THE UNIVERSITY 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

17 0

07:24 on Monday, 21 June 2021

Magugnano to Riva del Garda, Lake Garda

Add a description

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

Add private notes

With someone who didn't record? Add Friends

	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

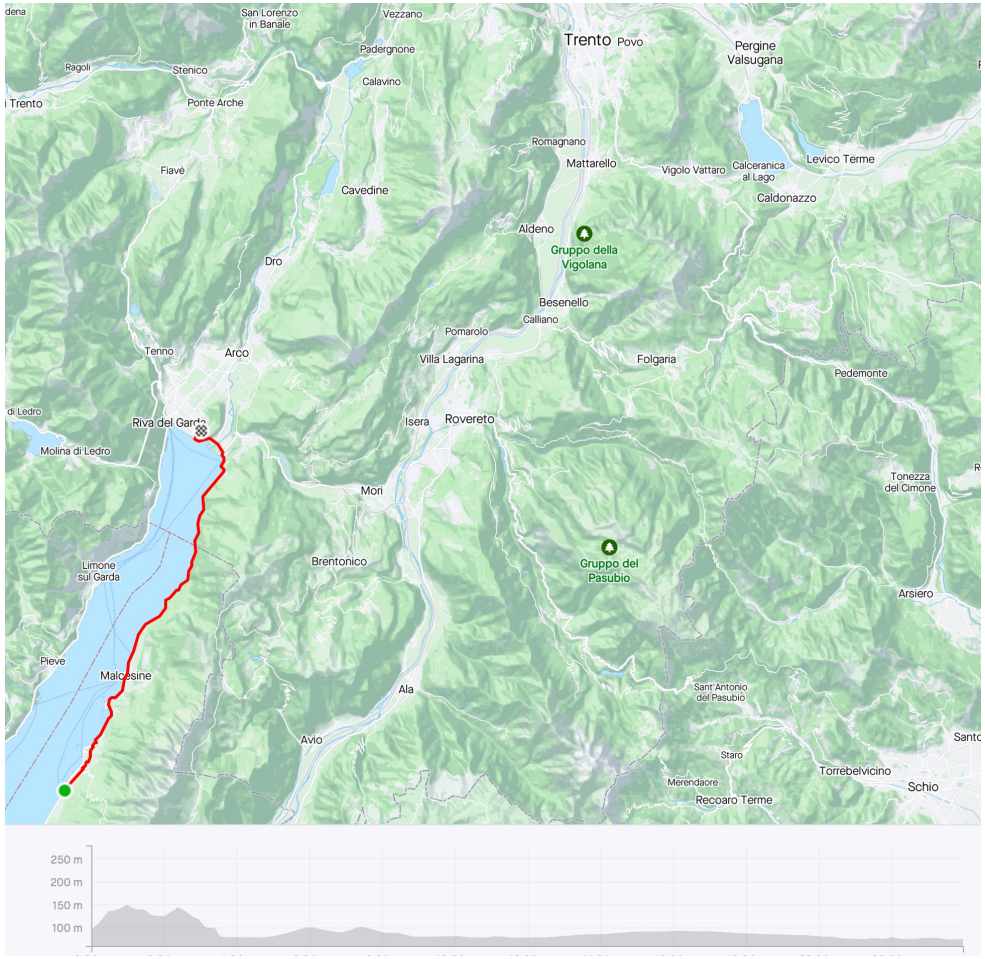
FulGaz

Bike: Brisbane Domane

4 Rides on this route

This Ride **26.8 km/h**

Trending Faster

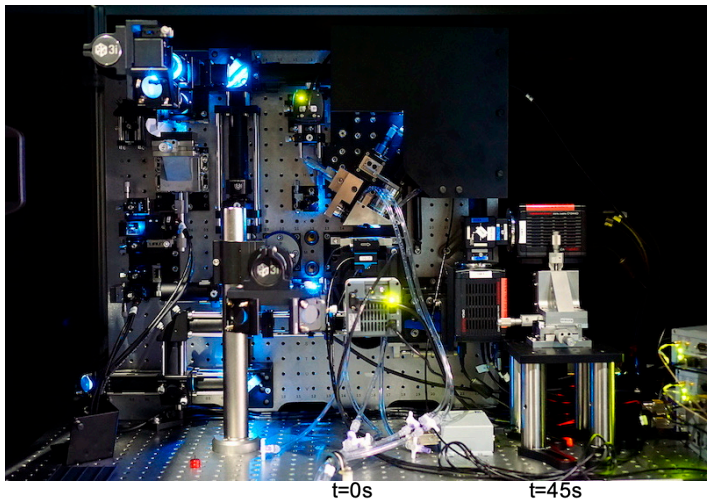


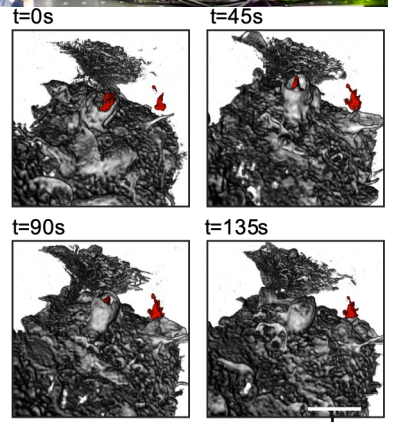
Introduction

- 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”.

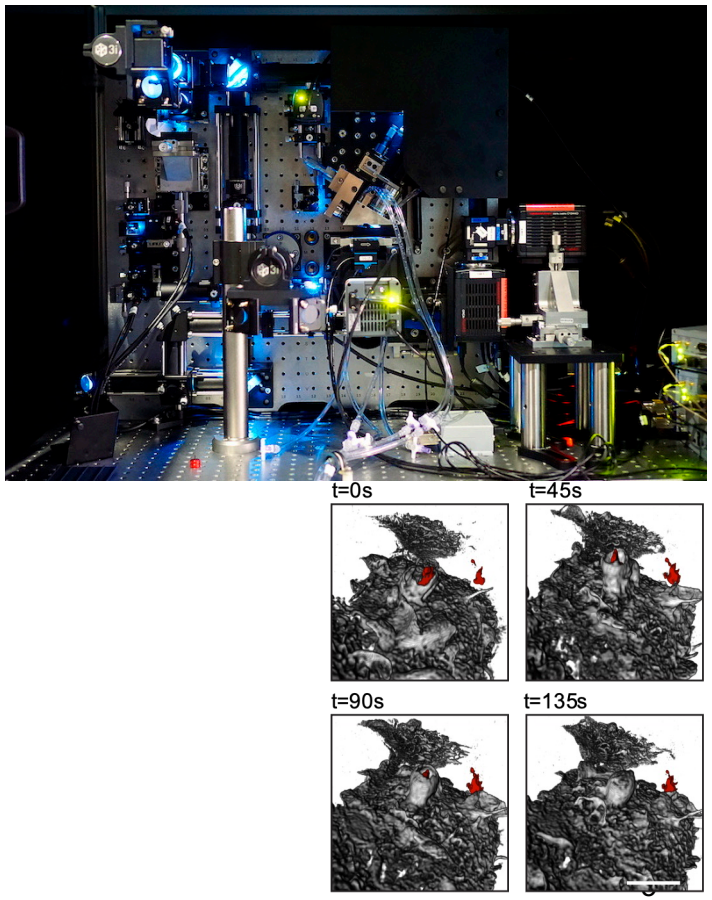
- Live-cell imaging optical microscope
  - Spatial resolution 512 x 2048 x 151 pixels,
  - Temporal resolution 60 volumes per minute
  - 5-10 TBytes per day!
- A researcher must contact the facility operator to book a time slot.
- Each 3 D volume must be pre-processed
  - multiple channel alignment,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



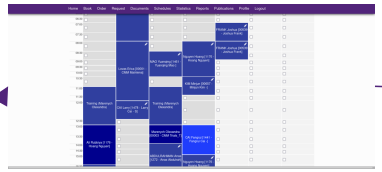


“I just want the pretty picture, movie and graph, not how the pipes are connected, nor why I need some big computer to process it”.

- 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.

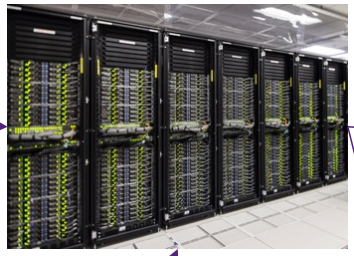


Instrument Researcher Workflow

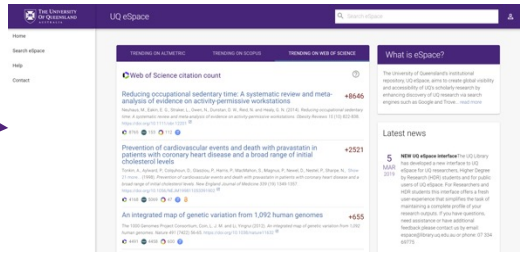


Book laboratory

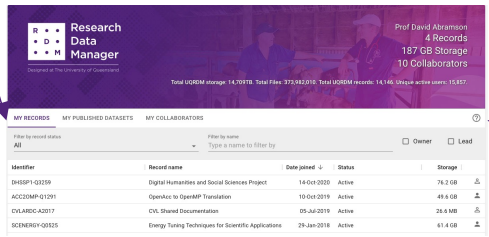
Perform experimental work



Analyze results



Publish



Reserve data collection

Storage

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

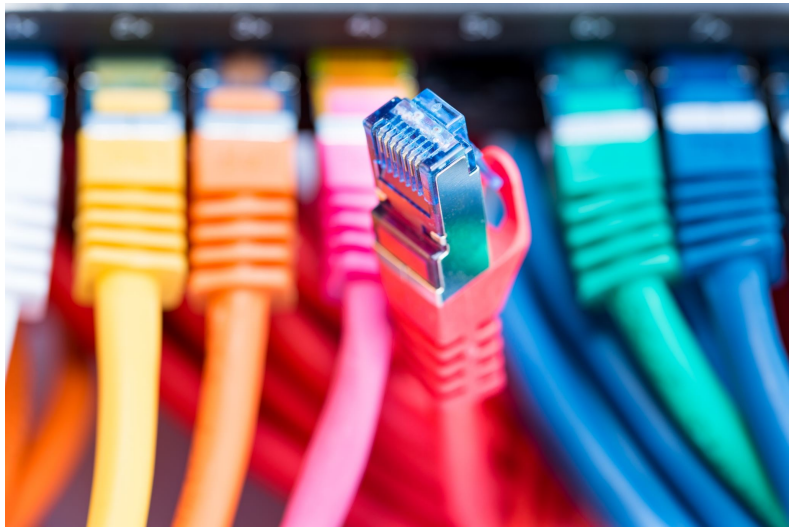
- *We envisage a system* that
  - allows researchers to book time on an instrument
  - required e-infrastructure to be simultaneously scheduled and managed.
  - For example
    - if a user needs to pre-process data sets on the fly, they also require access to processing software on the correct computational 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 is 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.

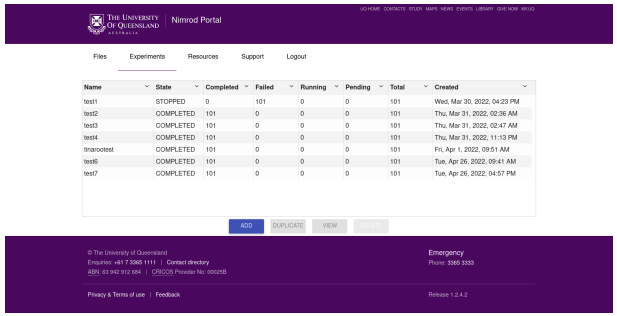
The removal of explicit data movement steps and the knowledge of the various storage subsystems

- *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.



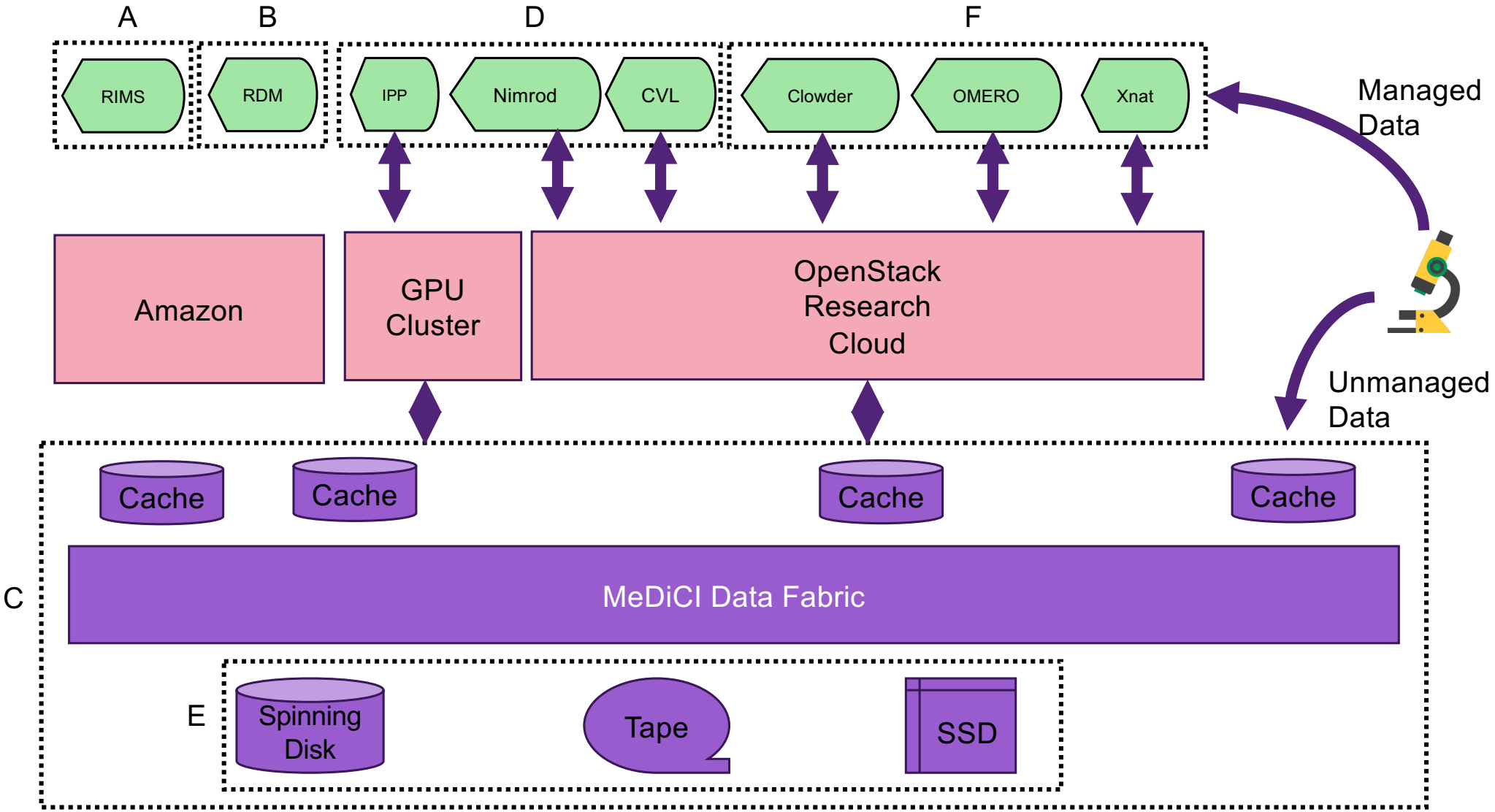
Automatic archiving and sharing of both primary and secondary data sets

- *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.

