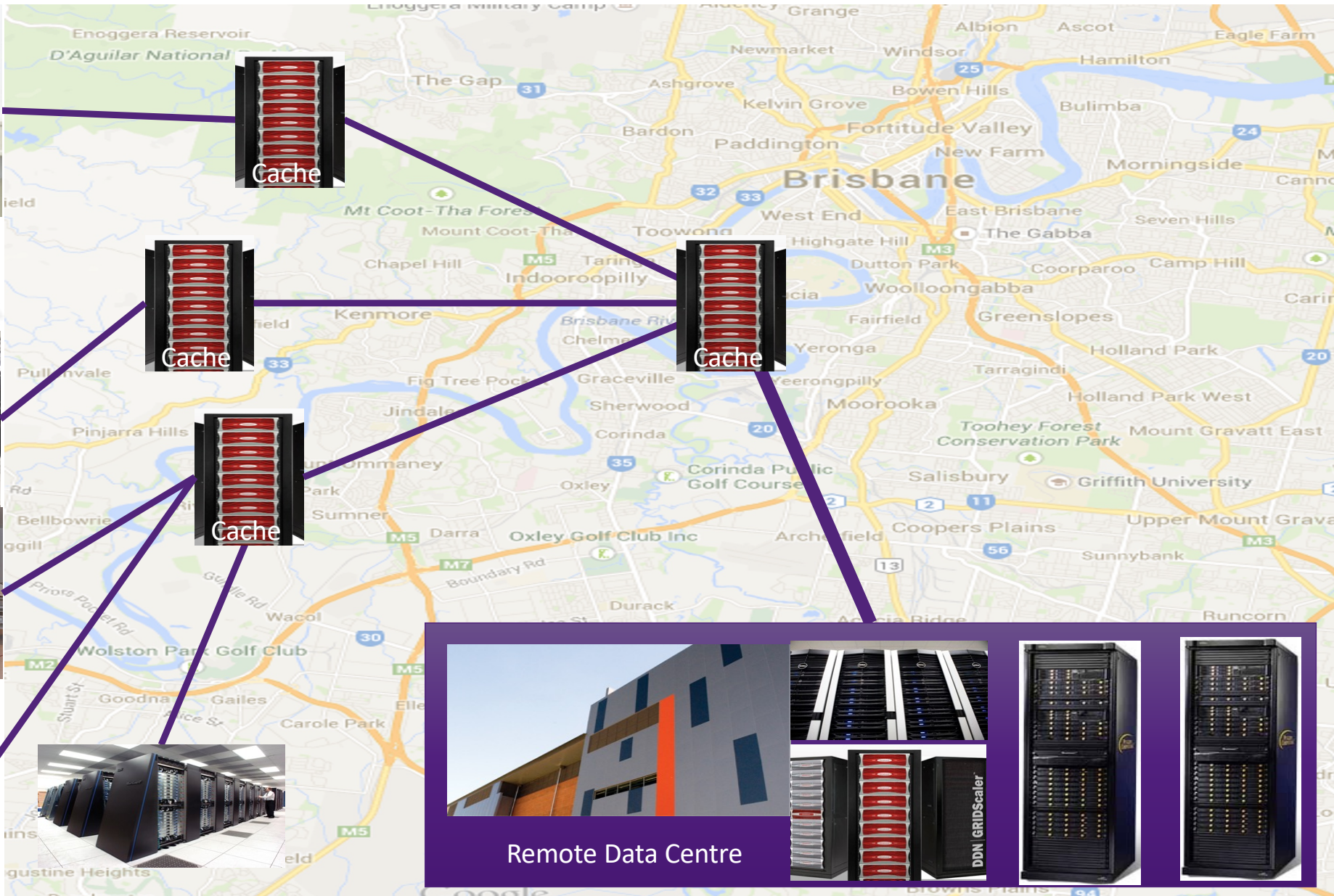
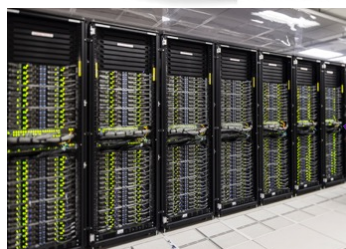
Implementing on campus caching

Automatic data movement

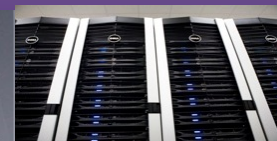
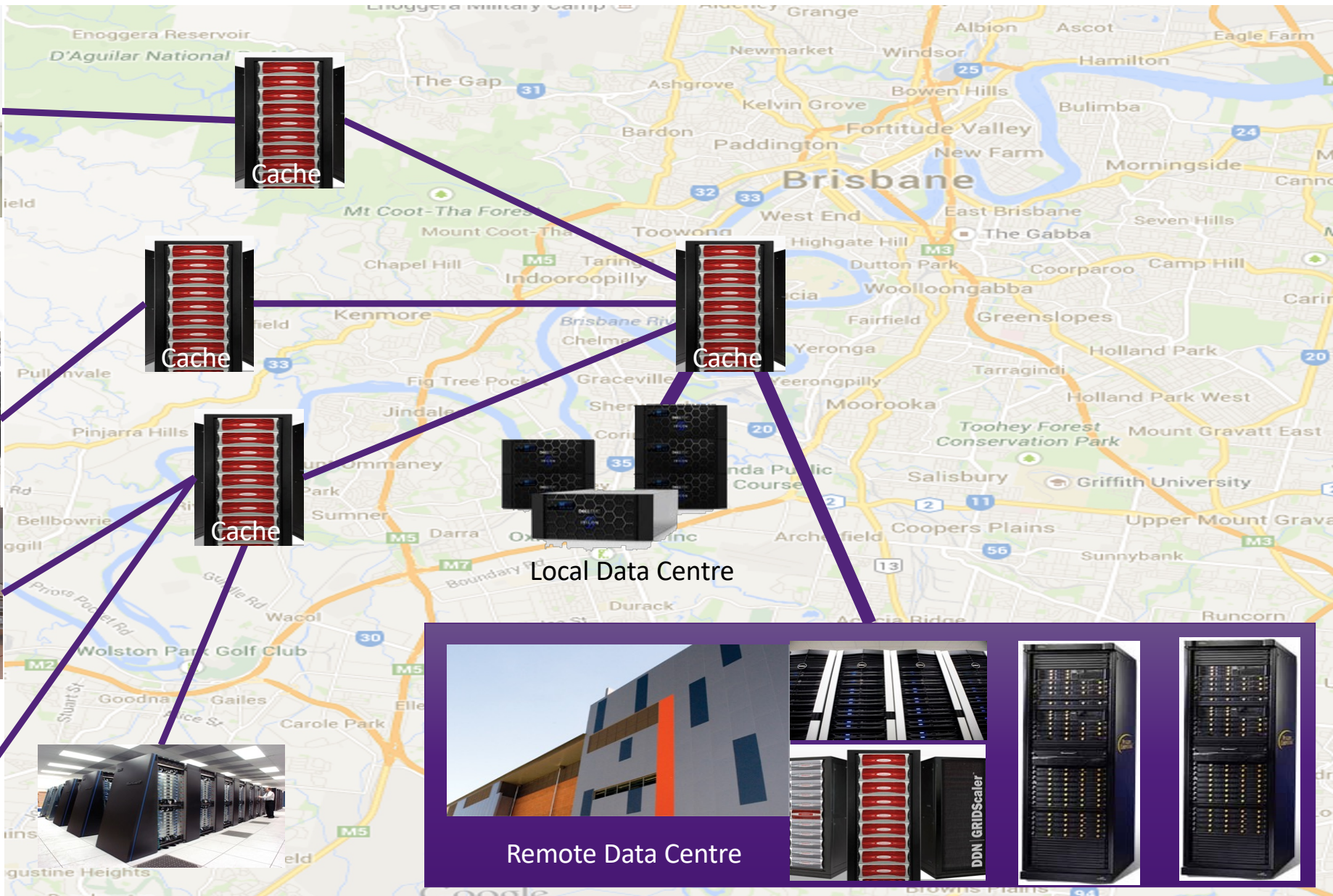
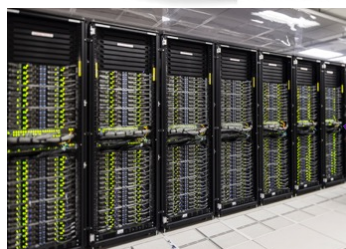
- Current implementation based on IBM Spectrum Scale (GPFS) and HPE DMF





