An Australian Government Initiative

National Collaborative Research Infrastructure Strategy

ANFF

Surface analysis: new approaches to access, data and analyses

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La Trobe University,
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LA TROBE UNIVERSITY

Outline

- Project participants
- La Trobe University: research and instrumentation
- Remote access to instrumentation
- Creating an integrated, immersive environment
- Dealing with data
- Building a *Virtual Research Laboratory*

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Project participants

La Trobe University

- Paul Pigram
- Robert Jones
- Daniel Tosello

- Mark Kosten
- Emma Curtis-Bramwell

Victorian eResearch Strategic Initiative

- Chris Myers
- Michael D'Silva
- Conal Tuohy

- Ann Borda

Funding: La Trobe University
Victorian Government through VeRSI
Australian National Data Service

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La Trobe University

- 30,000 students across 6 campuses
- Victoria's 3rd oldest established University

La Trobe University

- The principal campus is located in Melbourne's northern suburbs

La Trobe's principal campus is 15 km from Melbourne's CBD


Physics and
Surface Science

Centre for Materials and Surface Science

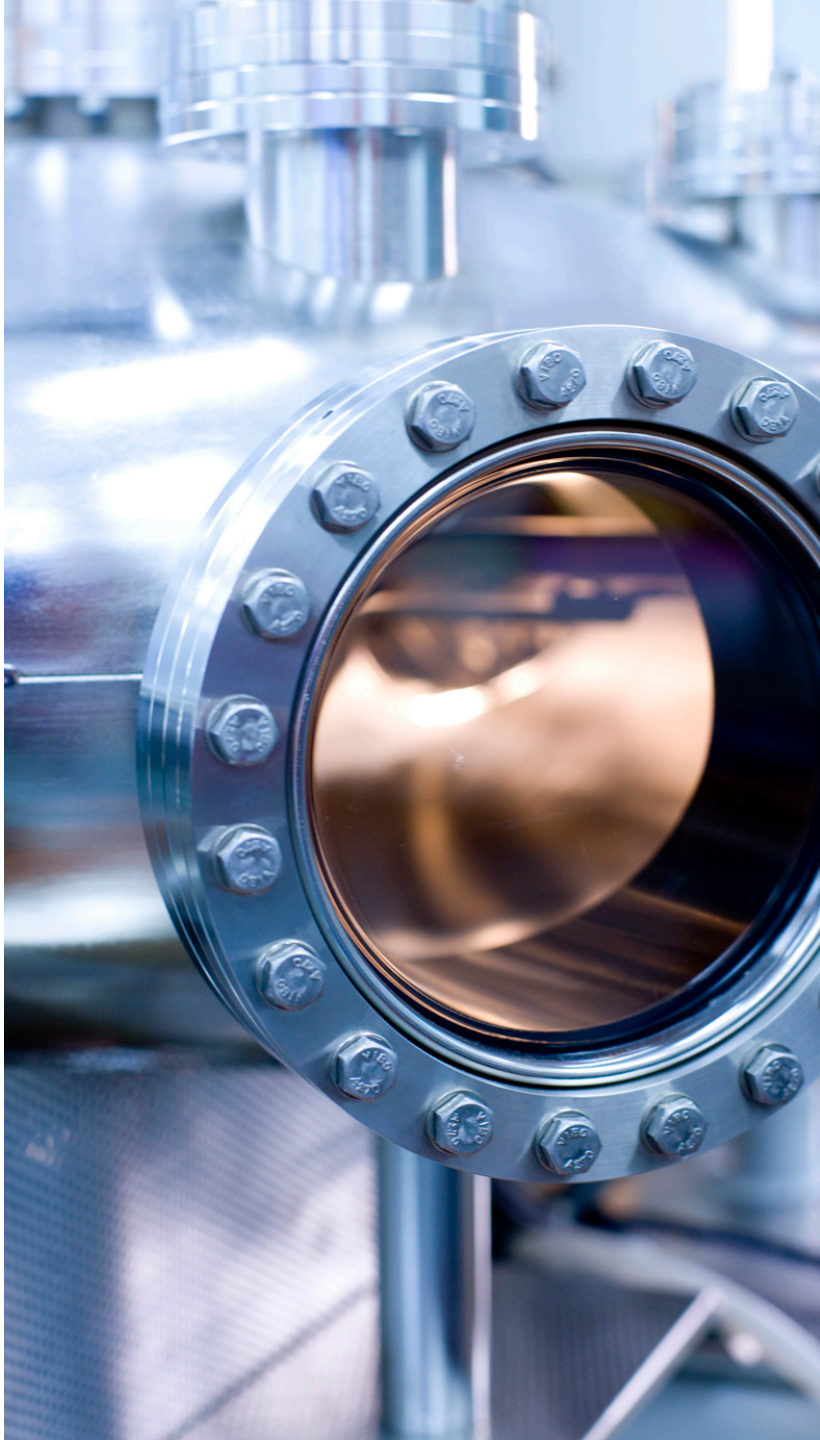
- Department of Physics
- Department of Chemistry
- Department of Electronic Engineering