Implementation @ UQ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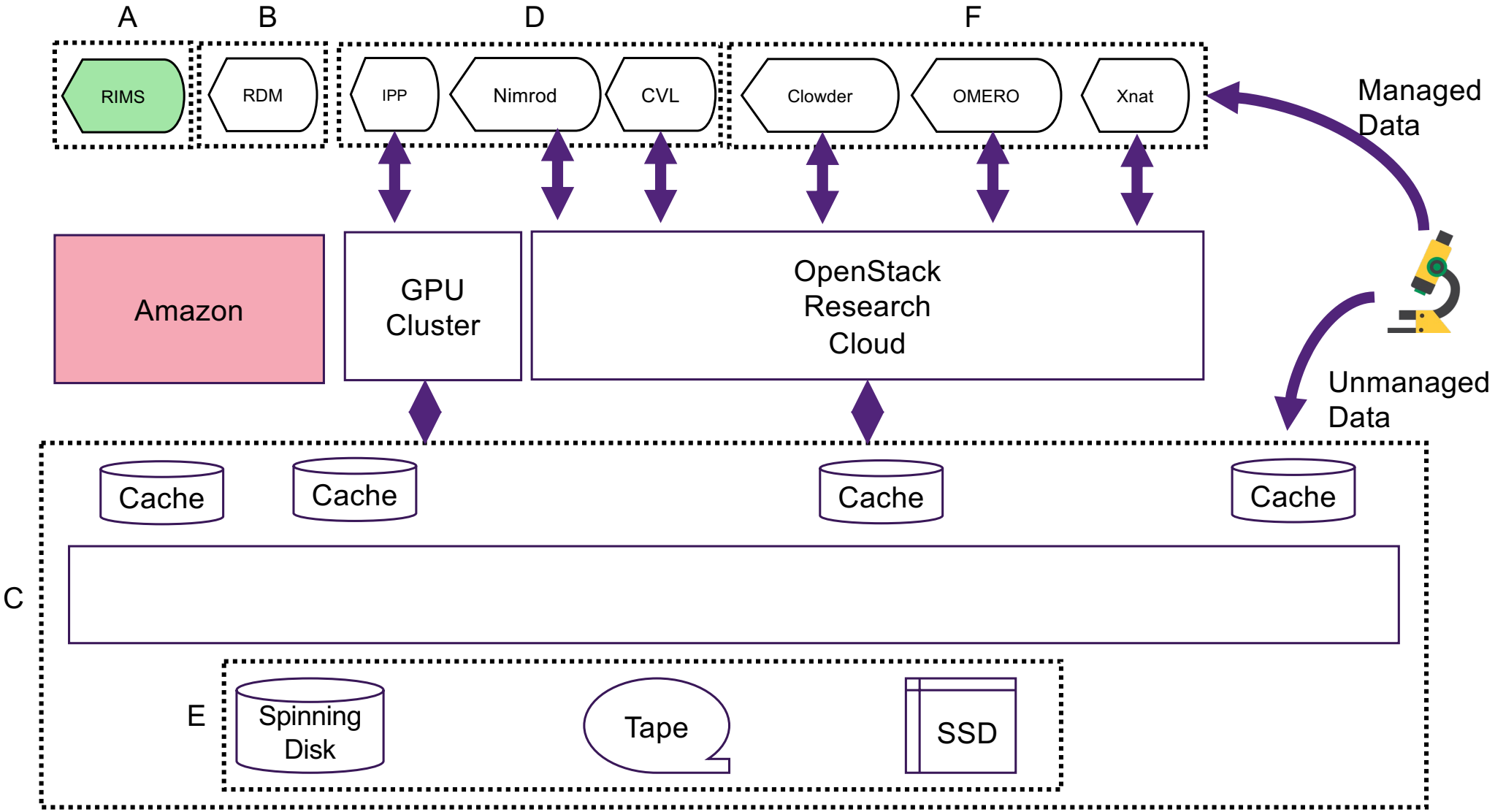
Booking an instrument and associated laboratory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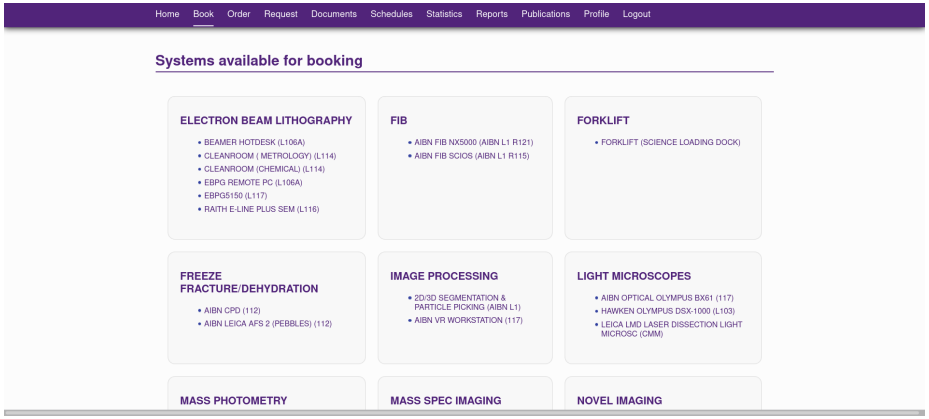
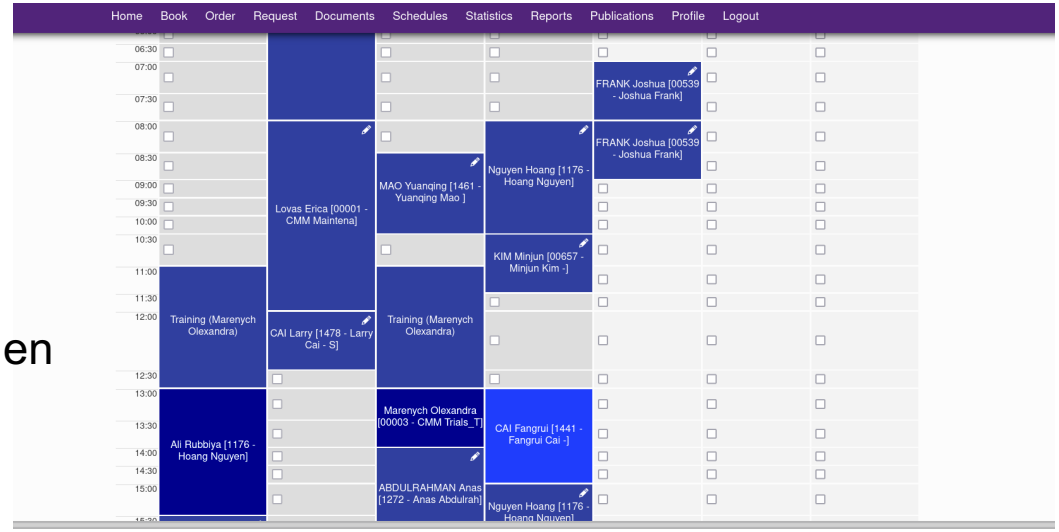
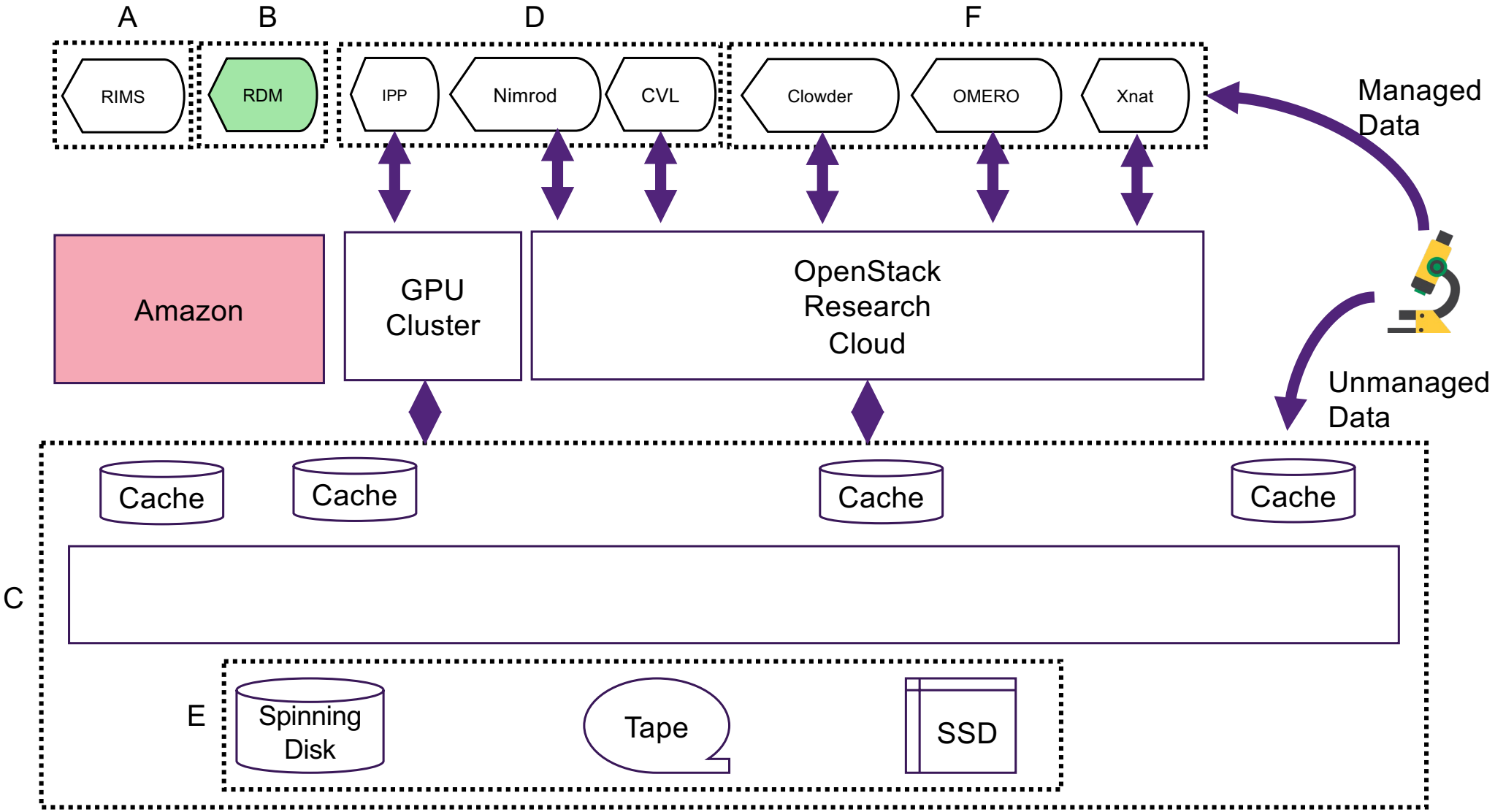
RIM - PPMS

- Cloud-based, online research infrastructure register and booking system
  - search
  - book specific research instruments and equipment across UQ.
- Provides cost-saving benefits for UQ as a single enterprise software system
- Greater asset utilisation and strategic reporting.
- Benefits include;
  - Easier online access to find and book UQ research equipment and infrastructure
  - Consistent user experience every time a system is used
  - Online support from facility admin staff if/when required





Automatic provisioning of sufficient storage capacity for the scale of the experiments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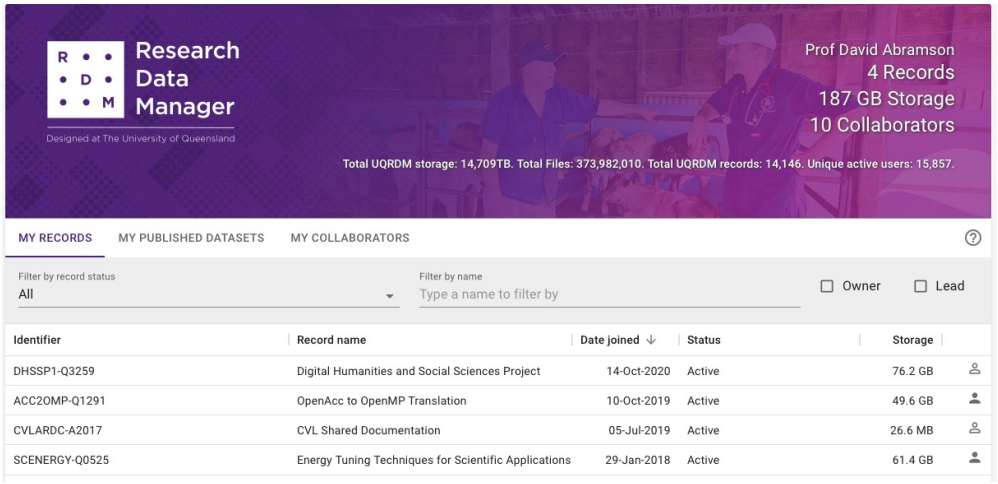
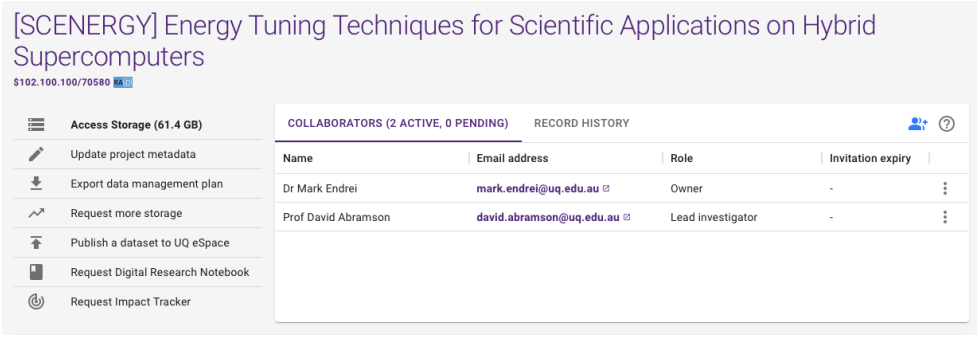
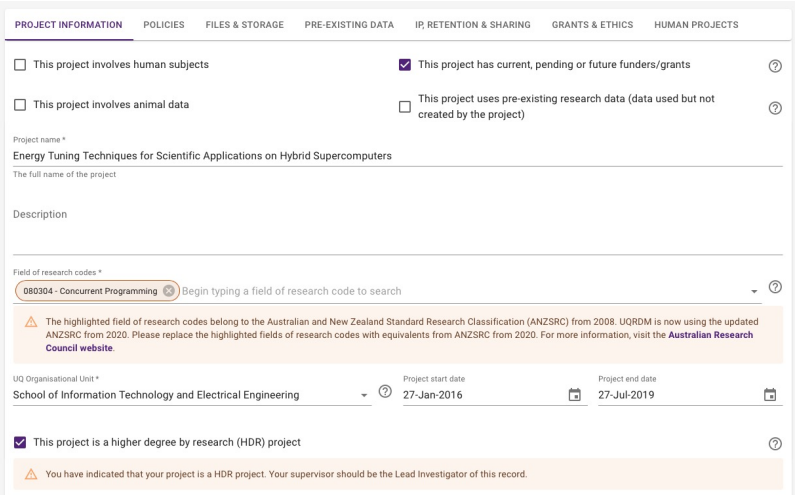
Research Data Manager (RDM)