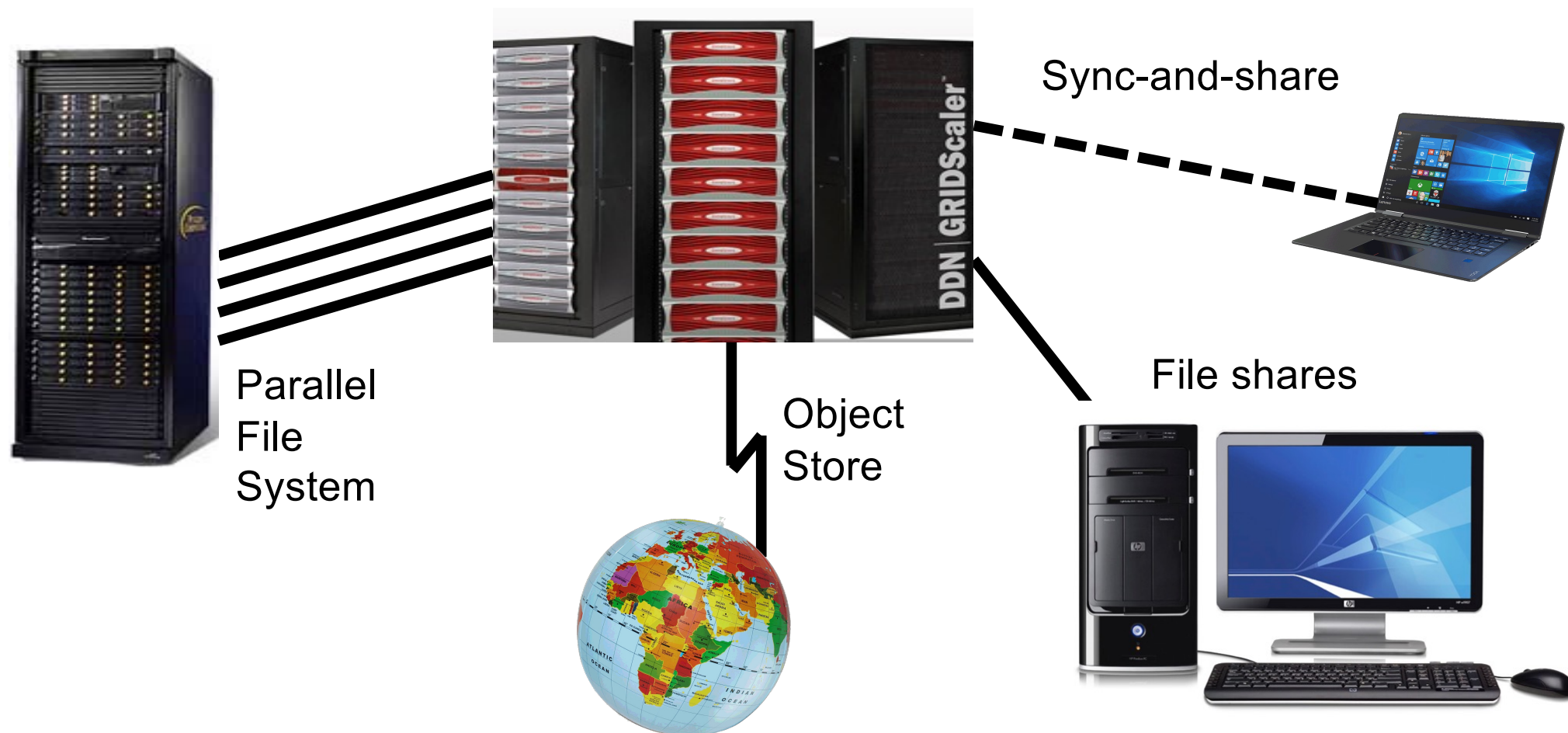






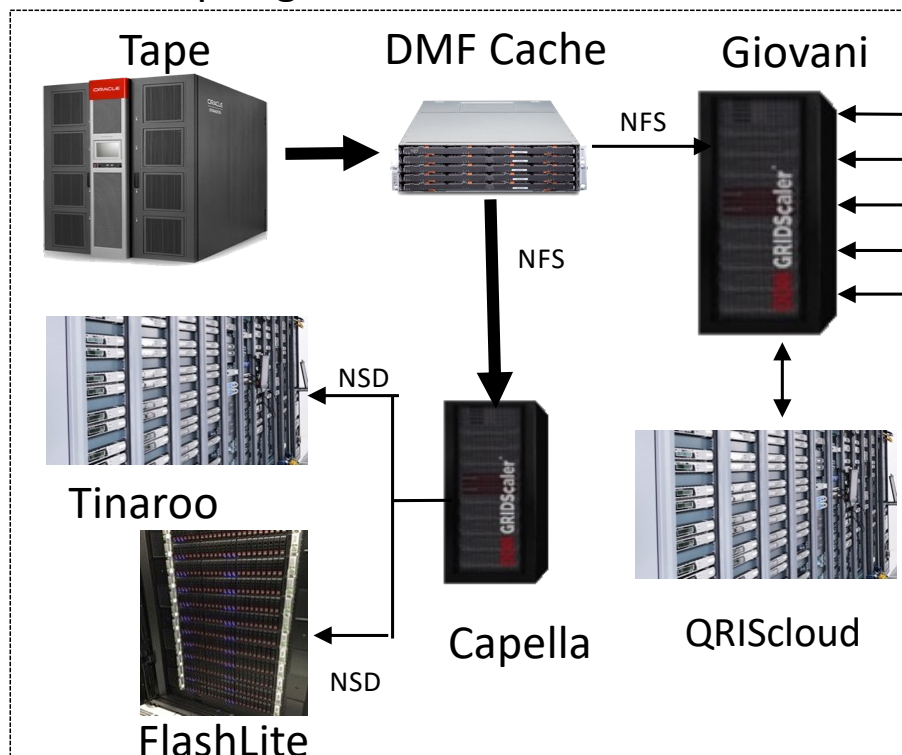
Remote Data Centre

# MeDiCI unifies data access

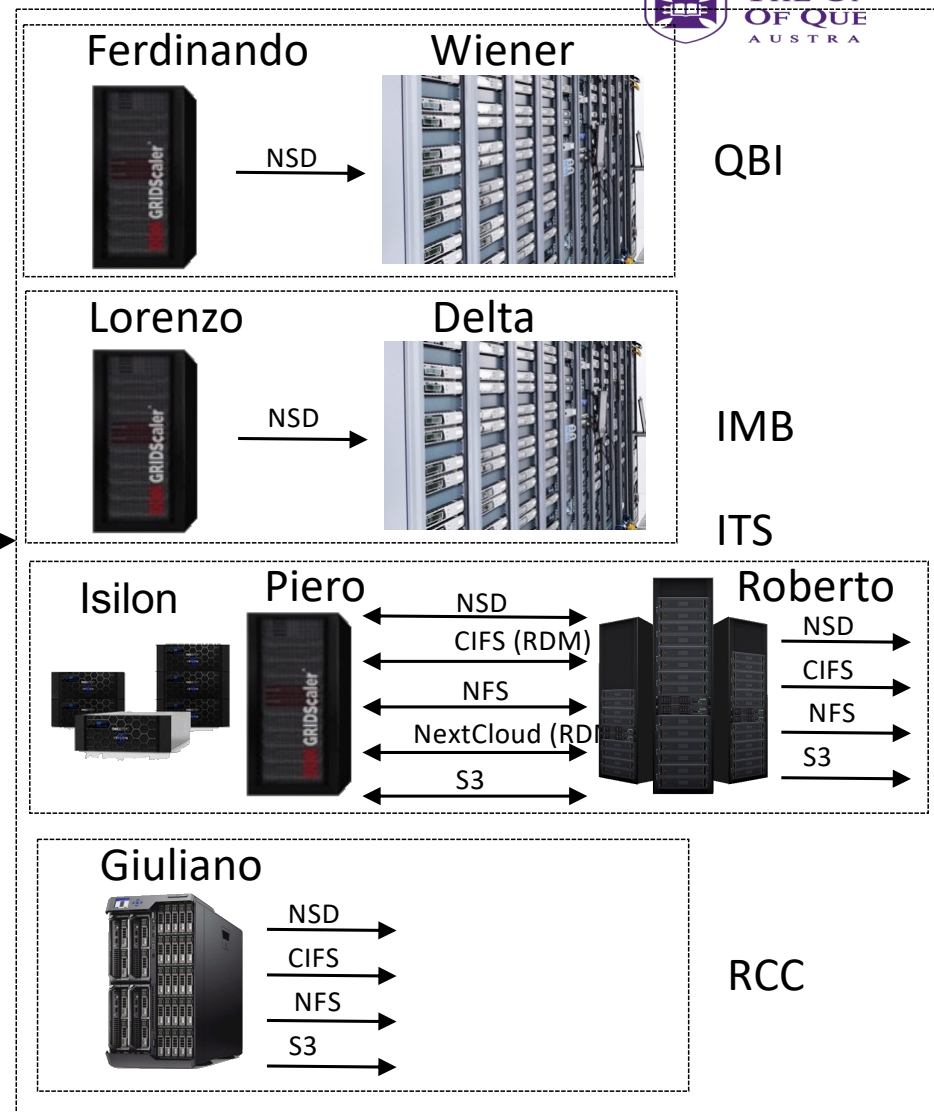




## Polaris Springfield



External (UCSD, AIST, JCU, NCI, Amazon EC2)

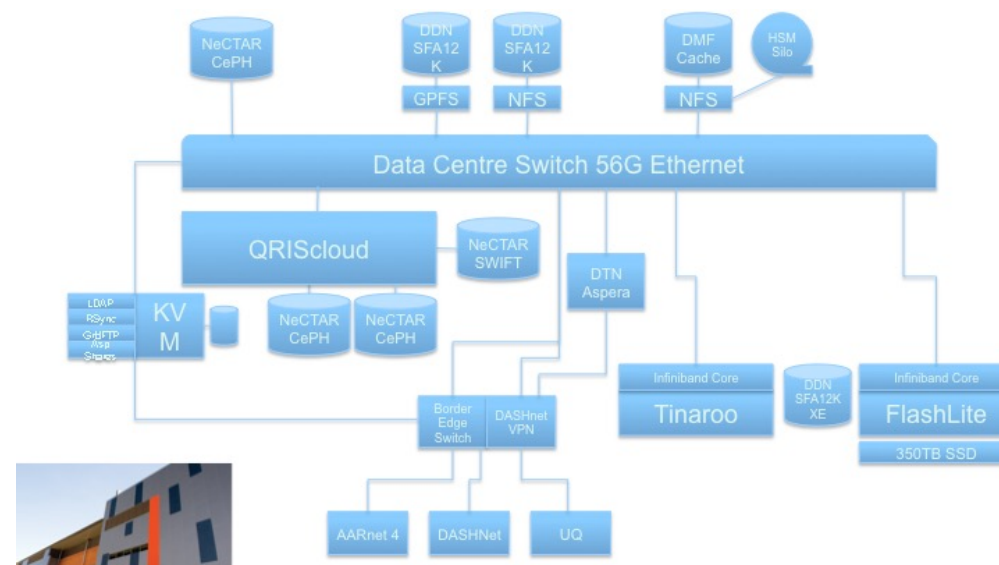


UQ St Lucia

## A Declarative Machine Room?

- Static allocation of disk and tape
- Policy driven allocation

RULE 'prefetch-list'  
LIST 'toevict'