- *Interdisciplinary research centre comprising 16 academic staff*

Our research program

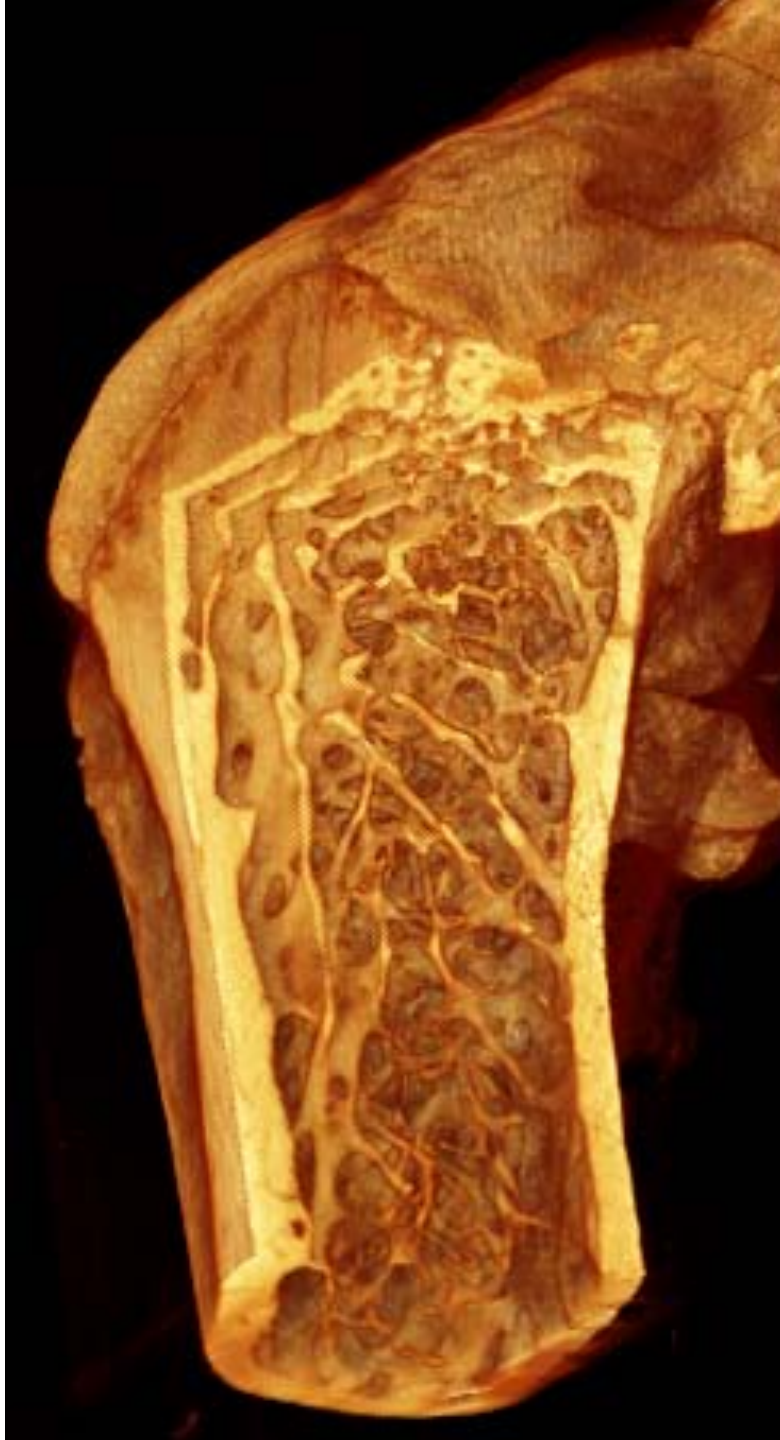
Surface science

- Molecular interactions at surfaces
- Carbon electronics
- Band structure studies of metals, alloys, semiconductors and magnetic materials
- Auger photoelectron coincidence spectroscopy
- Understanding bio-surfaces
- Functional nano-particle systems
- Understanding complex mineral systems at the nanoscale
- Electrochemical and electrochemiluminescent sensors



X-ray science

- Coherent diffractive imaging
- Phase contrast imaging
- Tomography - synchrotron and laboratory-based
- Nano-fabrication (partnering with MCN)
- Scanning X-ray Transmission Microscopy (STXM)
- ARC Centre of Excellence in Coherent X-ray Science