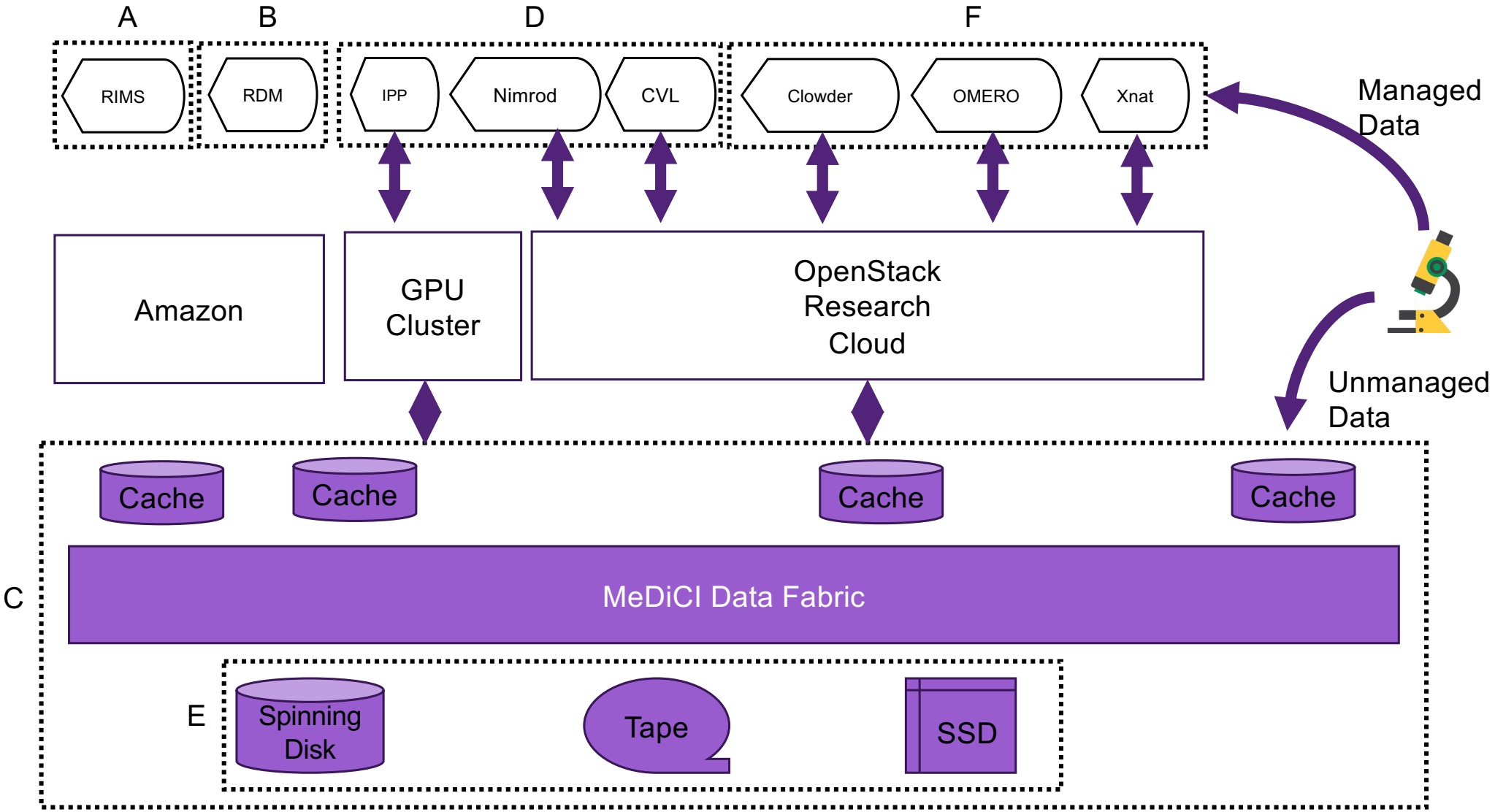
- Integrated data management system covering the entire research data lifecycle.
- Seamless provisioning of easily accessible, secure and sharable data storage in real-time
- Enables publication of datasets into UQ eSpace.







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

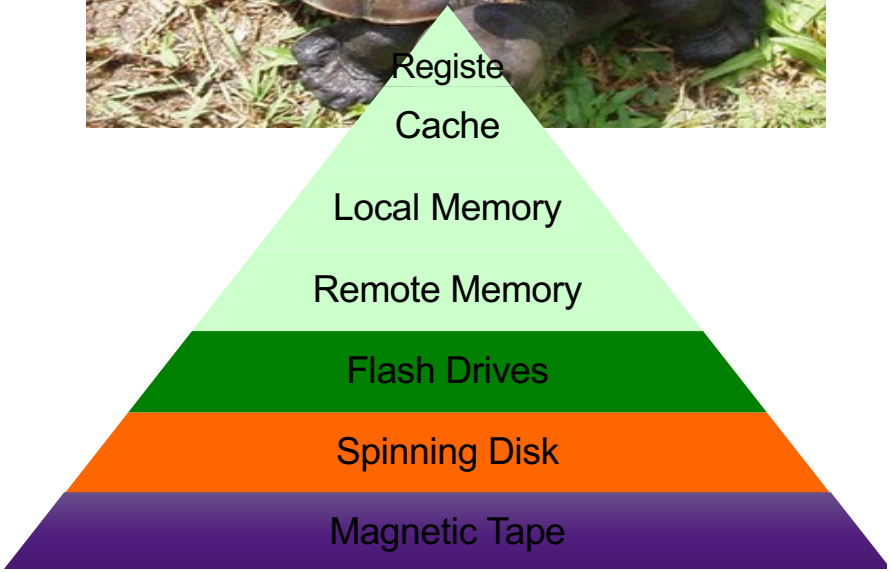
~~Turtles~~ Caches all the way down

“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.

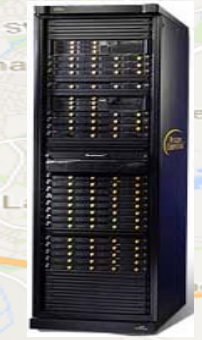
Questioning what the final turtle might be standing on, the anecdote humorously concludes that it is turtles all the way down””

https://en.m.wikipedia.org/wiki/Turtles_all_the_way_down



UQ Landscape: An inconvenient truth

30 kms



MeDiCI

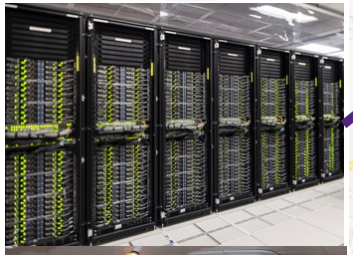
- Centralising research data storage and computation
- Distributed data is further from both the instruments that generate it, some of the computers that process it, and the researchers that interpret it.
- Existing mechanisms manually move data
- MeDiCI solves this by

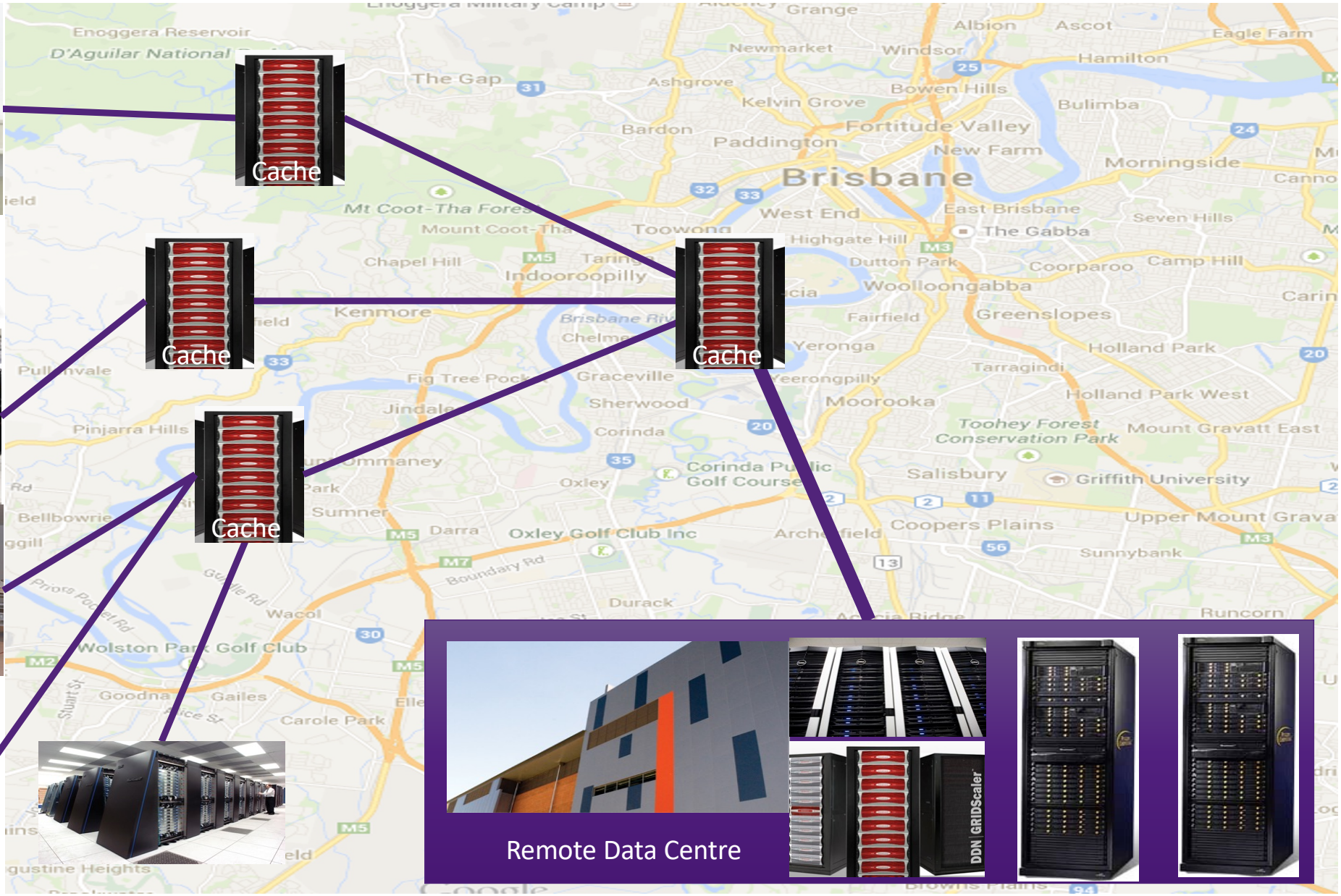
Augmenting the existing infrastructure,

Implementing on campus caching

Automatic data movement

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

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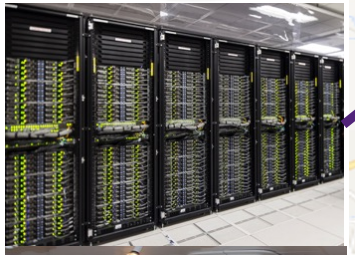
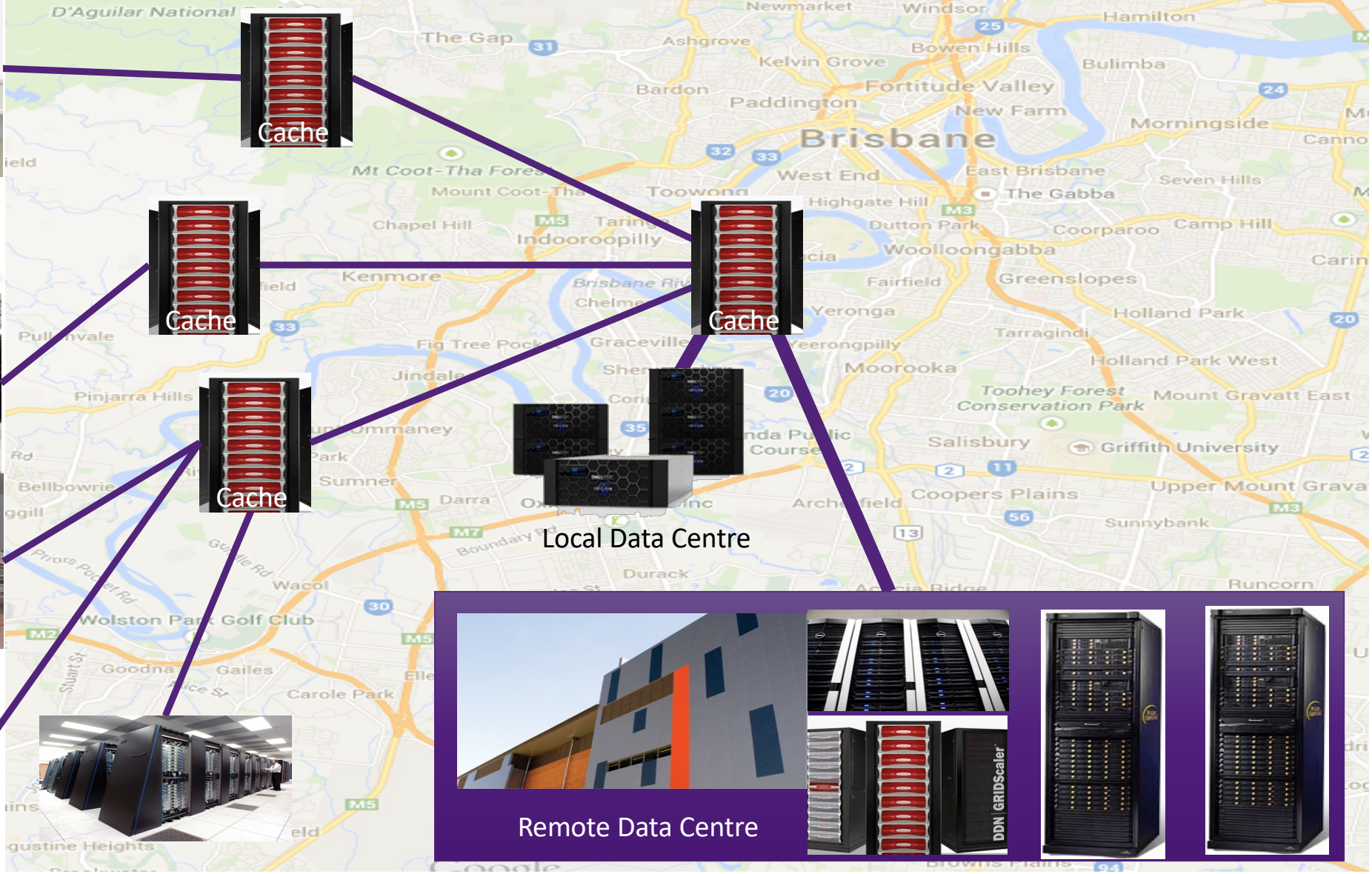
Brisbane
Remote Data Centre
DDN GRIDScaler