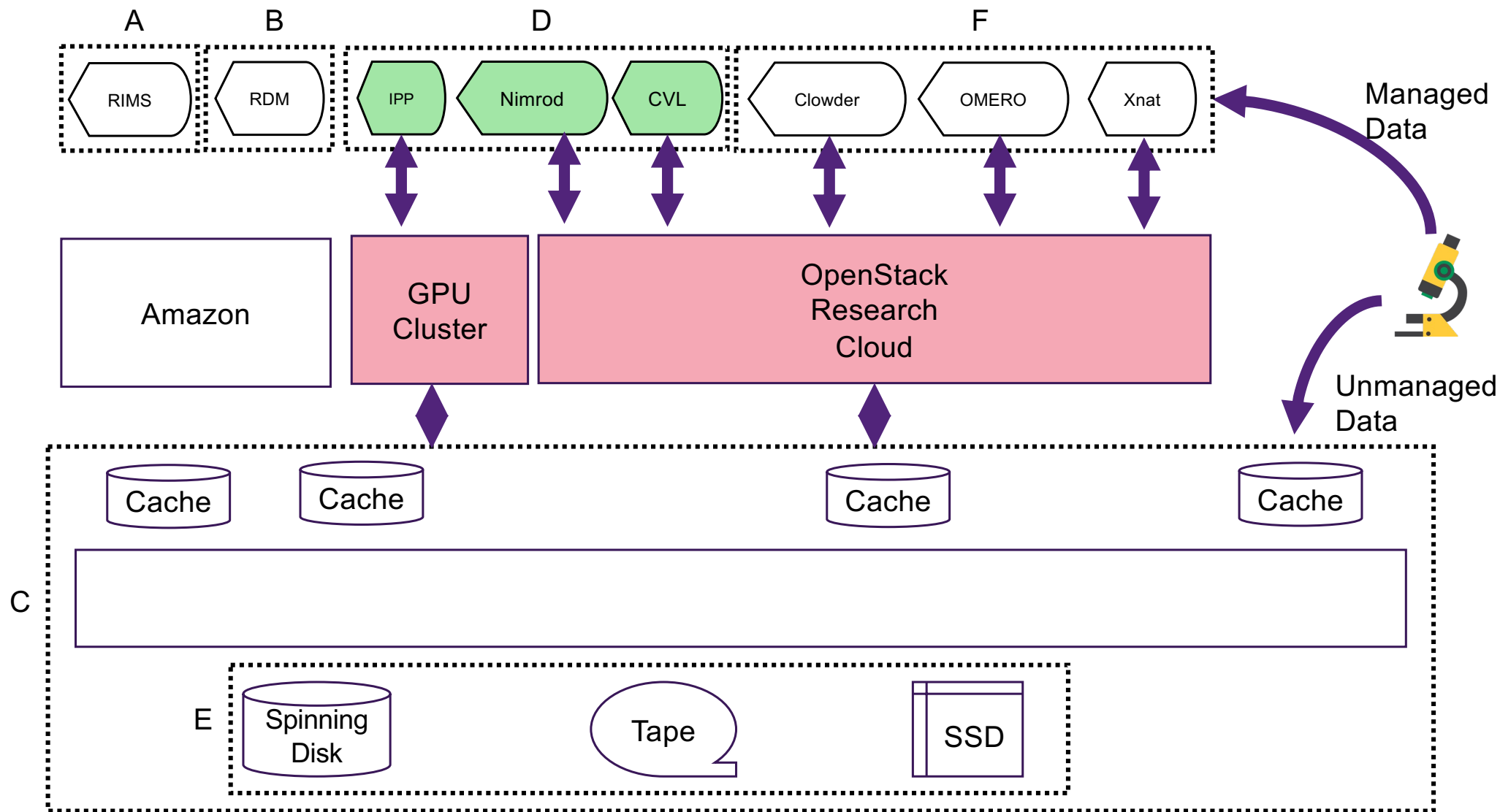


WHERE CURRENT\_TIMESTAMP - ACCESS\_TIME >  
INTERVAL '7' DAYS

AND REGEX(misc\_attributes, '[P]') /\* only list AFM managed files  
\*/

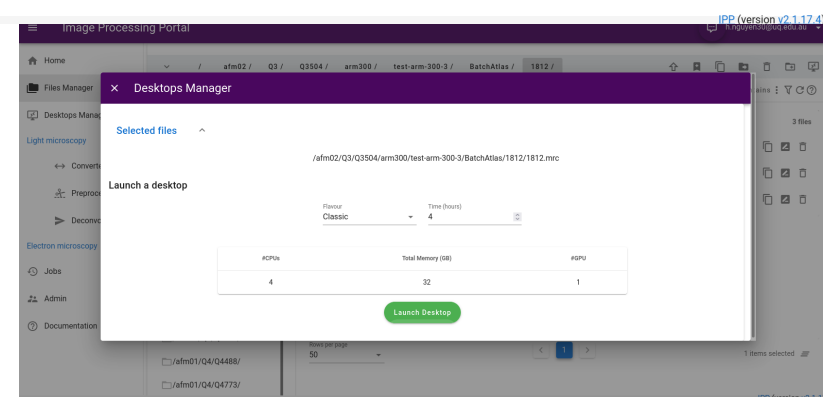
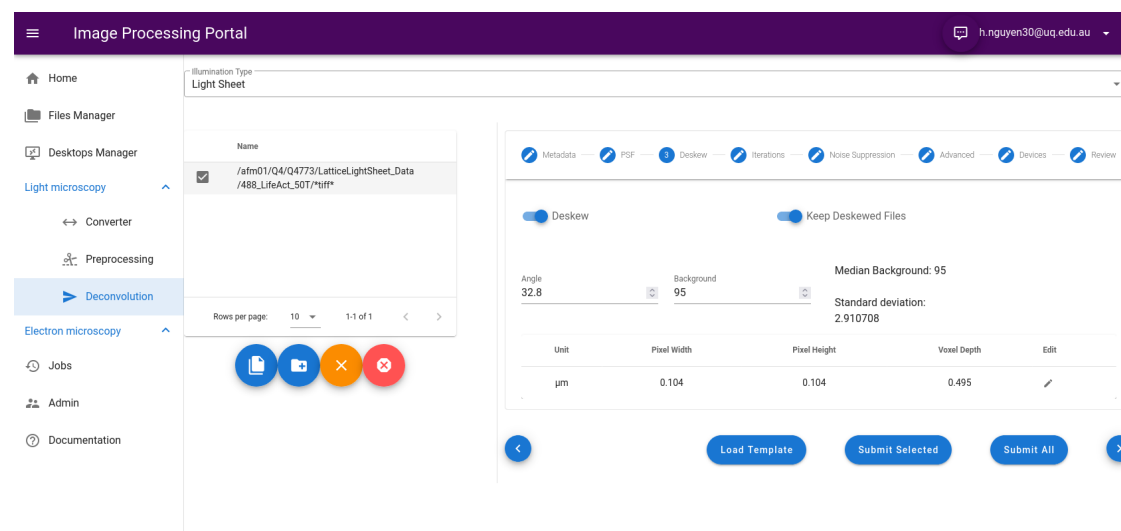


# Processing data on advanced computational platforms without complex manual configuration



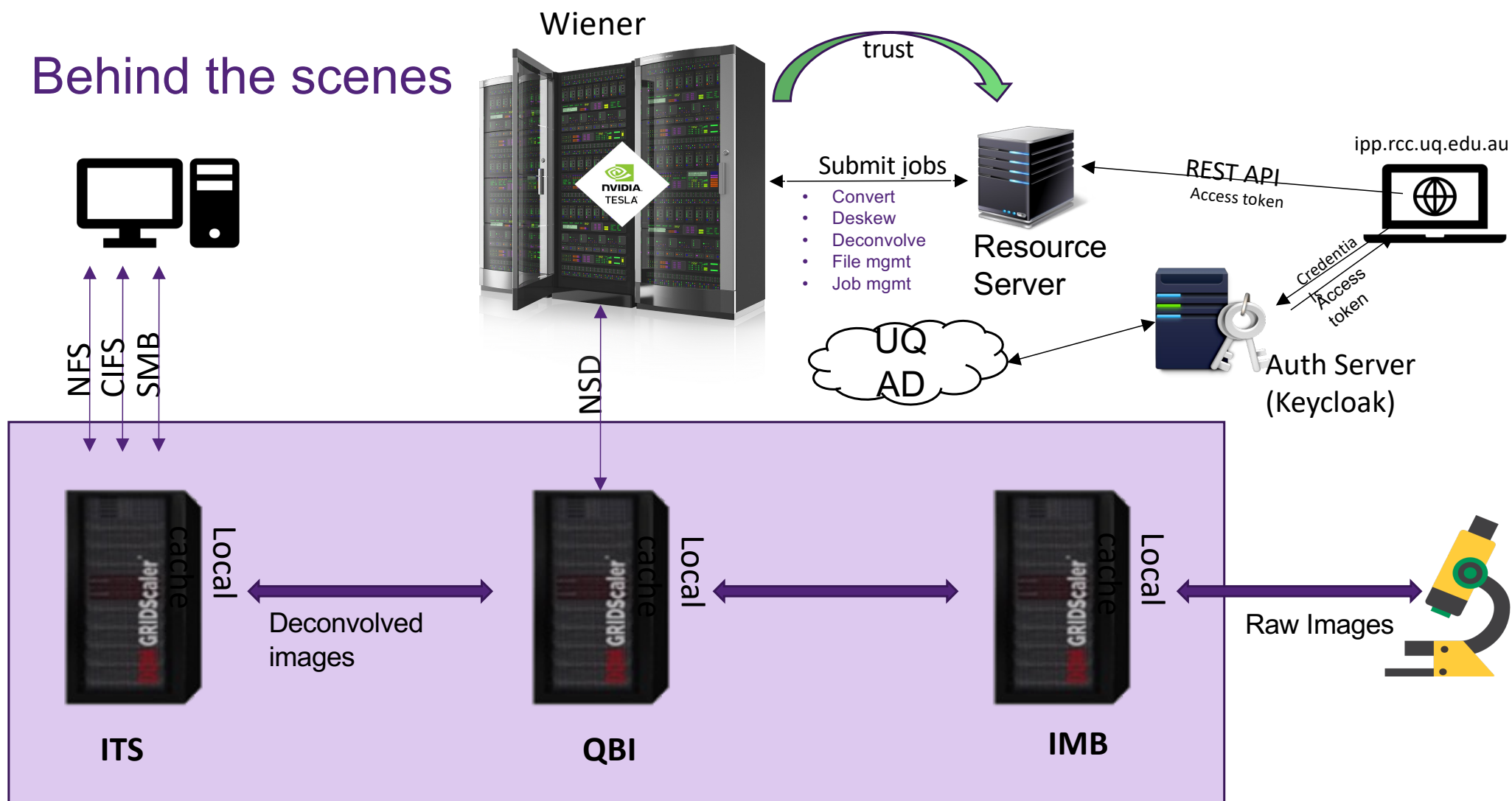
# The UQ Image Processing Portal (IPP)

- Cloud based Science Gateway to simplify image pre-processing steps
- File conversions between proprietary and open-source file types
- Pre-processing: this step is to deskew raw data from Lattice Light-Sheet microscopes
- Deconvolution: this is a compute-intensive image processing technique to improve image contrast and resolution.
  - Currently uses Microvolution, a commercial package
- Interfaces with SLURM based GPU supercomputer