Key instrumentation

1. **High throughput XPS** (Kratos Nova, 2009)
2. **Imaging XPS** (Kratos Ultra DLD, 2007; + RDC)
3. **Time-of-flight secondary ion mass spectrometry**
   (Ion-Tof TOF-SIMS IV, 2002/2004; Bi, Cs/O sources)
   (Next generation ToF-SIMS funded 2012)
4. **Scanning probe microscopy** (Asylum Research, 2 systems, 2007)
5. **Synchrotron end-station** – toroidal photoelectron spectroscopy
   System 1 – Berlin (La Trobe, 2003)
   System 2 – Melbourne (La Trobe, commissioning 2011)
6. Ultrahigh vacuum **surface physics** instruments incorporating:
   - UHV SPM (Specs, 2007) + UPS, MBE, LEED evaporation etc
   - UHV cryo-SPM (STM + Q-Plus AFM) (Createc, 2008)
7. **Auger coincidence photoelectron spectroscopy** (Murdoch design)
8. **X-ray microtomography and imaging** (Lab-based)
   (2 systems, Xradia, 2006; Fein Focus, commissioning 2011)
9. **X-ray tomography end-station** (Xradia + La Trobe: APS Argonne)

Our challenges

- Building strong collaborations
- Supporting our international instrumentation
- Best practice in surface science
- Open access for our partners
- Dealing with all that data

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Remote access to instrumentation

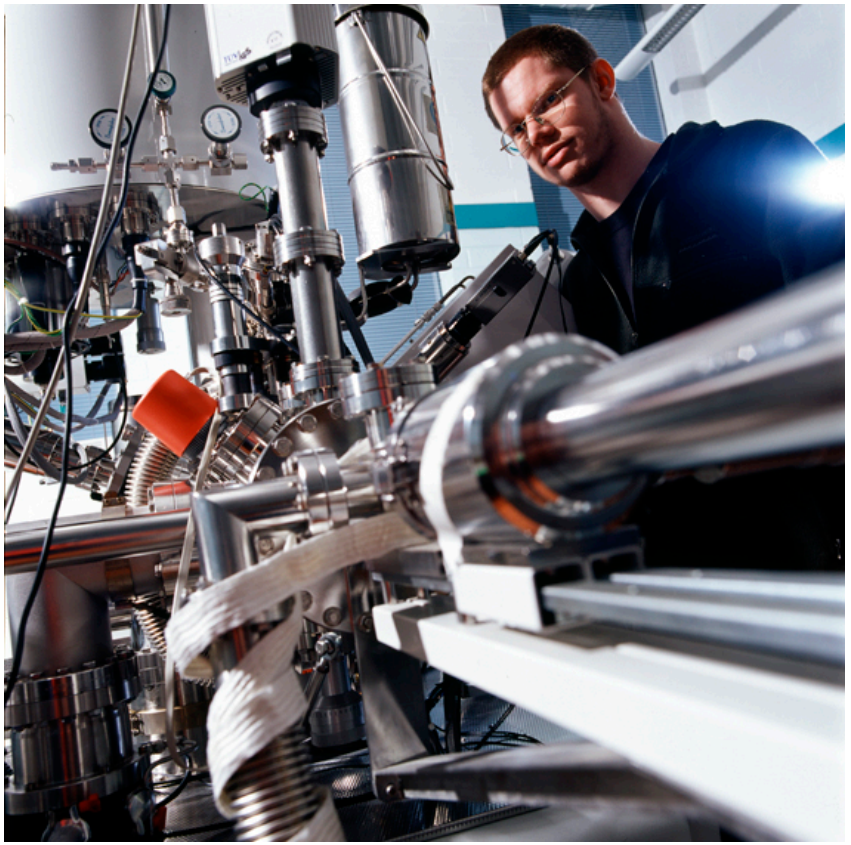
- Why do we need it?
- Why are we scared?
- What is happening now?
- What will be gained?

Why do we need remote access?