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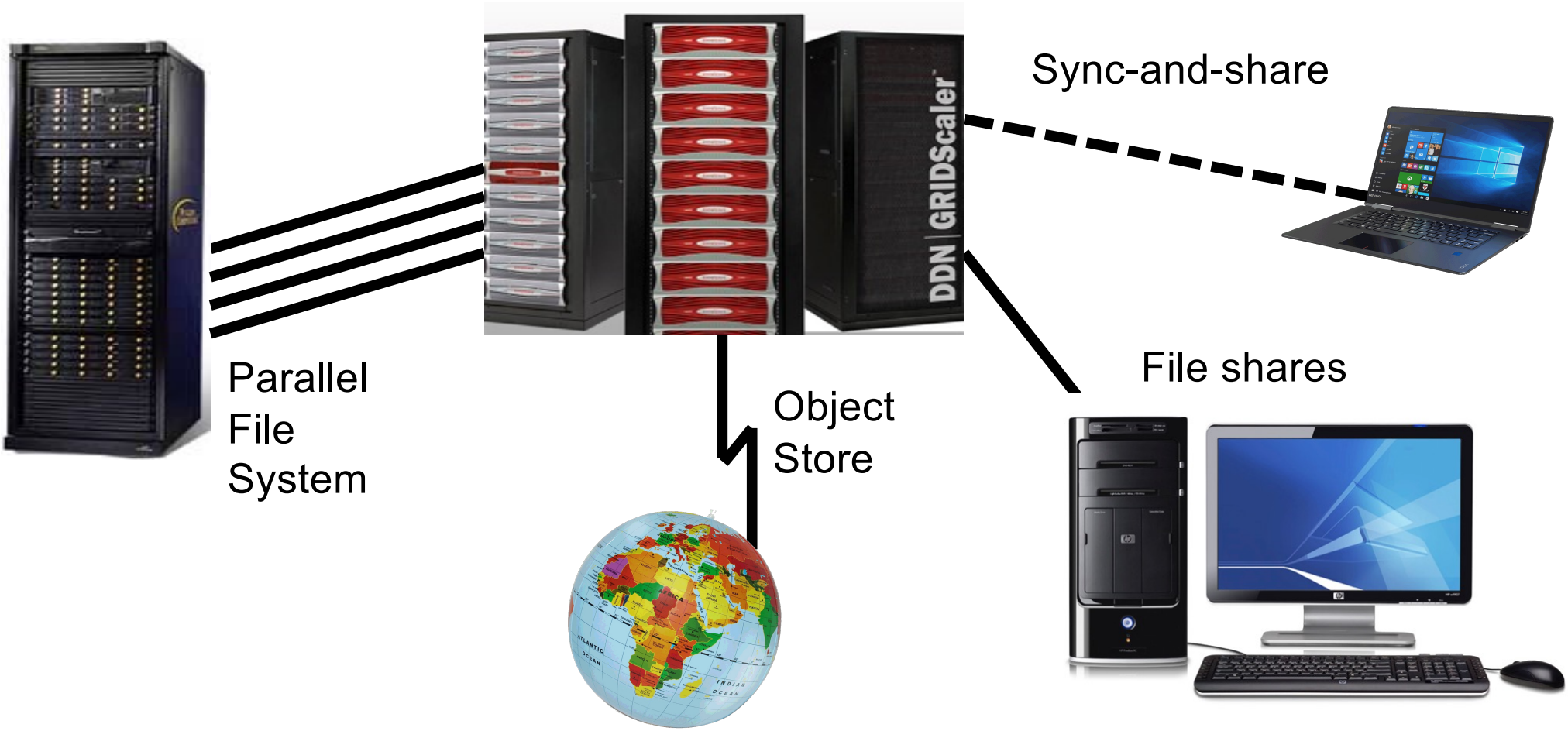
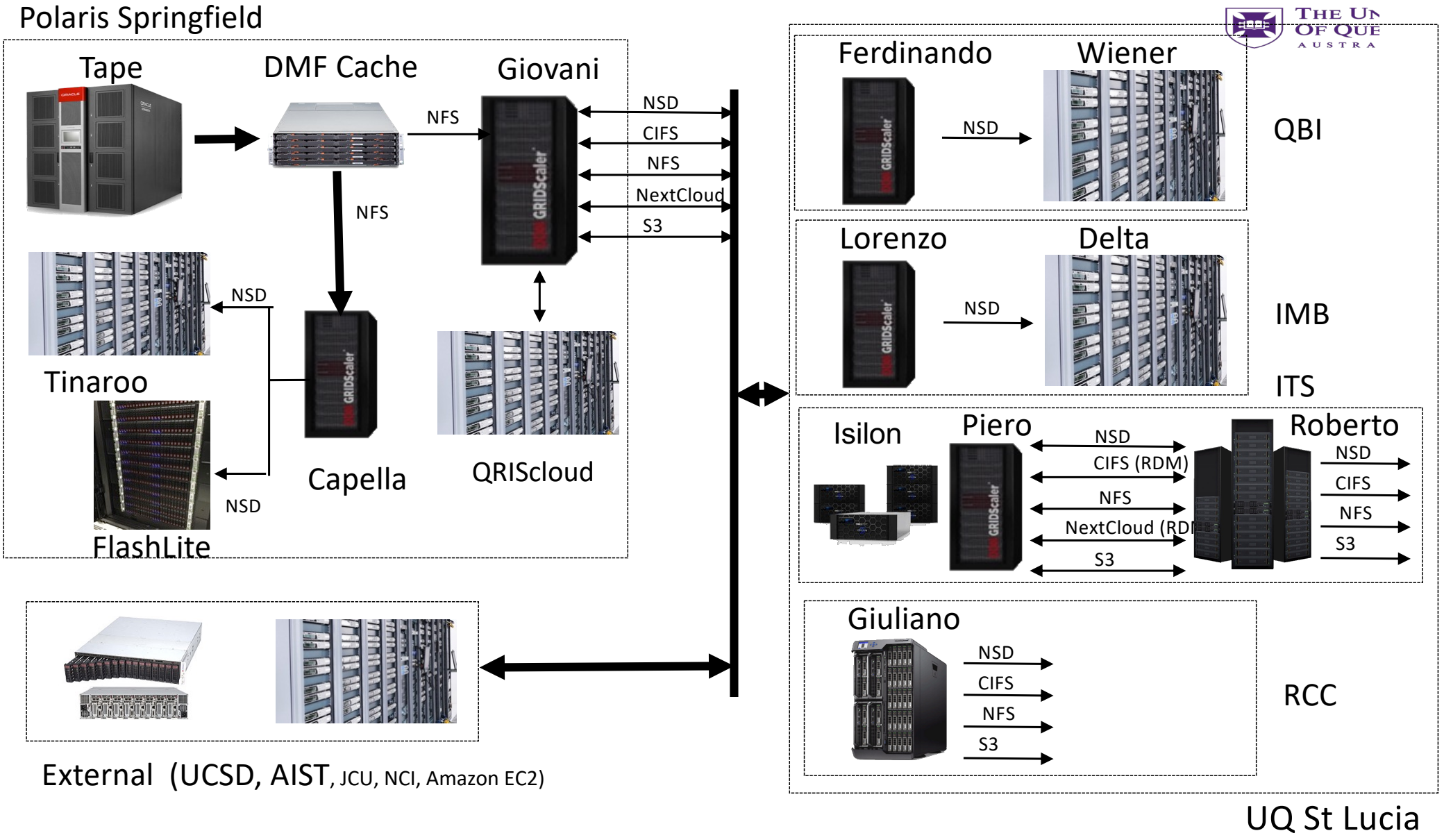
Remote Data Centre
DDN GRIDScaler

MeDiCI unifies data access

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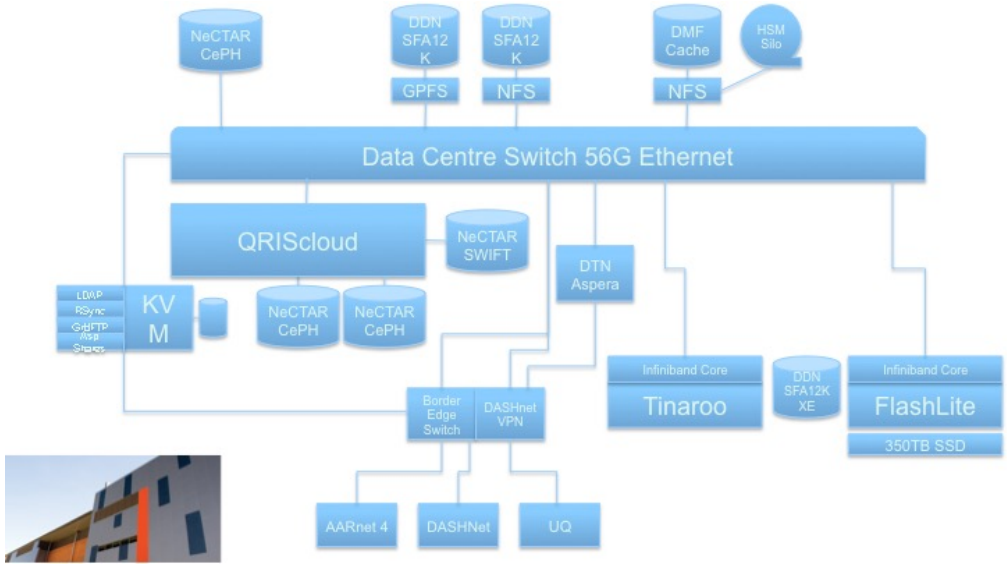
A Declarative Machine Room?