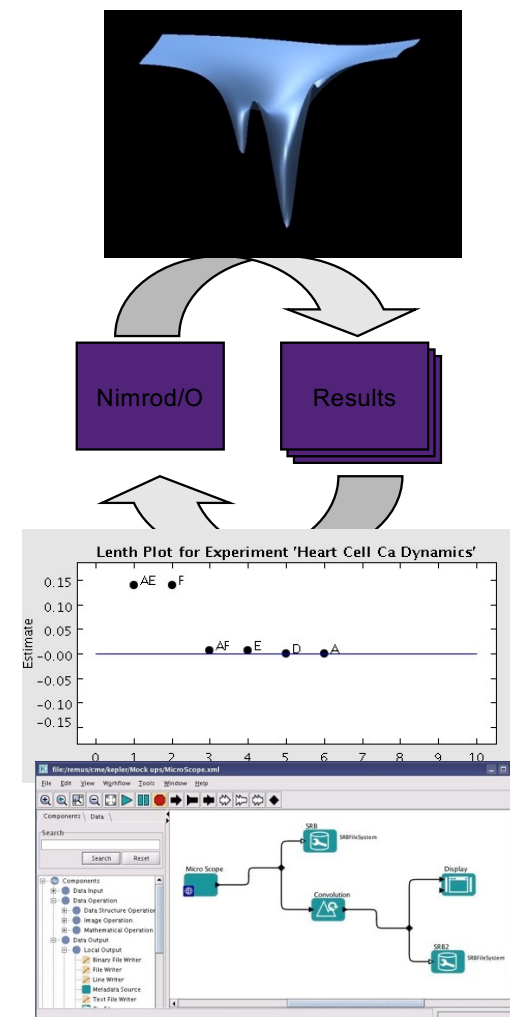


# Behind the scenes



## The UQ Nimrod Service

- 25 years supporting “real” science
  - A full parameter sweep is the cross product of all the parameters (Nimrod/G)
  - An optimization run minimizes some output metric and returns parameter combinations that do this (Nimrod/O)
  - Design of experiments limits number of combinations (Nimrod/E)
  - Workflows (Nimrod/K)

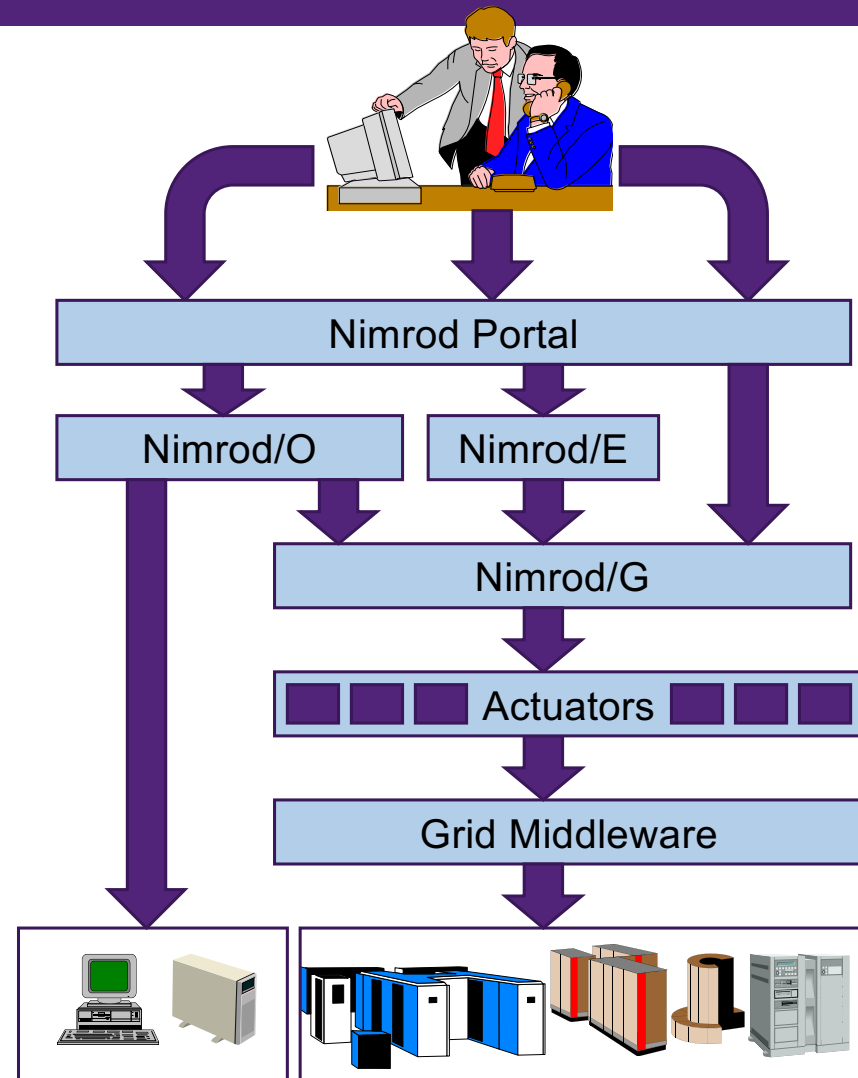


# A family of tools

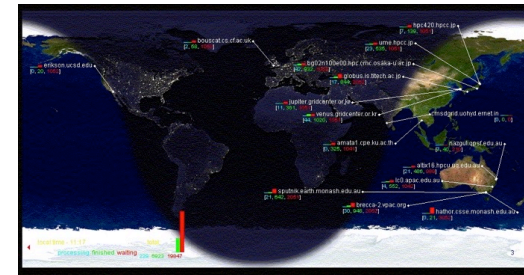
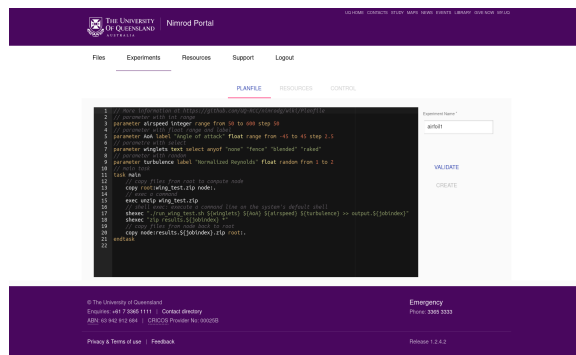


parameter pressure float range from 5000 to 6000 points 4  
parameter concent float range from 0.002 to 0.005 points 2  
parameter material text select anyof "Fe" "Al"

```
task main
  copy compModel node:compModel
  copy inputFile.skel node:inputFile.skel
  node:substitute inputFile.skel inputFile
  node:execute ./compModel < inputFile > results
  copy node:results results.$jobname
endtask
```

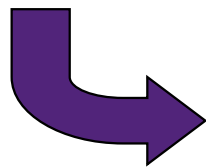


# Nimrod Development Cycle

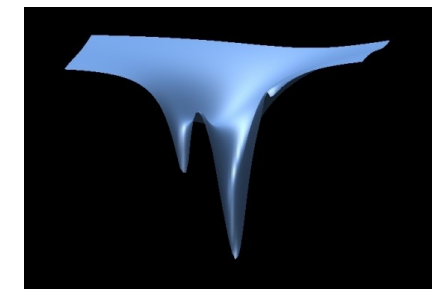


Sent to available machines

Prepare Jobs using Portal



Name	State	Completed	Failed	Running	Pending	Total	Created
test1	STOPPED	0	101	0	0	101	Wed, Mar 30, 2022, 04:23 PM
test2	COMPLETED	101	0	0	0	101	Thu, Mar 31, 2022, 02:36 AM
test3	COMPLETED	101	0	0	0	101	Thu, Mar 31, 2022, 02:47 AM
test4	COMPLETED	101	0	0	0	101	Thu, Mar 31, 2022, 11:15 PM
Unproctored	COMPLETED	101	0	0	0	101	Fri, Apr 1, 2022, 09:51 AM
test5	COMPLETED	101	0	0	0	101	Tue, Apr 26, 2022, 09:41 AM
test7	COMPLETED	101	0	0	0	101	Tue, Apr 26, 2022, 04:57 PM

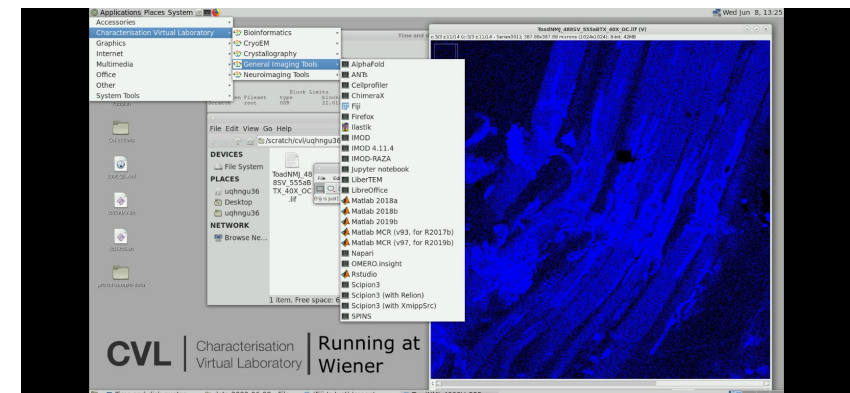
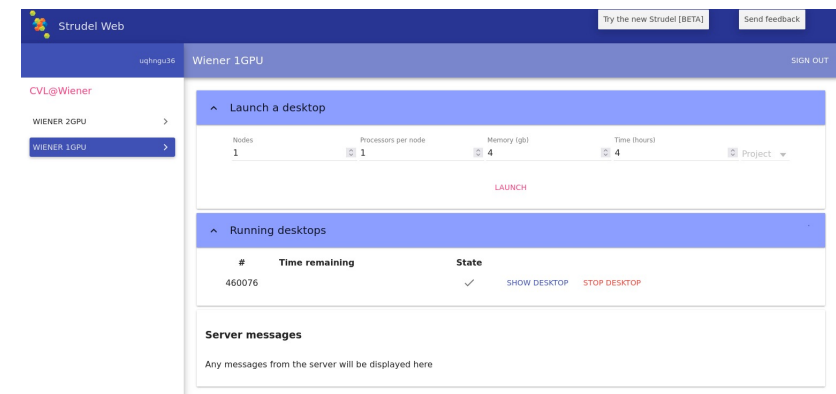


Results displayed & interpreted

Jobs Scheduled Executed Dynamically

# Characterisation Virtual Laboratory (CVL)

- Virtual desktop environment that provides researchers with access to imaging tools and data
- Each CVL desktop is pre-configured with imaging tools, wrapped as singularity containers or HPC modules.
- End users can choose the size and wall-time of the virtual desktop before launch.
- Once launched, user storage collections are automatically mounted into the virtual desktop as network mounts.