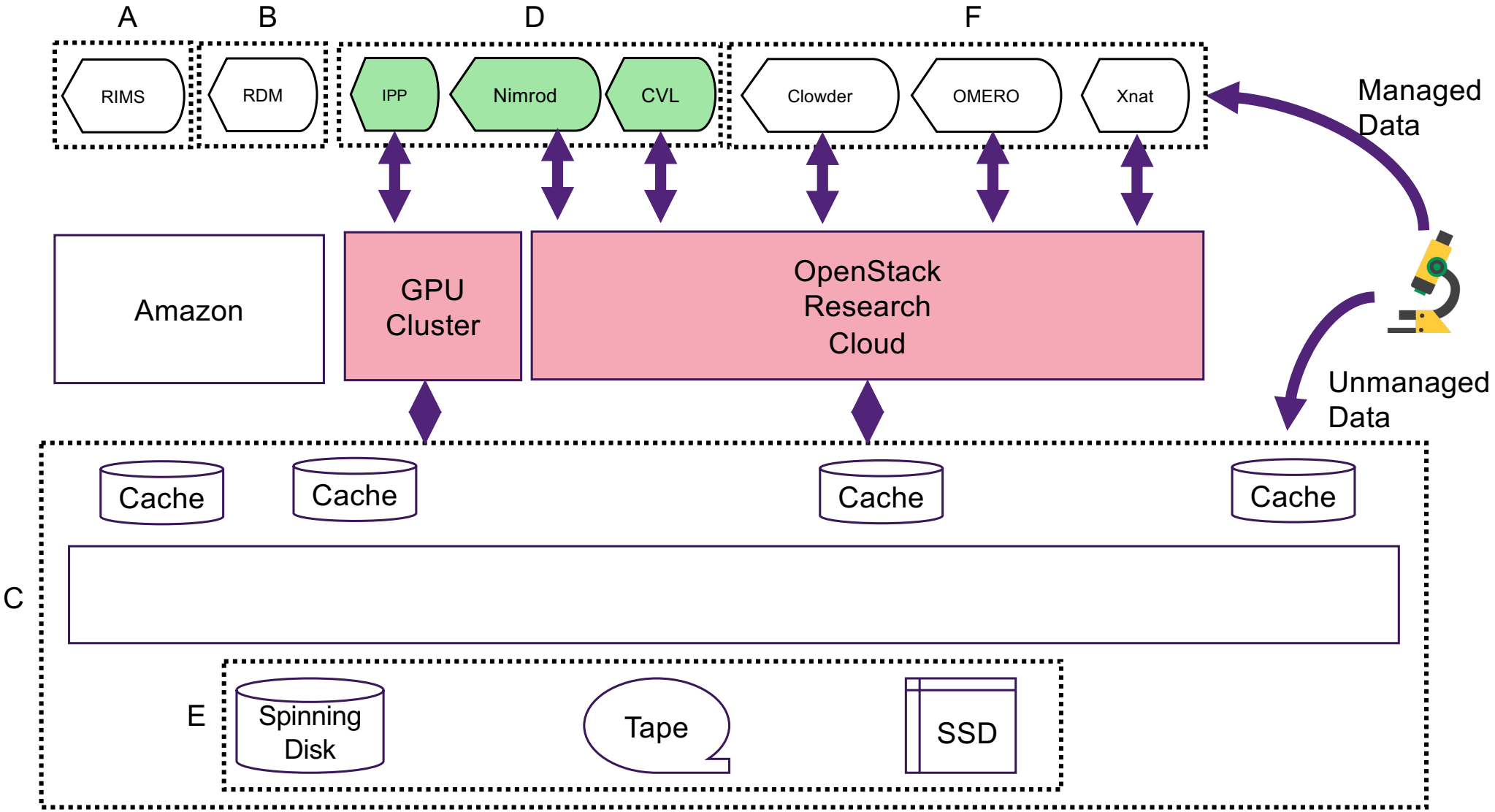
- Static allocation of disk and tape
- Policy driven allocation




```
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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OMERO
Xnat
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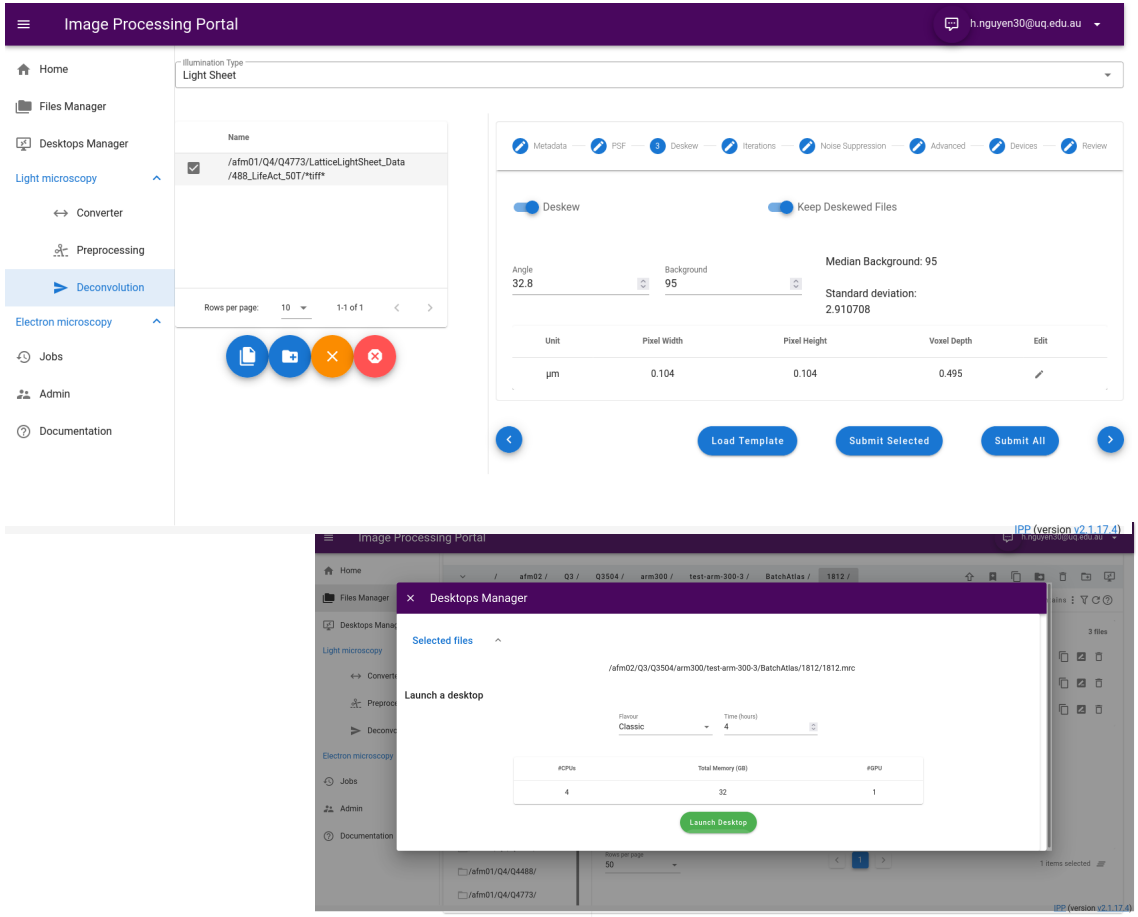
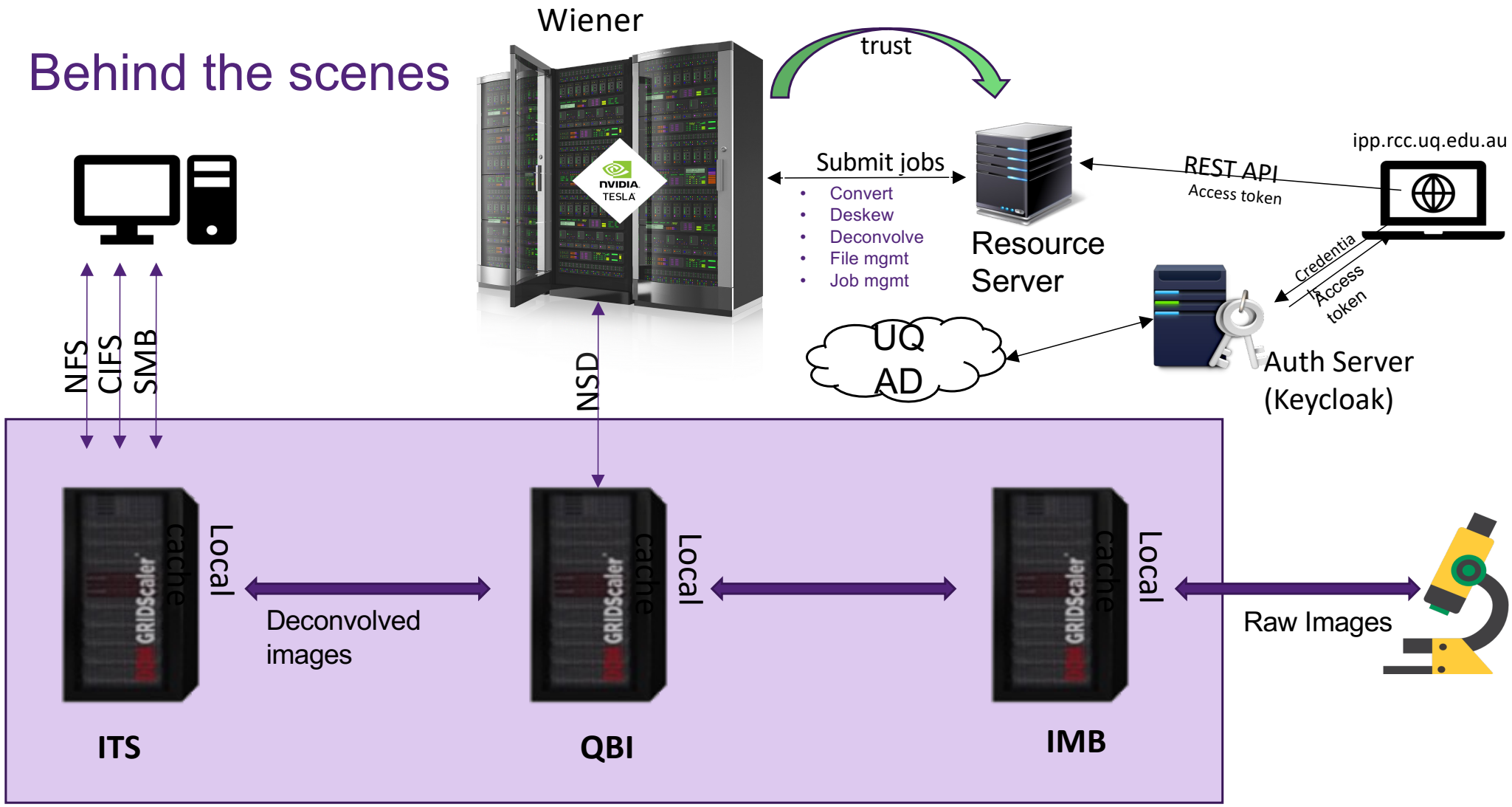
The UQ Image Processing Portal (IPP)

- 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

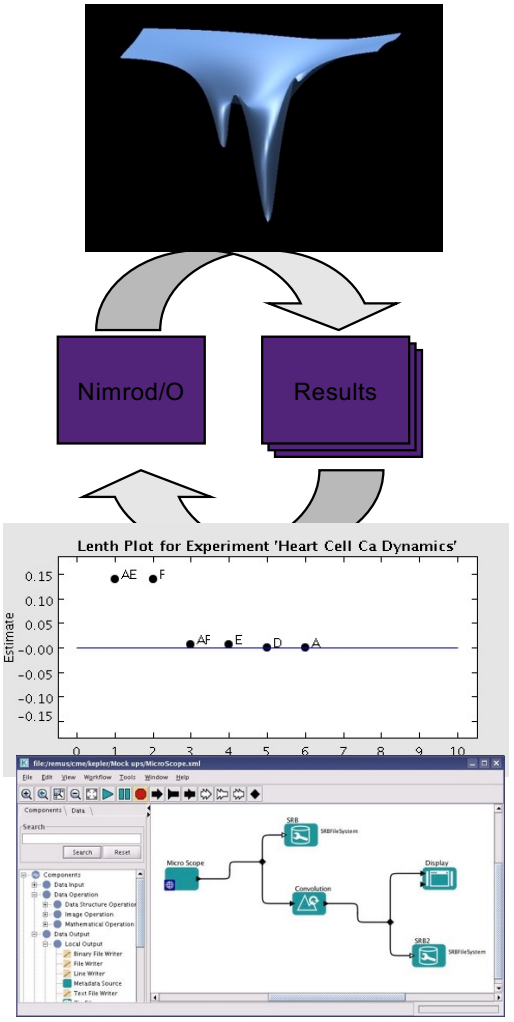


Behind the scenes



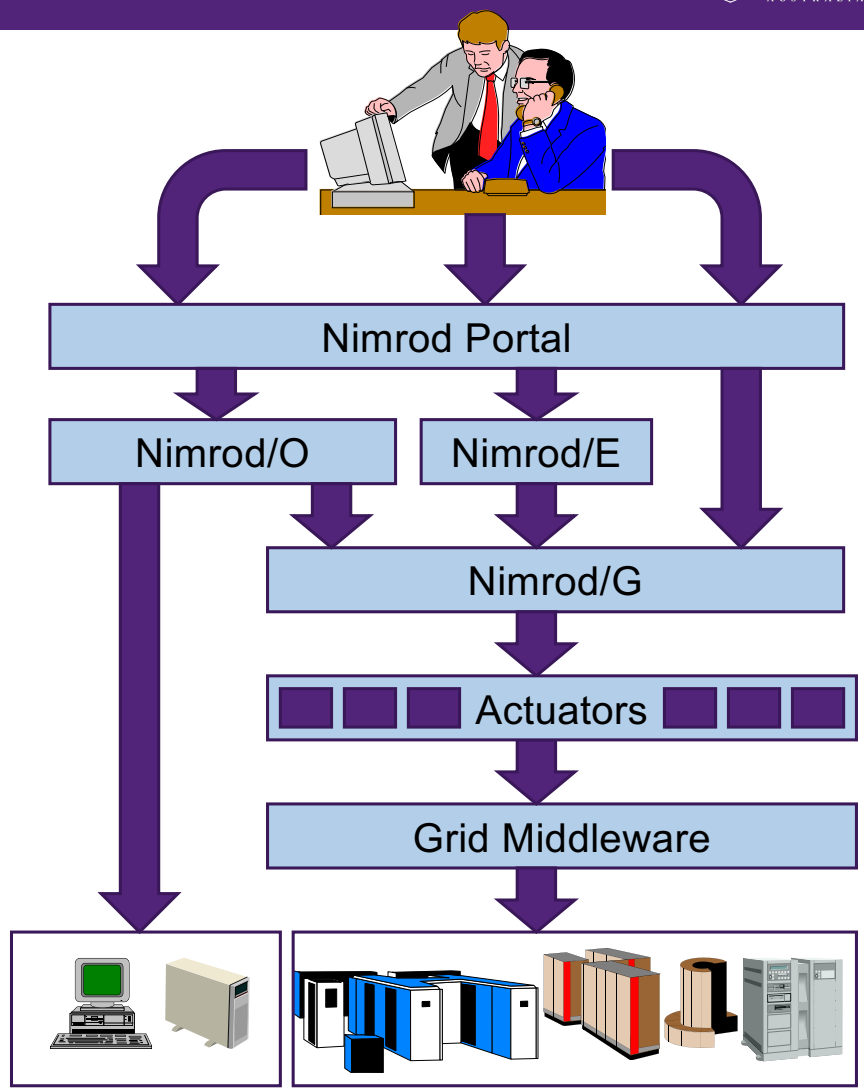
The UQ Nimrod Service

- 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)

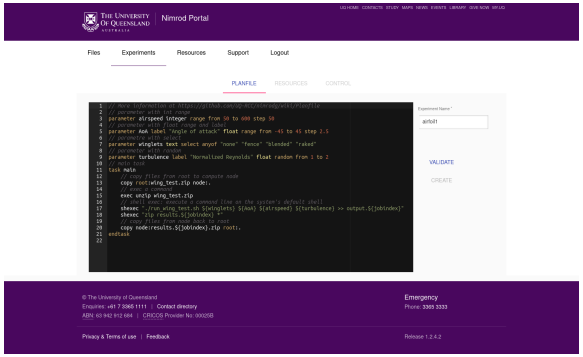


A family of tools

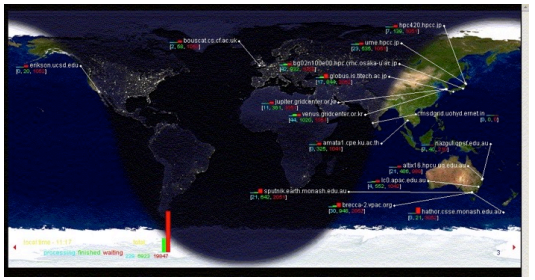

```
parameter pressure float range from 5000 to 6000 points 4
parameter concent float range from 0.002 to 0.005 points 2
parameter material text select anyof “Fe” “Al”