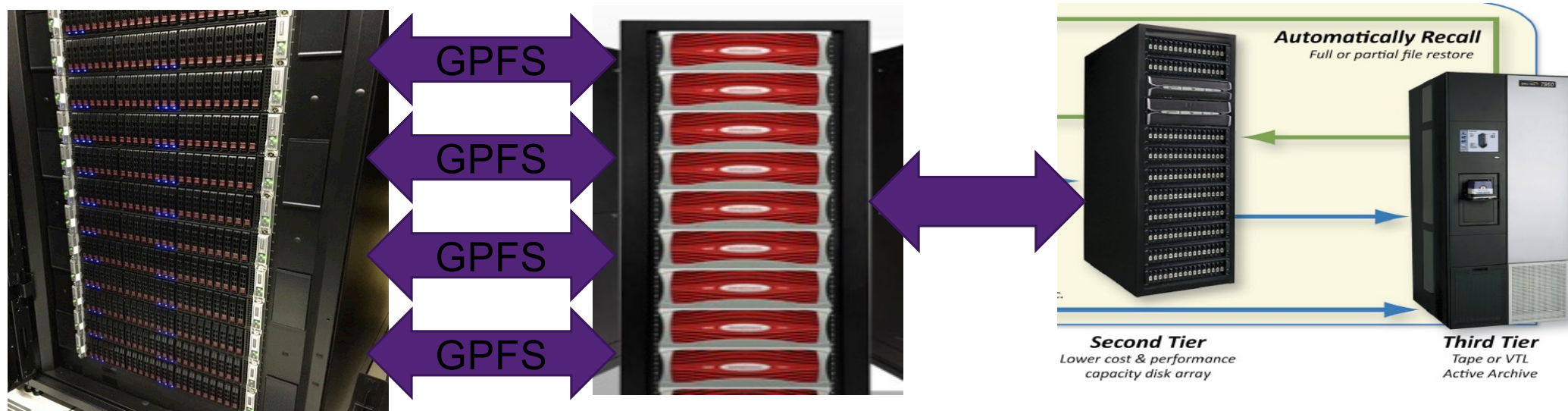




# Automatic archiving and sharing of both primary and secondary data sets



## Accessing long term collections



HPC

IBM Spectrum Scale

Parallel file system

HPE DMF Disk/Tape

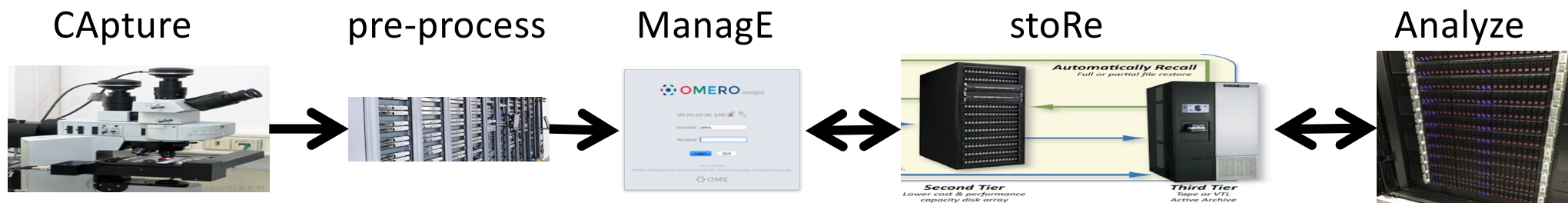
Long term data collections



# Automatic capture of instrument and experiment meta-data.

## CAMERA: MeDiCI meets instruments

- MeDiCI abstracts storage location and protocol issues
- RDM captures experiment level meta-data and provisions storage
- Repository captures instrument level meta-data
- Collections can be attached to repository stacks



# Unmanaged data workflow



Designed at The University of Queensland



# Managed data workflow



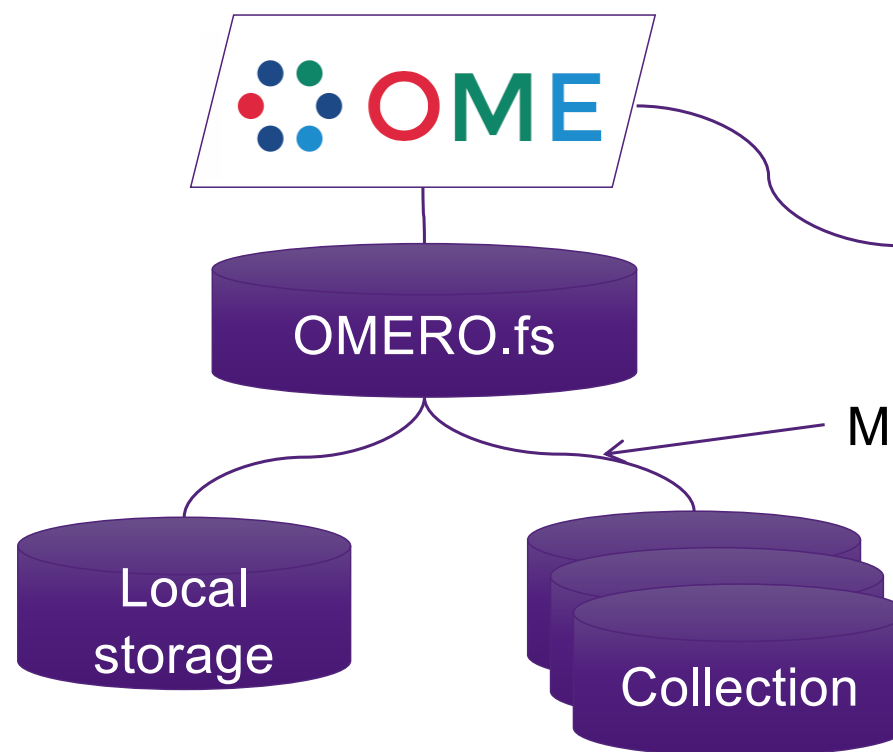
Designed at The University of Queensland



## Leveraging unmanaged data collections



Cloud  
Hosted  
OMERO  
server

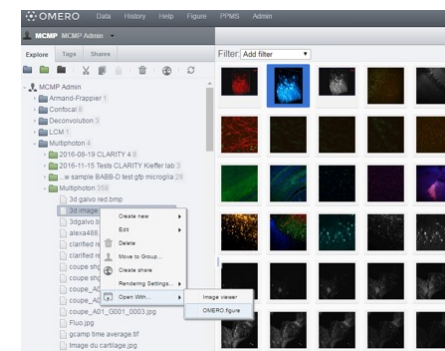


Web front end

Magic happens here

Data ingest  
and  
presentation

Collections  
are mapped  
to OMERO  
groups

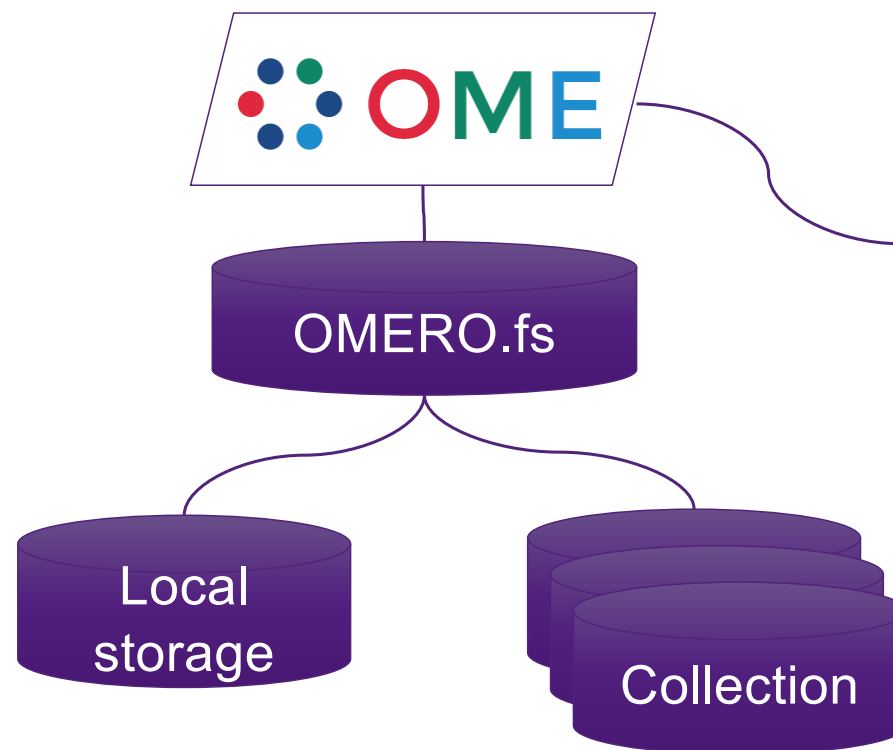




## Leveraging unmanaged data collections



Cloud  
Hosted  
OMERO  
server

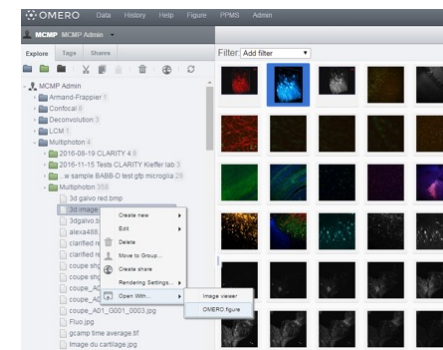


Web front end

Data ingest  
and  
presentation

Analyse

Read  
Only





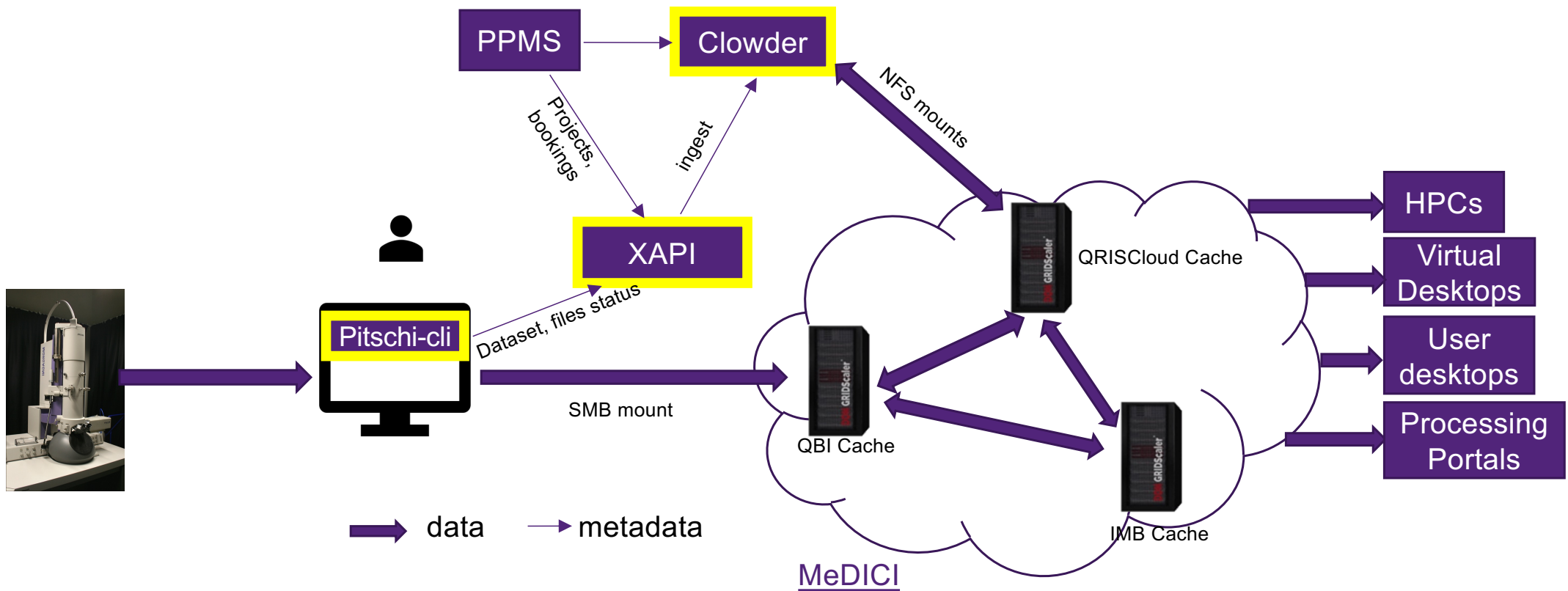
Pitchi: A Clowder based repository for EM data

The image displays a screenshot of the Pitchi web application. The top navigation bar features the Pitchi logo, 'Pitchi', 'Explore', and 'Help' links, along with a search bar and a 'Login' button. The main content area shows a dataset titled '20220428' with a 'Download All Files' button and a 'Download' button. The dataset is described as 'All Rights Reserved Pitchi Clowder'. The right sidebar contains 'Statistics' (Views: 1, Downloads: 0), 'Sources containing the Dataset' (Pitchi Clowder Data Platform (2 datasets)), and 'Collections containing the Dataset'.

[illegible]

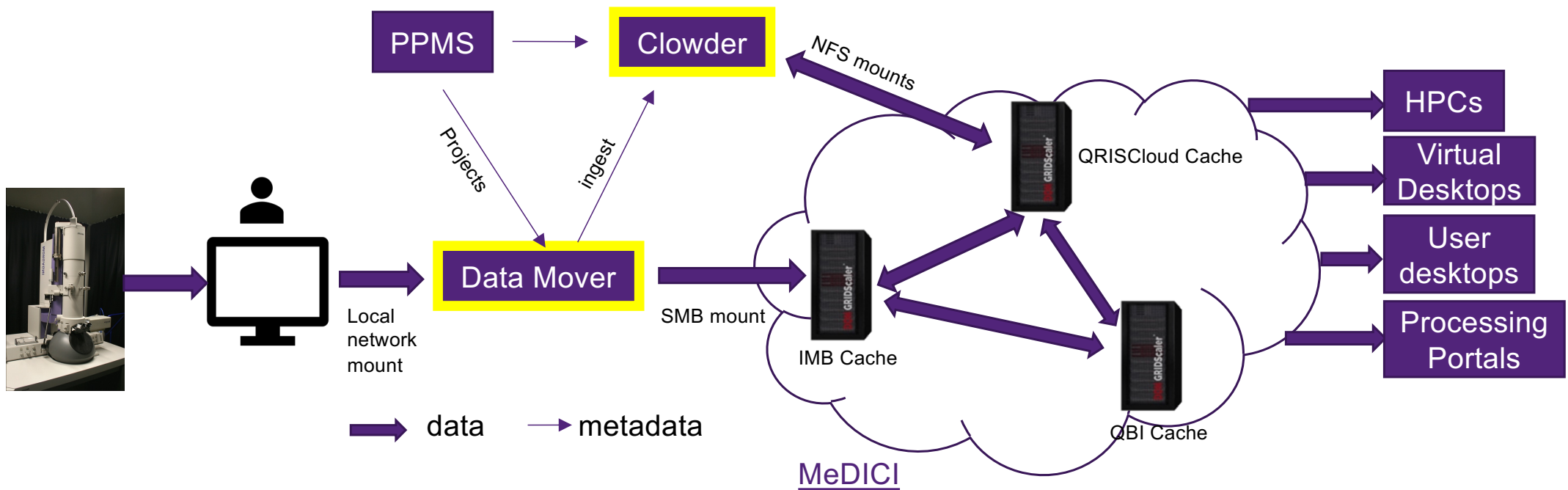
# Pitschi – direct transfer

<https://pitschi.rcc.uq.edu.au/>

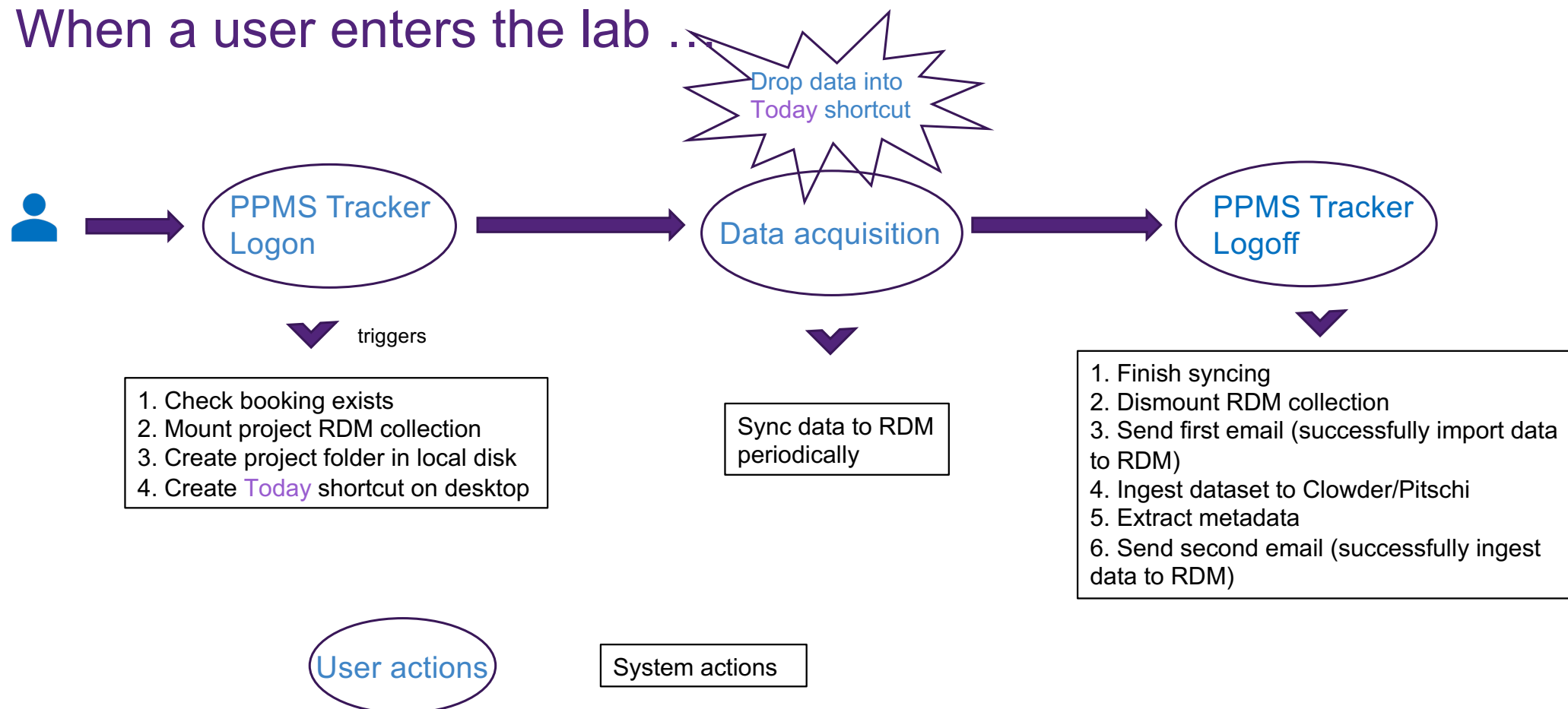


# Pitschi – indirect transfer

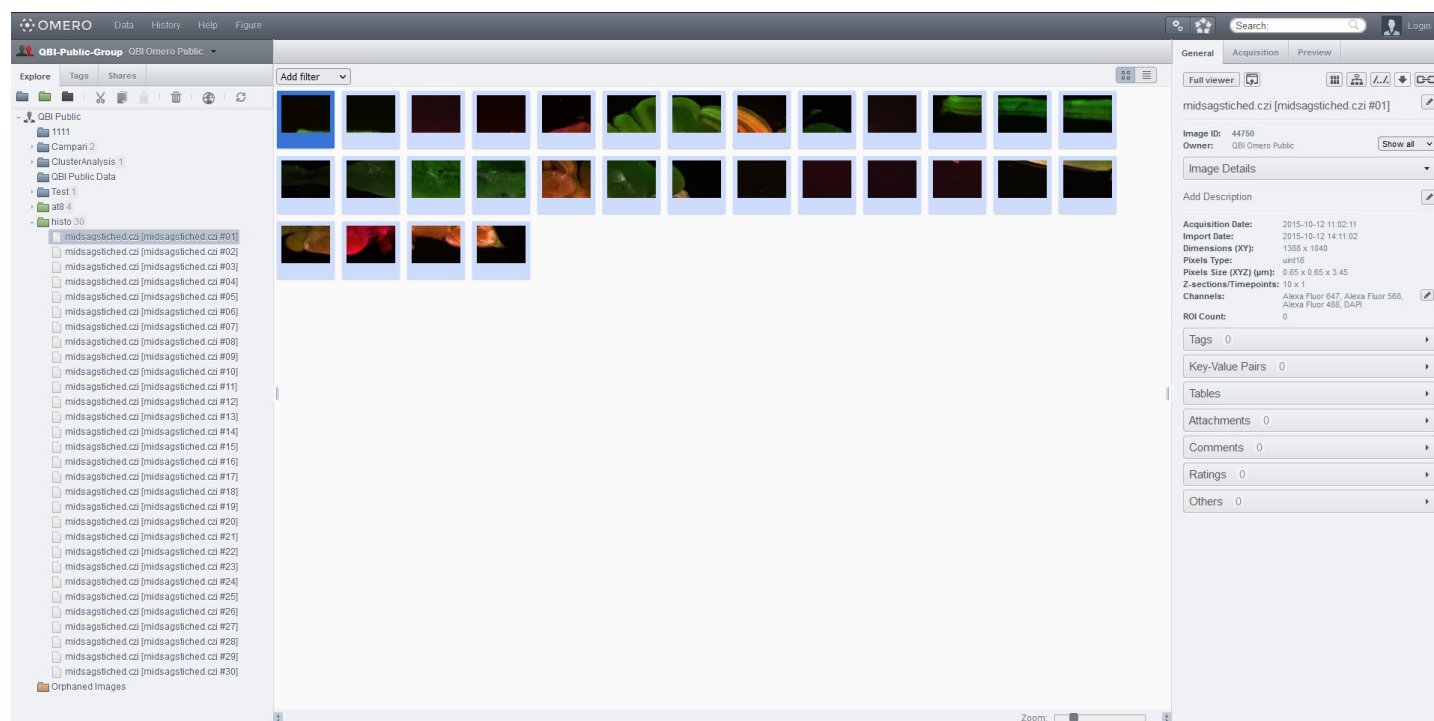
<https://pitschi.rcc.uq.edu.au/>



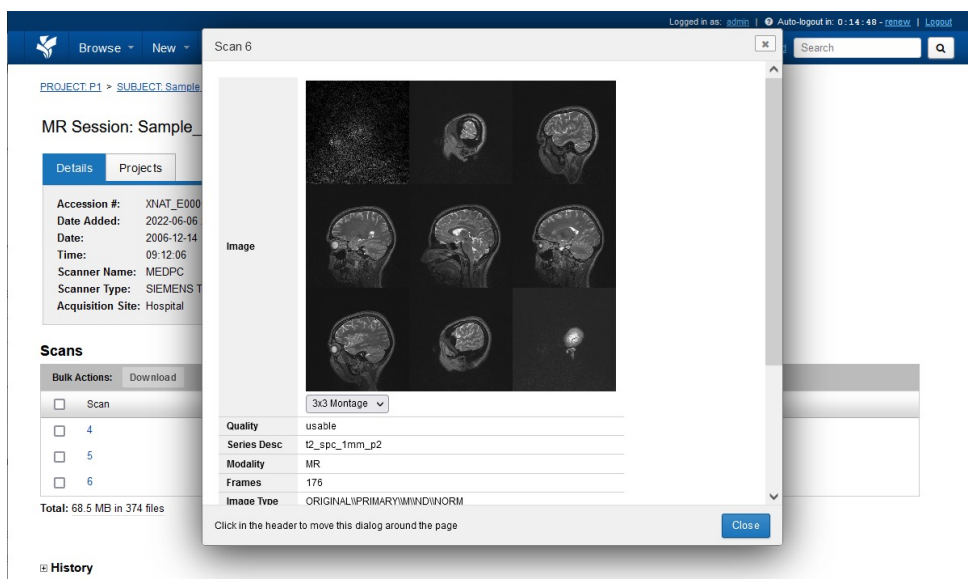
# When a user enters the lab ...



# The UQ Open Microscopy Environment: OMERO



# The UQ XNAT service



Logged in as: admin | Auto-logout in: 0:14:48 - renew | Logout

PROJECT: P1 > SUBJECT: Sample

### MR Session: Sample

Details Projects

Accession #: XNAT\_E000  
Date Added: 2022-06-06  
Date: 2006-12-14  
Time: 09:12:06  
Scanner Name: MEDPC  
Scanner Type: SIEMENS T  
Acquisition Site: Hospital

### Scans

Bulk Actions: Download

☐ Scan

☐ 4

☐ 5

☐ 6

Total: 68.5 MB in 374 files

@ History

Scan 6

Image

3x3 Montage

Quality: usable

Series Desc: t2\_spc\_1mm\_p2

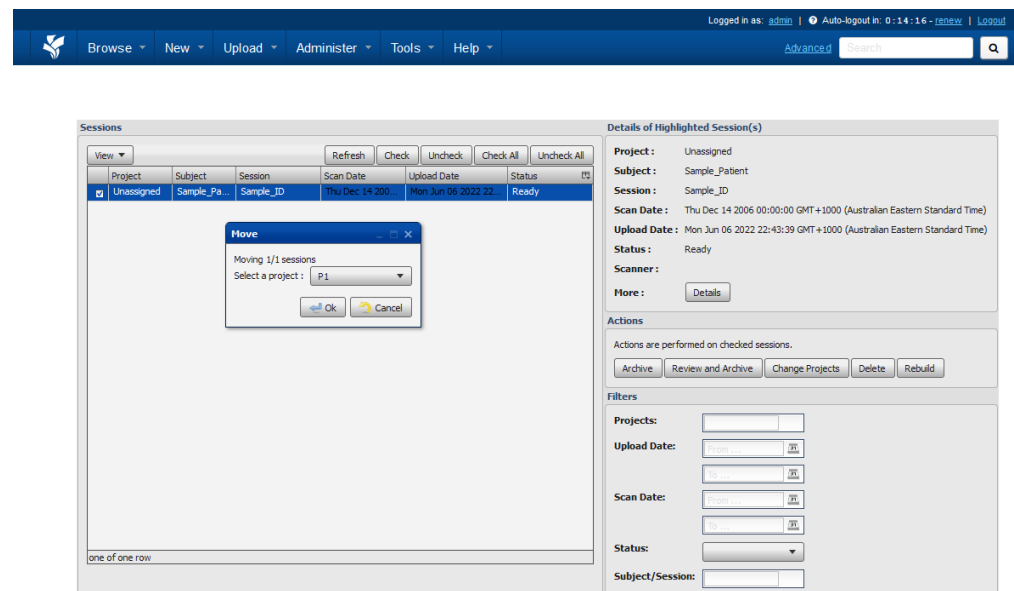