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
```



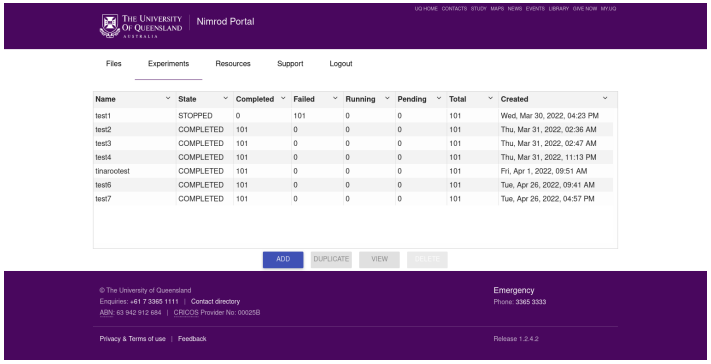
Nimrod Development Cycle



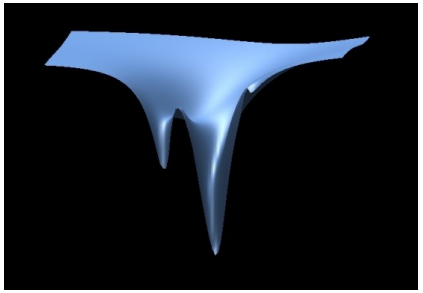
Prepare Jobs using Portal



Sent to available machines



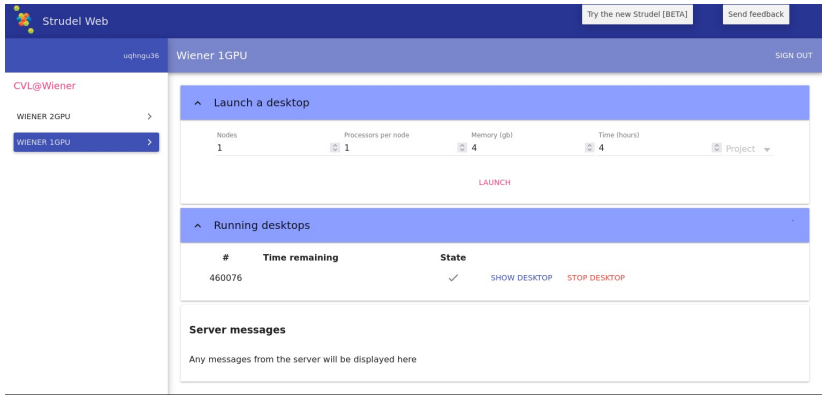
Jobs Scheduled Executed Dynamically

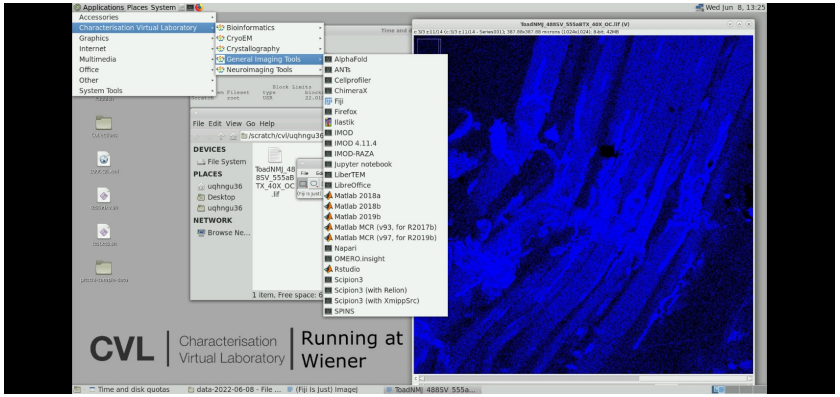


Results displayed & interpreted

Characterisation Virtual Laboratory (CVL)

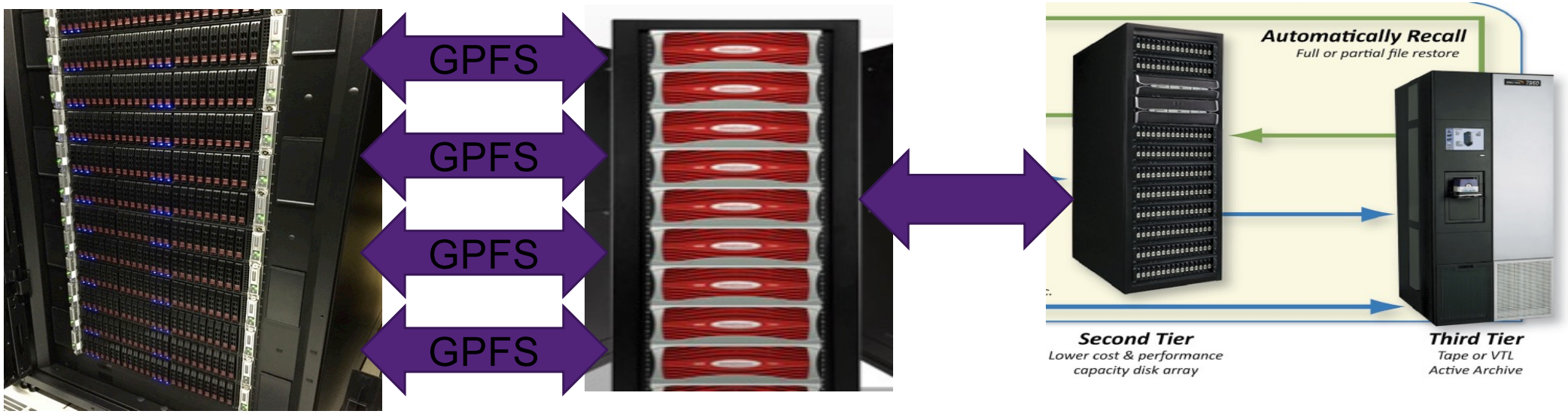
- Virtual desktop environment that provides researchers with access to imaging tools and data
- Each CVL desktop is pre-configured with imaging tools, wrapped as singularity containers or HPC modules.
- End users can choose the size and wall-time of the virtual desktop before launch.
- Once launched,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



IBM Spectrum Scale

HPE DMF Disk/Tape

HPC

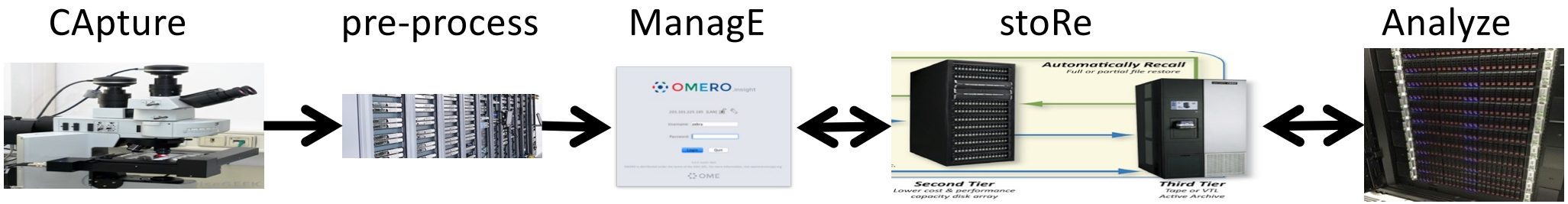
Parallel file system

Long term data collections

Automatic capture of instrument and experiment meta-data.

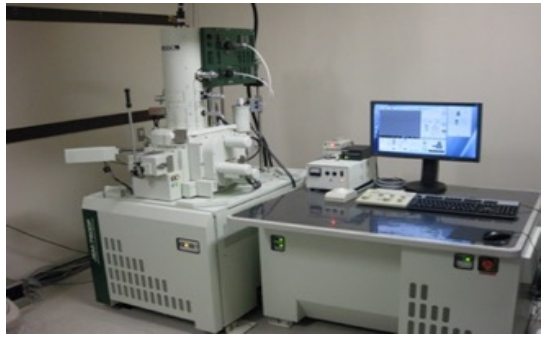
CAMERA: MeDiCI meets instruments

- 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

Research Data Manager
Designed at The University of Queensland

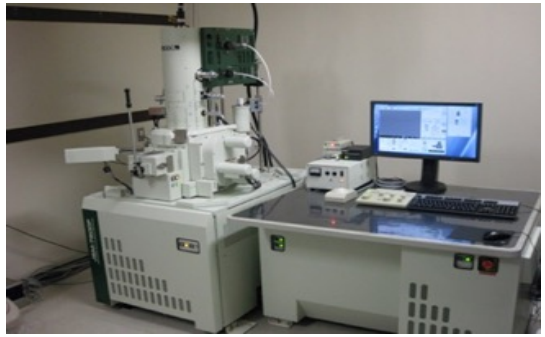


RDM creates collection → Collection mounted on scope → Data copied to collection → Collection mounted on HPC for analysis