Modality: MR

Frames: 176

Image Type: ORIGINAL/PRIMARY/MIND/NORM

Click in the header to move this dialog around the page

Close



Logged in as: admin | Auto-logout in: 0:14:16 - renew | Logout

Browse New Upload Administrator Tools Help

Advanced Search

### Sessions

View Refresh Check Uncheck Check All Uncheck All

Project	Subject	Session	Scan Date	Upload Date	Status
Unassigned	Sample_Pa...	Sample_ID	Thu Dec 14 2006	Mon Jun 06 2022 22	Ready

Move

Moving 1/1 sessions

Select a project: P1

Ok Cancel

### Details of Highlighted Session(s)

Project: Unassigned  
Subject: Sample\_Patient  
Session: Sample\_ID  
Scan Date: Thu Dec 14 2006 00:00:00 GMT+1000 (Australian Eastern Standard Time)  
Upload Date: Mon Jun 06 2022 22:43:39 GMT+1000 (Australian Eastern Standard Time)  
Status: Ready  
Scanner:   
More: Details

### Actions

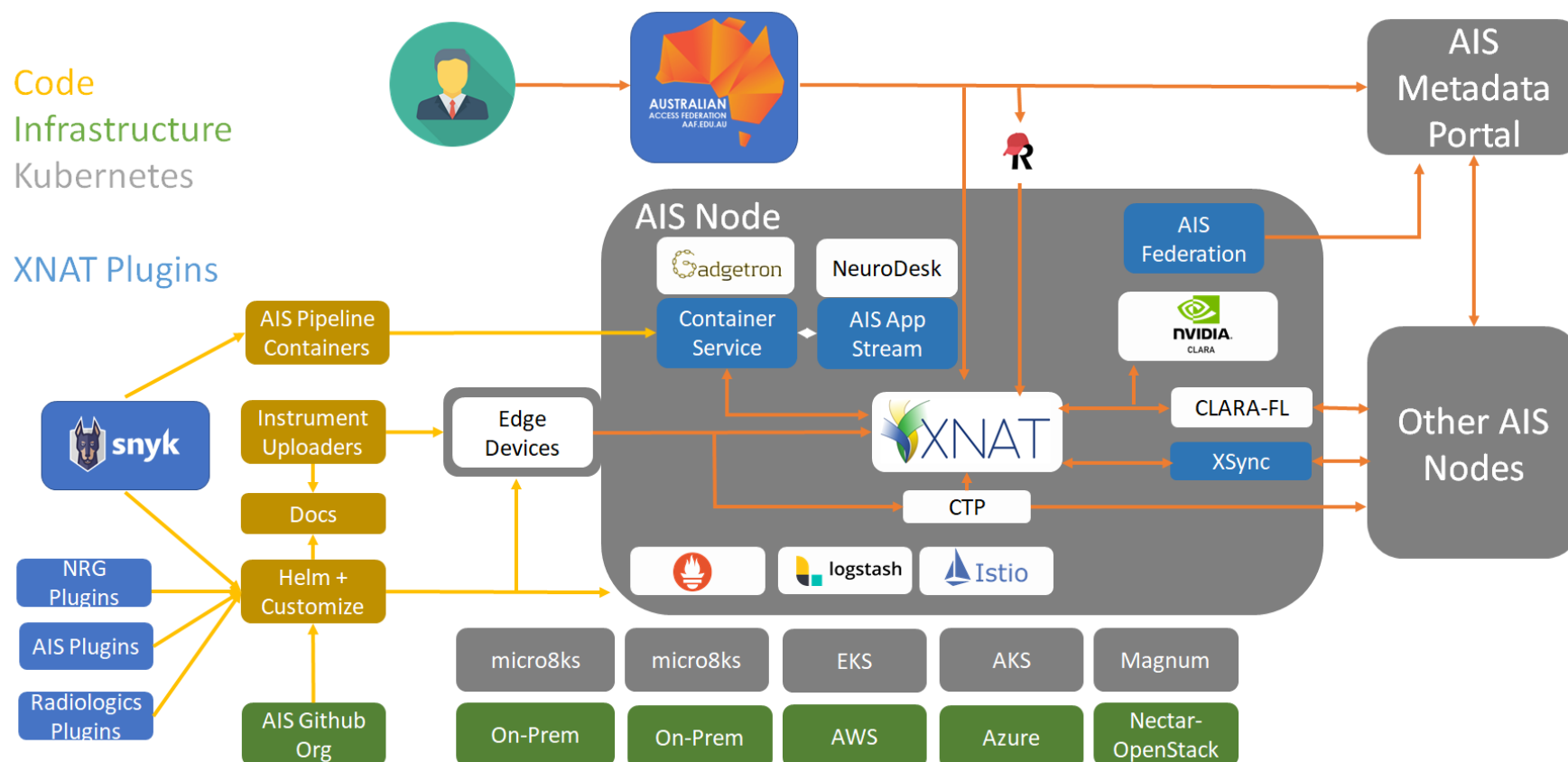
Actions are performed on checked sessions.