Managed data workflow

Research Data Manager

Designed at The University of Queensland



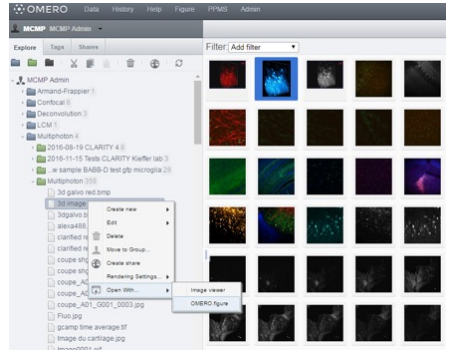
RDM creates collection

Collection mounted on repository

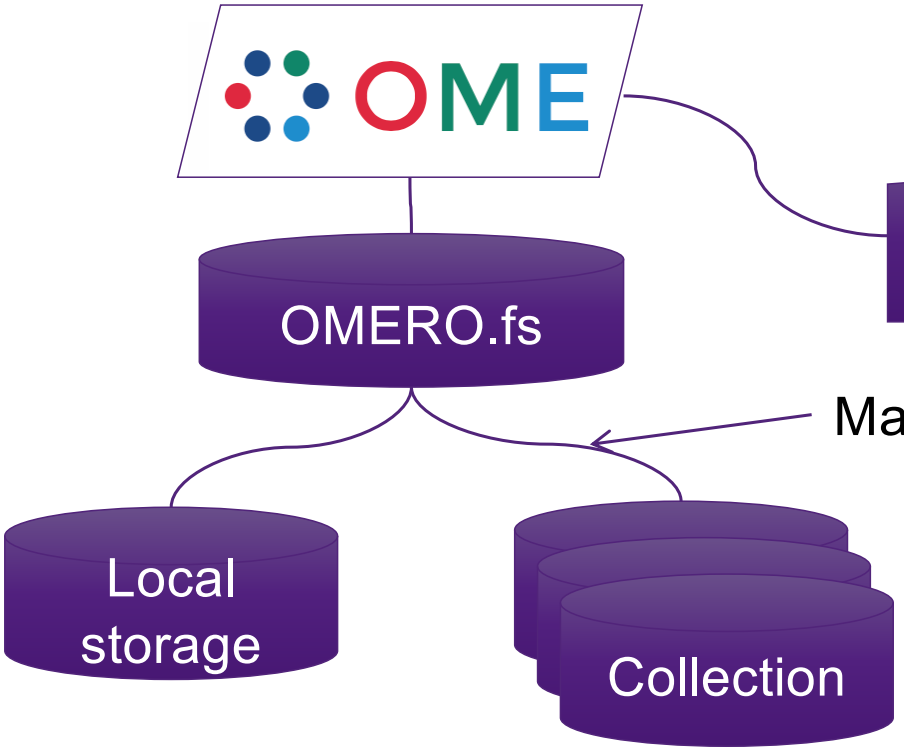
Data ingested into repository

Collection mounted on HPC for analysis

Leveraging unmanaged data collections



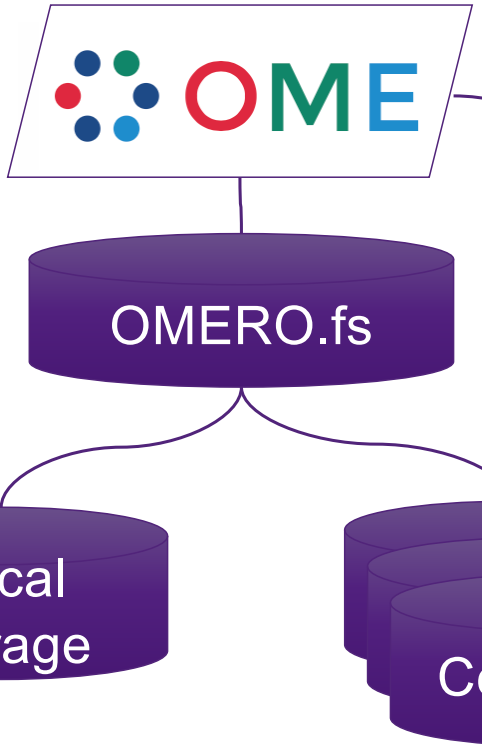
Cloud Hosted OMERO server

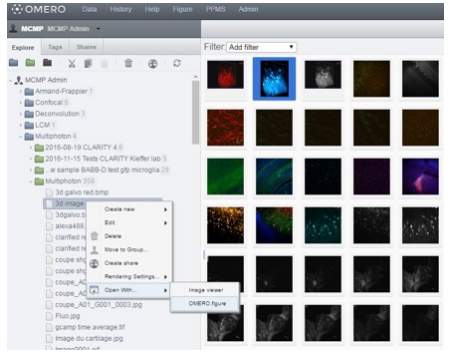


Collections are mapped to OMERO groups

Leveraging unmanaged data collections

Cloud Hosted OMERO server





Web front end

Data ingest and presentation

Read Only

Analyse

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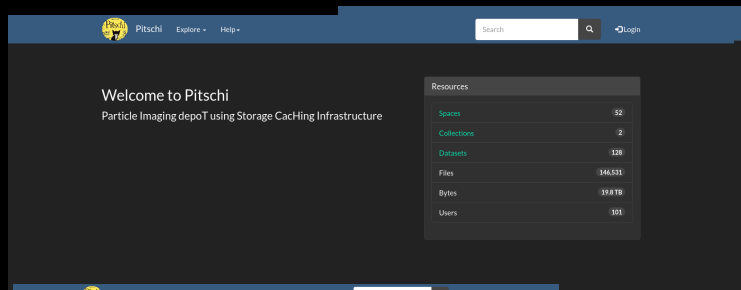
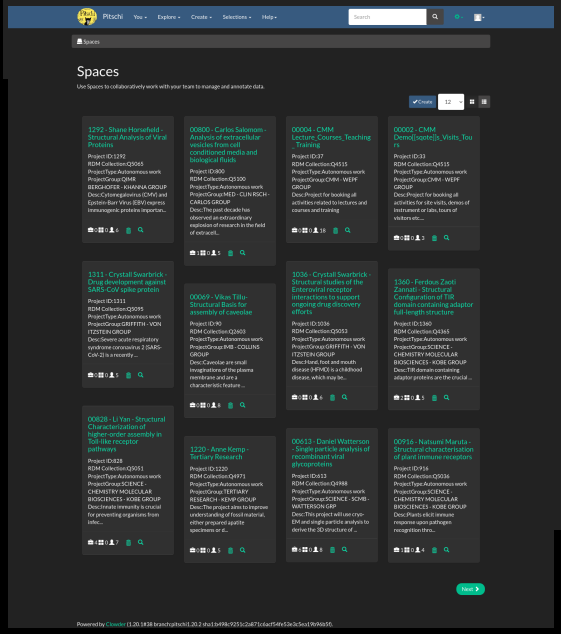
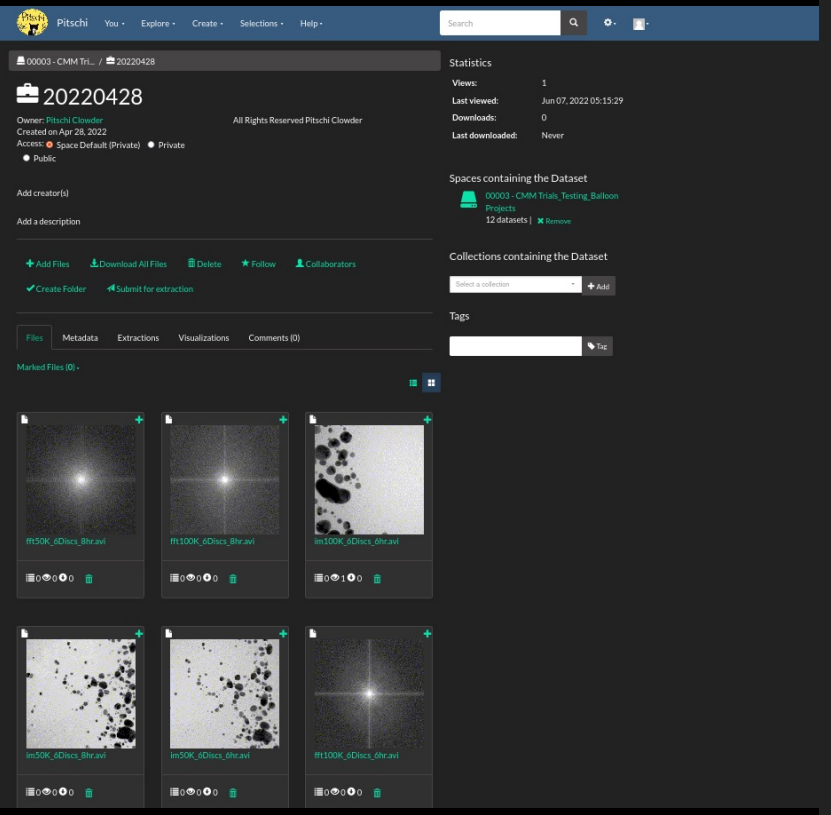
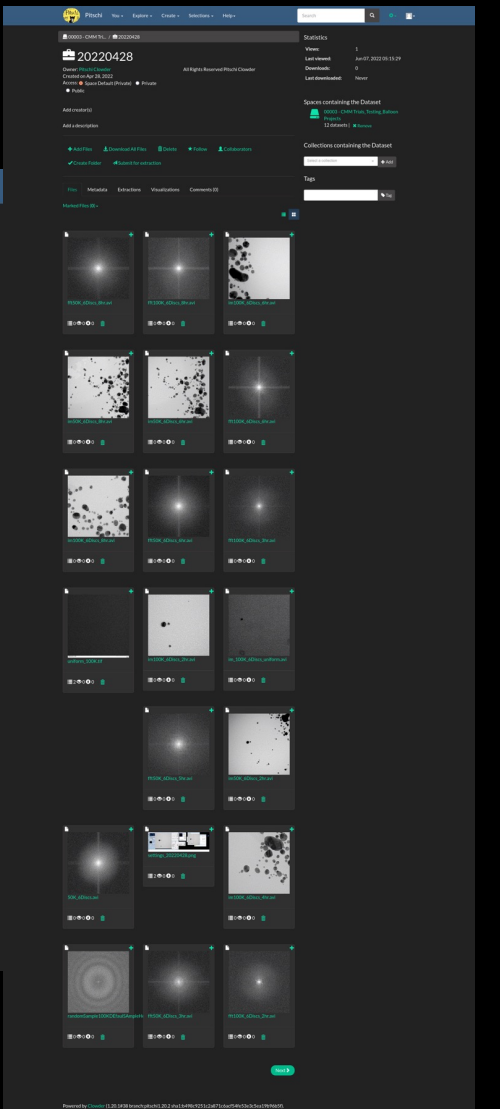
AUSTRALIA

Pitchi: A Clowder based repository for EM data



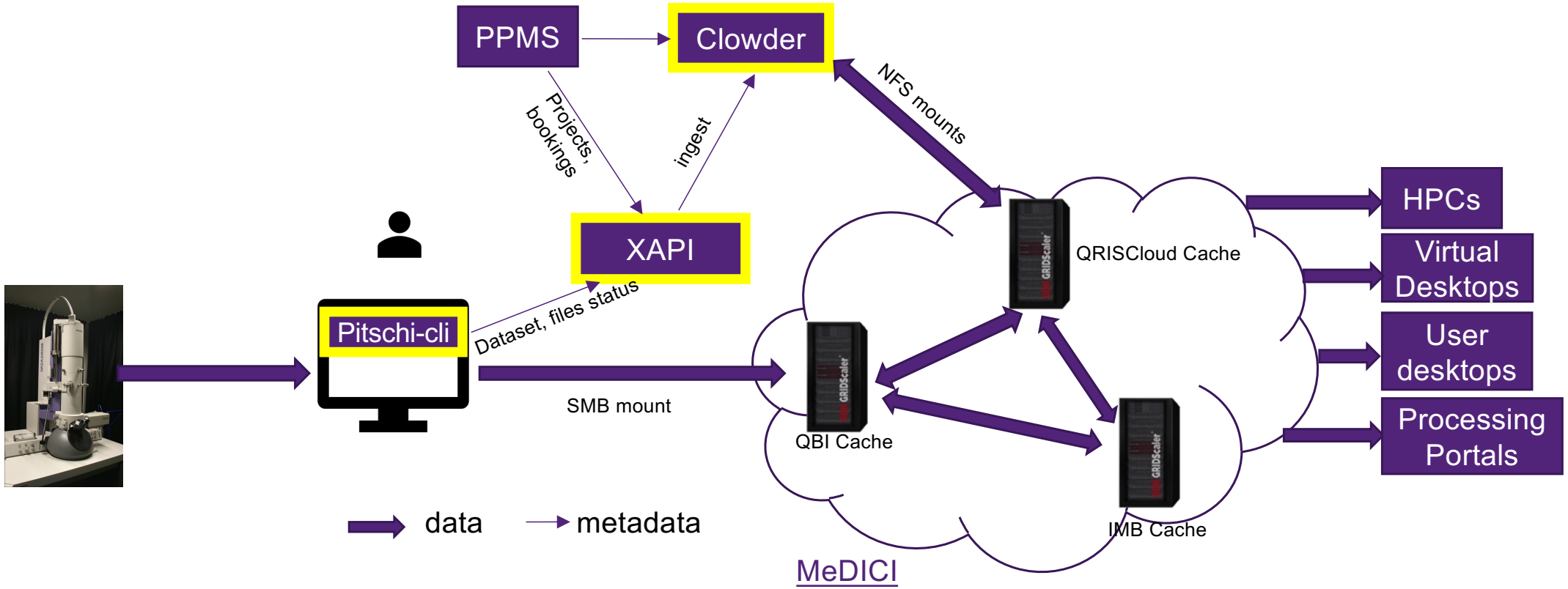






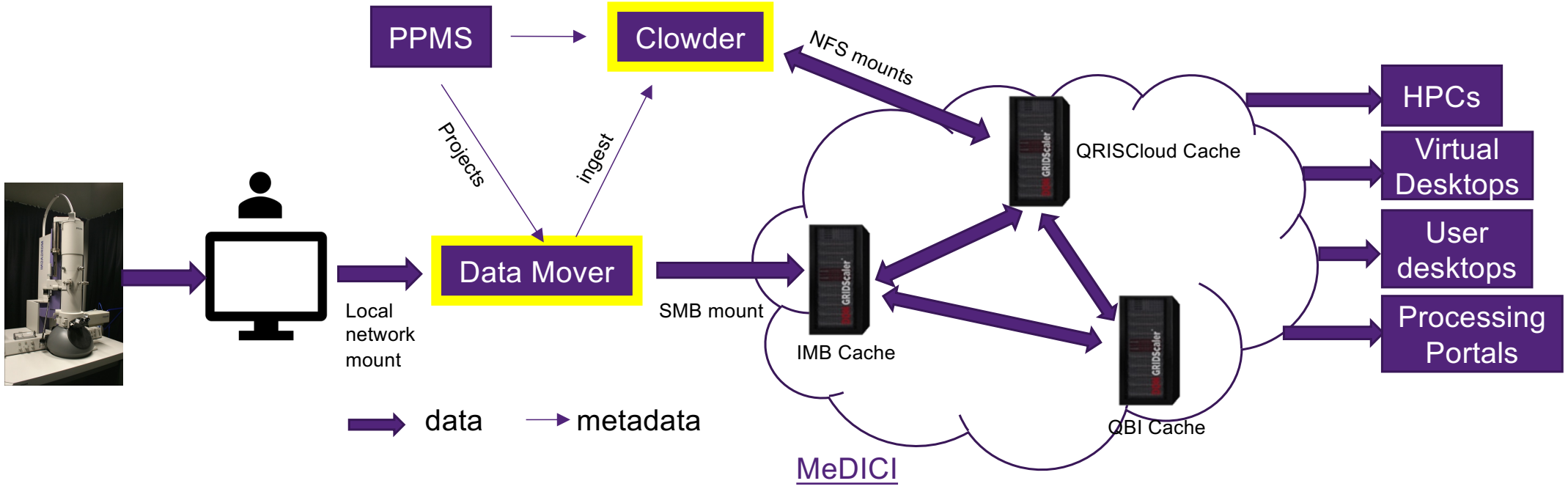
Pitschi – direct transfer

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

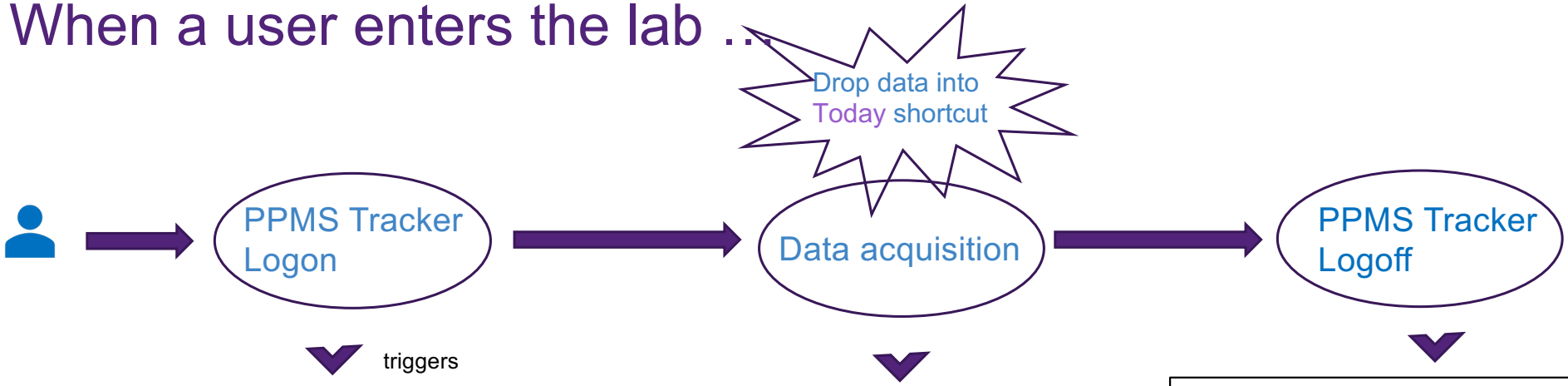


Pitschi – indirect transfer

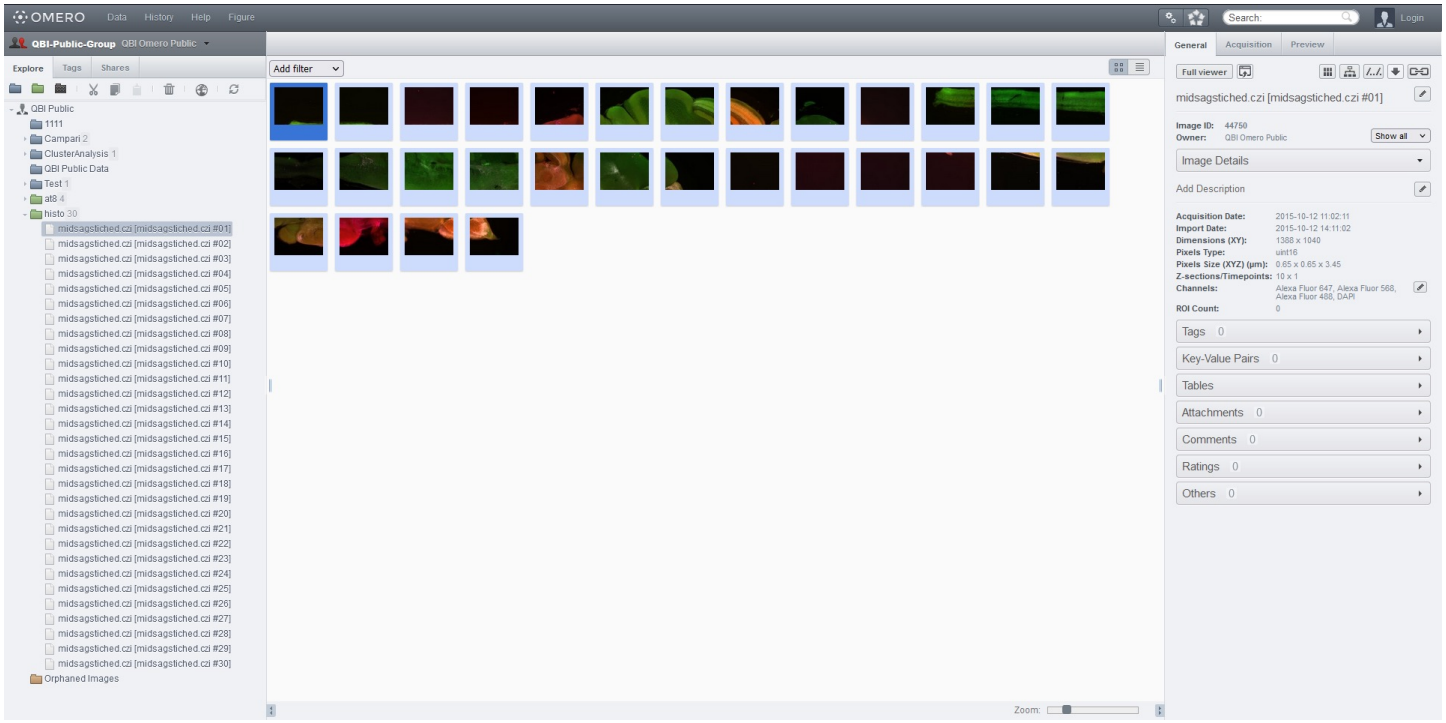
https://pitschi.rcc.uq.edu.au/



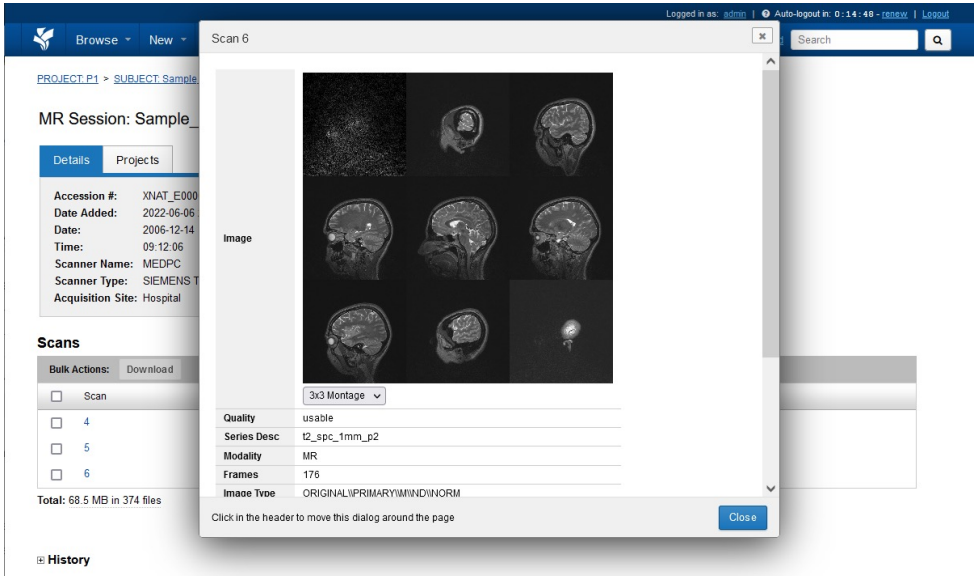
When a user enters the lab …

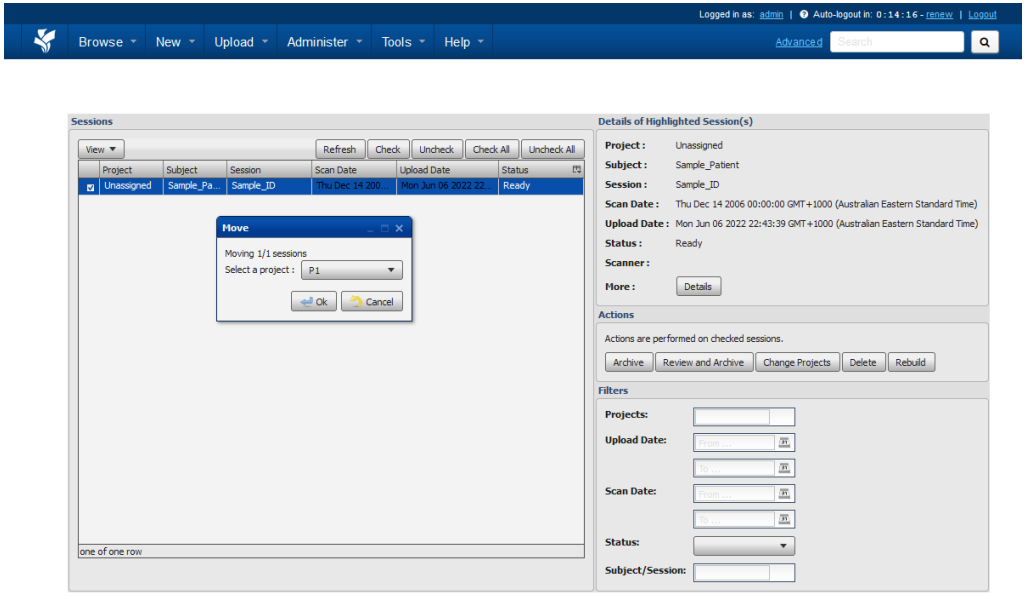


The UQ Open Microscopy Environment: OMERO

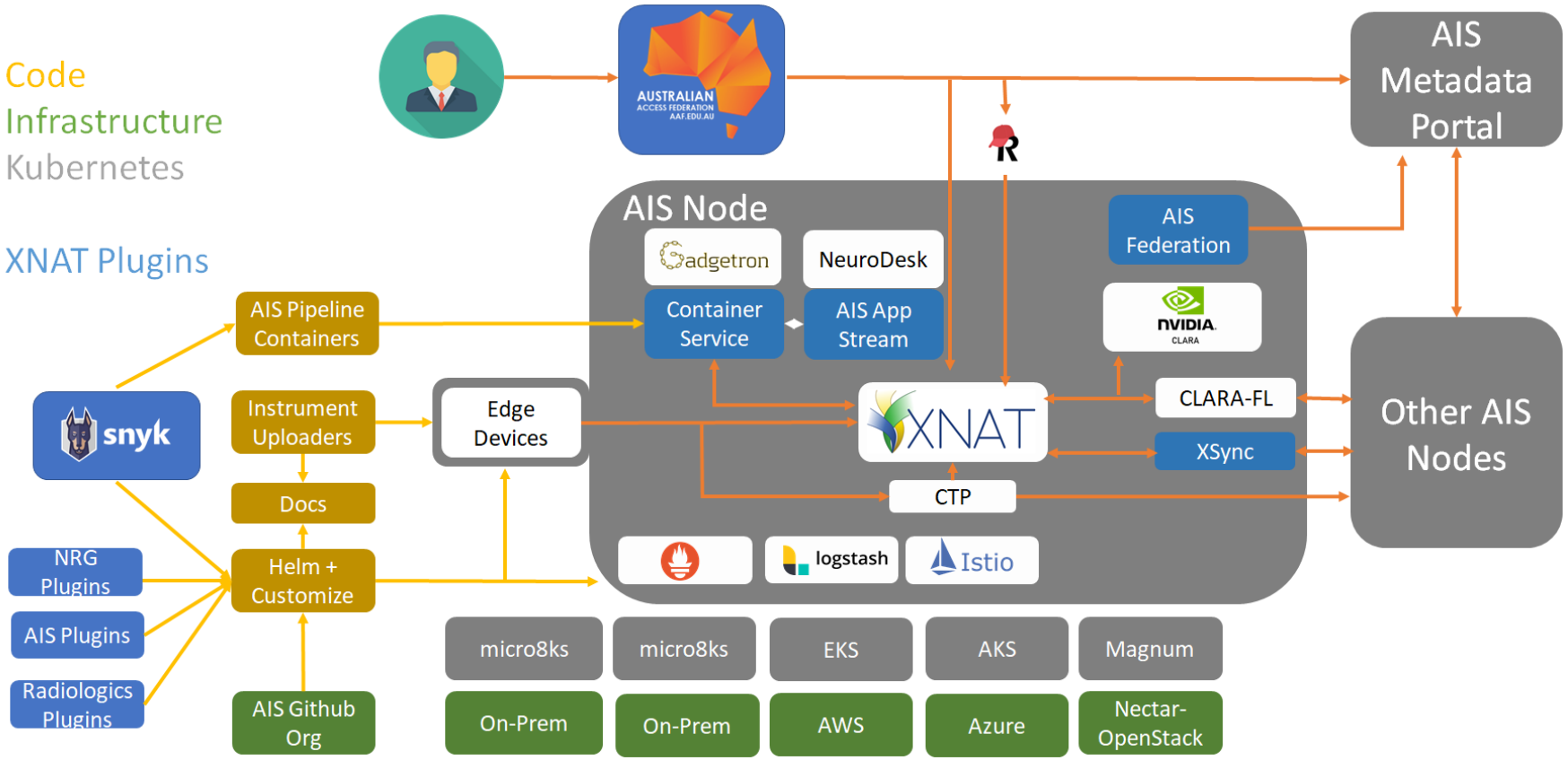


The UQ XNAT service





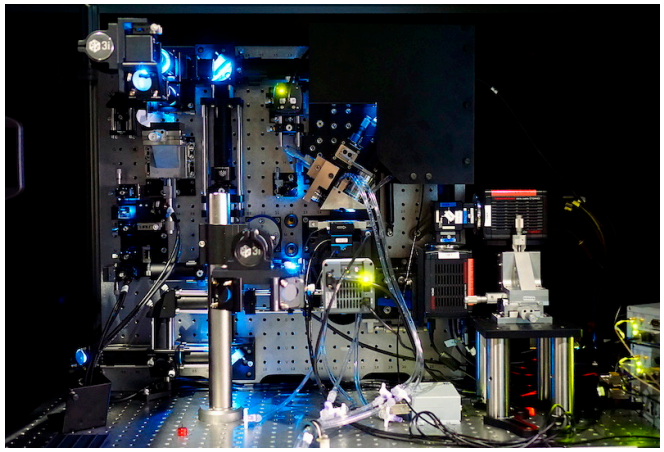
UQ XNAT: Under the covers



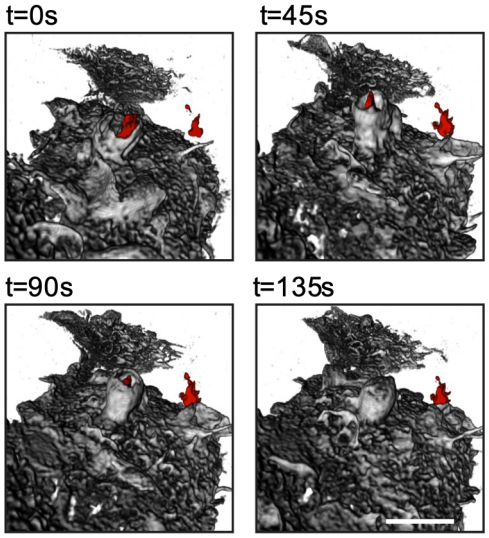
Case studies

Imaging immunology in near real-time

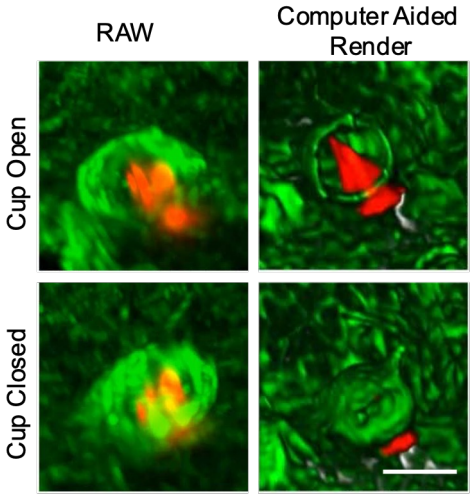
Nicholas D Condon
James Springfield
Deborah S. Barkauskas
UQ Institute for Molecular Bioscience



IMB: Janelia Lattice
Light-sheet Microscope



Yeast particle being engulfed by the macrophage cell

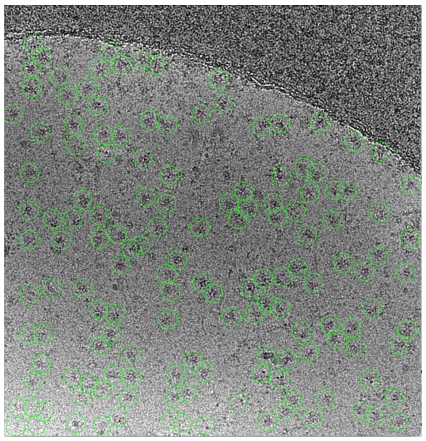


Two key stages of phagocytosis shown as both a RAW image maximum intensity projection (MIP) and as a computer aided 3D surface render

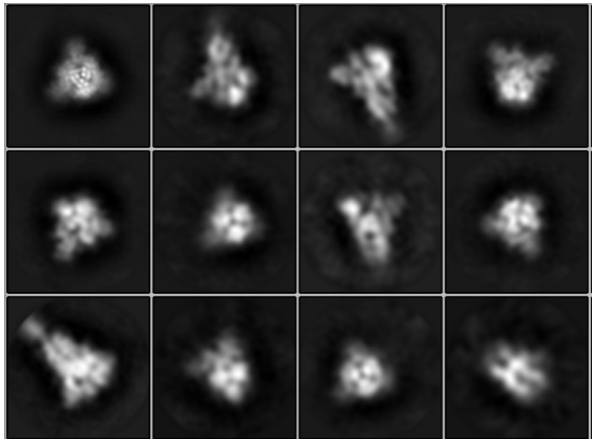
Cryo-electron microscopy for determining protein structure

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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AUSTRALIA
CREATE CHANGE

Thank you

David Abramson| Professor and Director
Research Computing Centre
David.Abramson@uq.edu.au
07 0000 000

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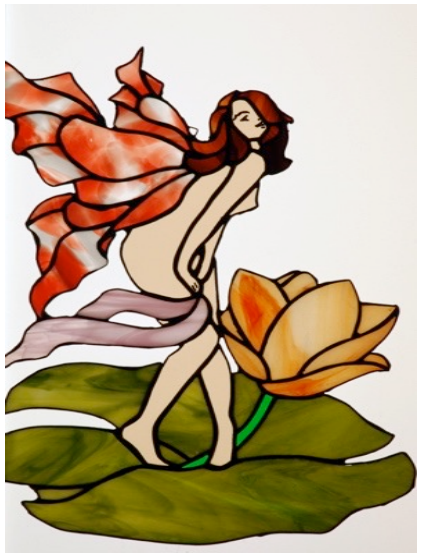
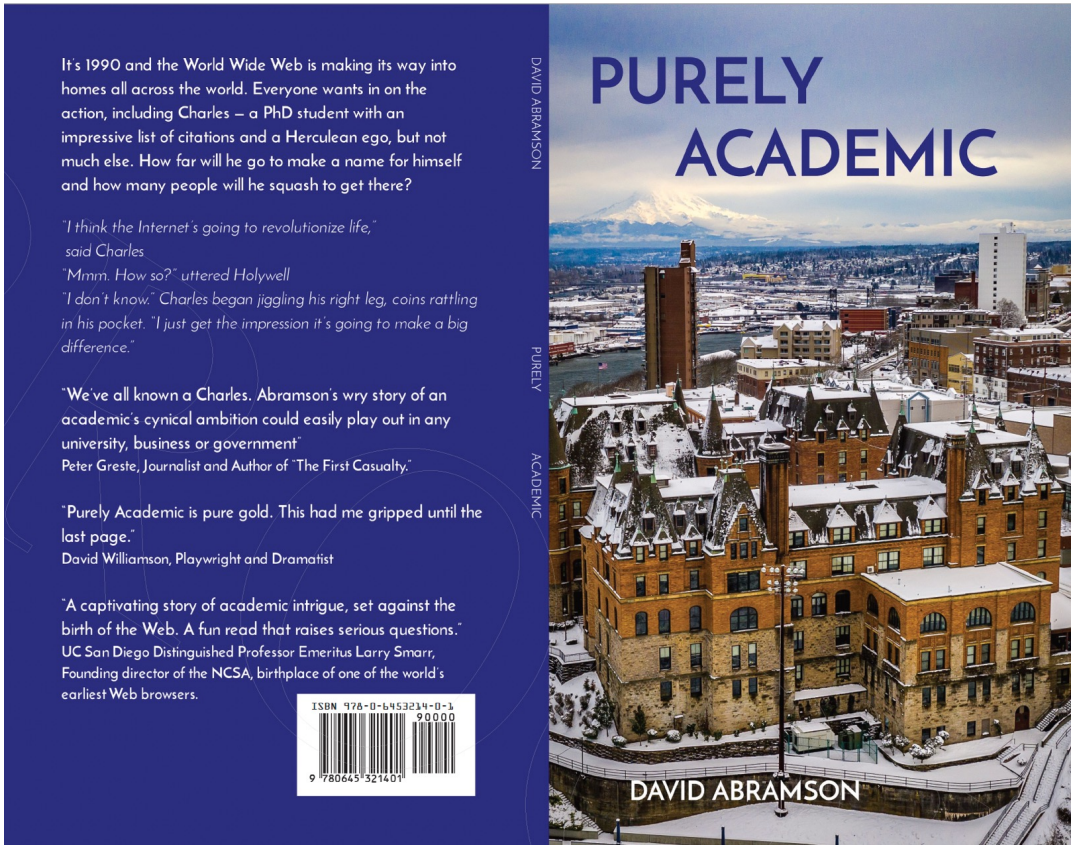
rcc.uq.edu.au

Thank you and Questions



Translation to the arts



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