Archive Review and Archive Change Projects Delete Rebuild

### Filters

Projects:   
Upload Date:   
Scan Date:   
Status:   
Subject/Session:

## UQ XNAT: Under the covers







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# Case studies

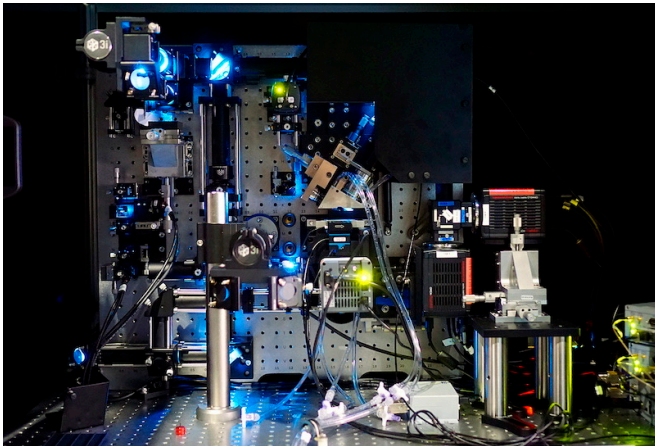
# Imaging immunology in near real-time

Nicholas D Condon

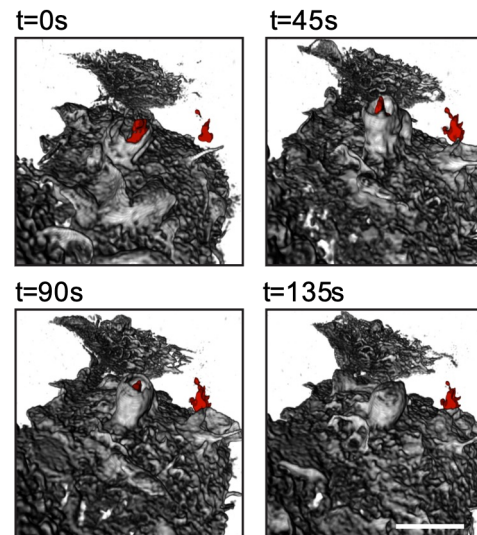
James Springfield

Deborah S. Barkauskas

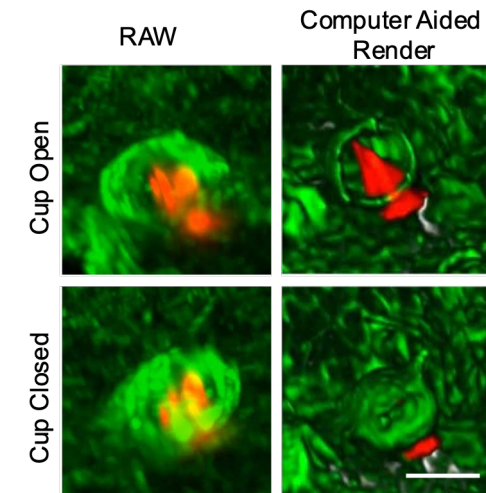
UQ Institute for Molecular Bioscience



IMB: Janelia Lattice  
Light-sheet Microscope



Yeast particle being  
engulfed by the  
macrophage cell



Two key stages of  
phagocytosis shown as both a  
RAW image maximum  
intensity projection (MIP) and  
as a computer aided 3D  
surface render

# Cryo-electron microscopy for determining protein structure

Naphak Modhiran

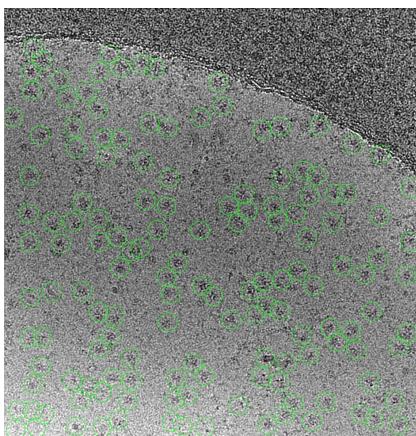
Daniel Watterson

School of Chemistry and Molecular Bioscience

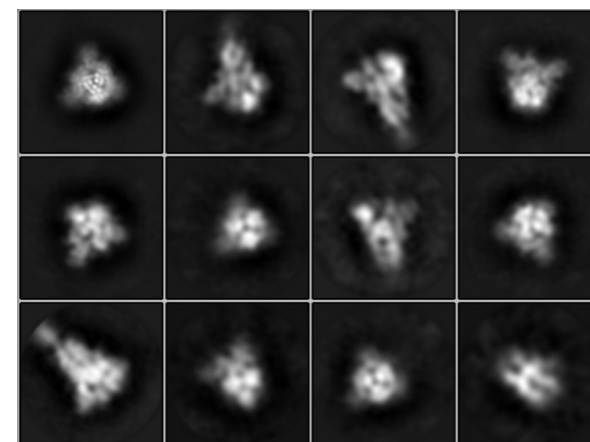
Centre for Microscopy and Microanalysis (CMM)



CMM: CRYO ARM™  
300 Field Emission  
Cryo-Electron  
Microscope



Representative  
micrographs of frozen-  
SARS-CoV-2 spike  
particle. Green circle  
represents picked  
particles



2D classification obtained from obtained  
from CryoARM300, equipped with Gatan  
K3, 50 frames, 9e-/pix/s, 5 sec. Pixel size  
=0.48 using super-resolution mode.

## Conclusions and further work

- Promised you a journey, not a product
- Mind the gaps
- Missing functionality?
  - More general workflows. But which one?
  - How to integrate into existing gateways?
- Journey from unF.A.I.R. to F.A.I.R. is hard





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# Thank you

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Research Computing Centre  
David.Abramson@uq.edu.au  
07 0000 000



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[Instagram.com/uniofqld](https://Instagram.com/uniofqld)



[twitter.com/RCCUQ](https://twitter.com/RCCUQ)

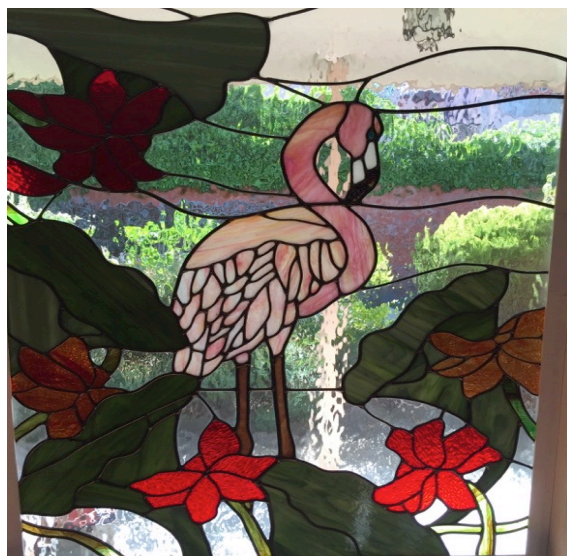


[facebook.com/rccuq](https://facebook.com/rccuq)

[rcc.uq.edu.au](https://rcc.uq.edu.au)

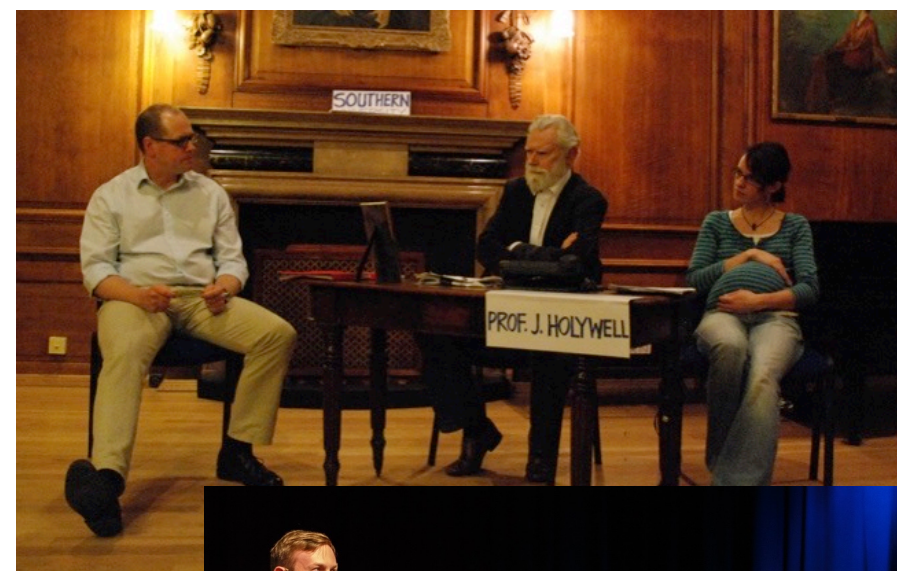
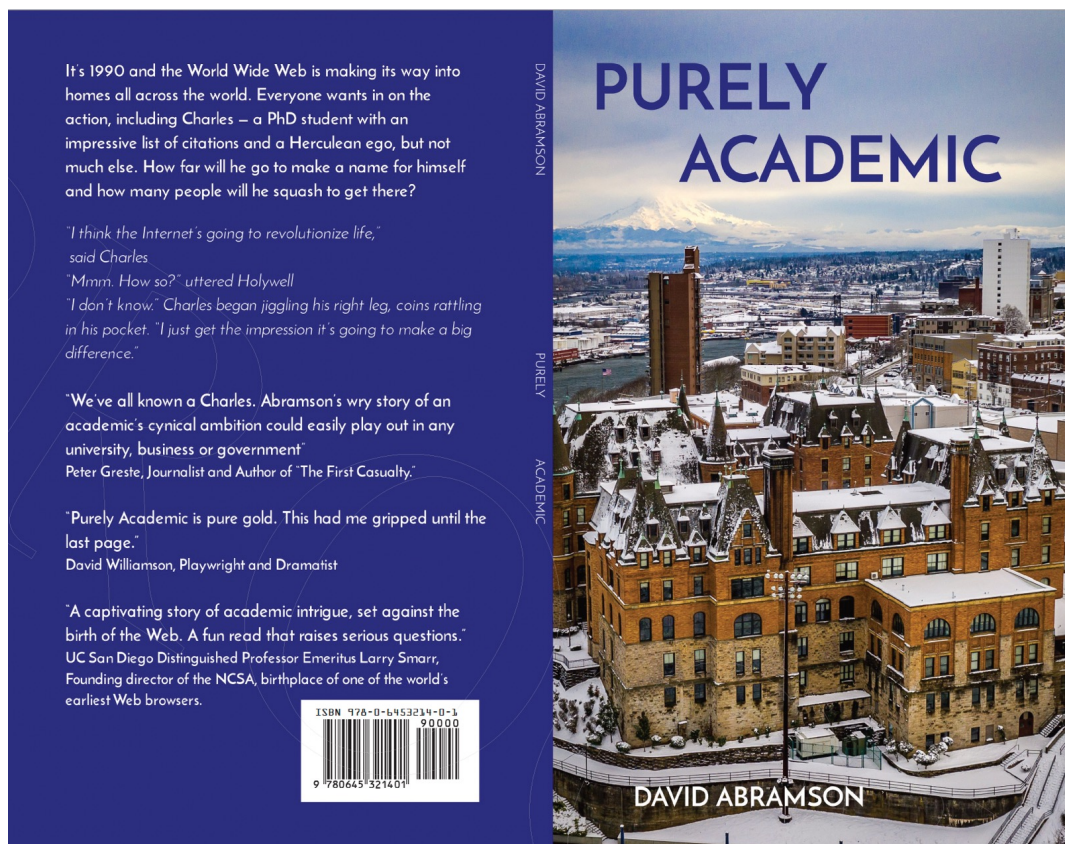


## Thank you and Questions





## Translation to the arts



[purely-academic.com](http://purely-academic.com)