- Distributed, global research collaborations enabled by the internet (particularly activities centred around large instruments)
- Very large scale data sets - emergence of data repositories
- High performance computing resources are frequently used
- Collaborative visualisation of data.
- Tele-science (remote access and control of instrumentation)
- Aiming for best practice in distributed access

Goals

- User Friendly
- Safe
- Reliable
- Fast
- Modular design



Sharing a common platform

- La Trobe University
- Australian Synchrotron
- ANSTO
- Future partners

Bringing everything together

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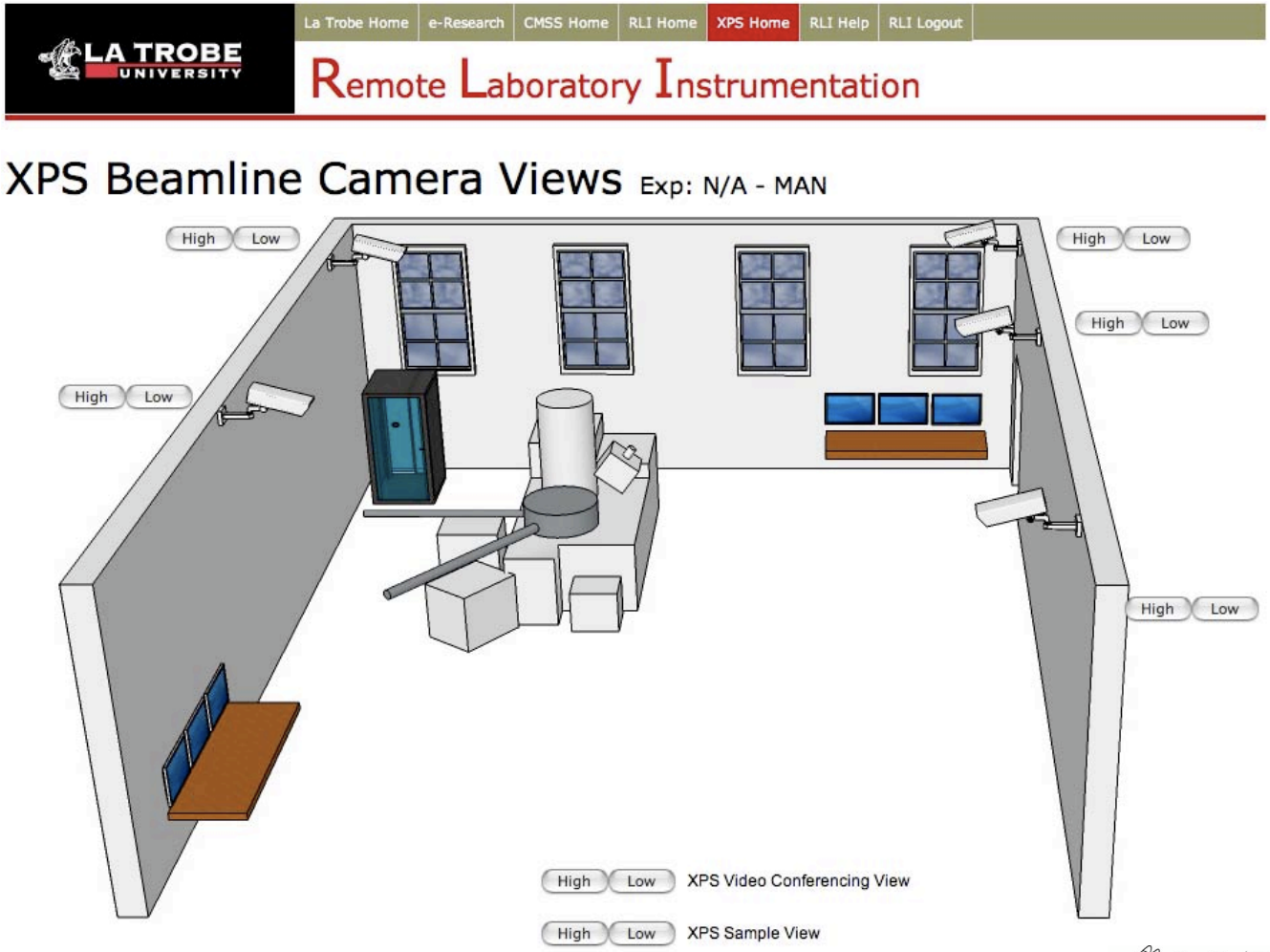
Building an immersive environment

- secure instrument remote control
- storage gateway
- data transfer services, metadata capture and repository integration
- videoconferencing / collaboration tools
- video streams - lab and instrument
- scheduling and access control
- training and induction
- laboratory information management

Building an immersive environment



Work Area Overview

- Video captured from the lab and instrument.
- Refreshes at close to video rate.
- WEB 2.0
- Camera views can be moved and resized.

Secure remote control - basic requirements

- Security critical for safe operations and instrument owner “buy-in”
- Avoid modification to proprietary datasystems
  (ie Kratos Vision)
- Ease of deployment to any user, anywhere
- Cost and quality of connection

comparison with current WebEx-based systems and KVM hardware

Secure remote control:
the La Trobe approach

- New XPS server hardware installed (Dell, rack mounted)
    - Connected to Kratos datasystem using a dedicated VNC link

      short run - high speed

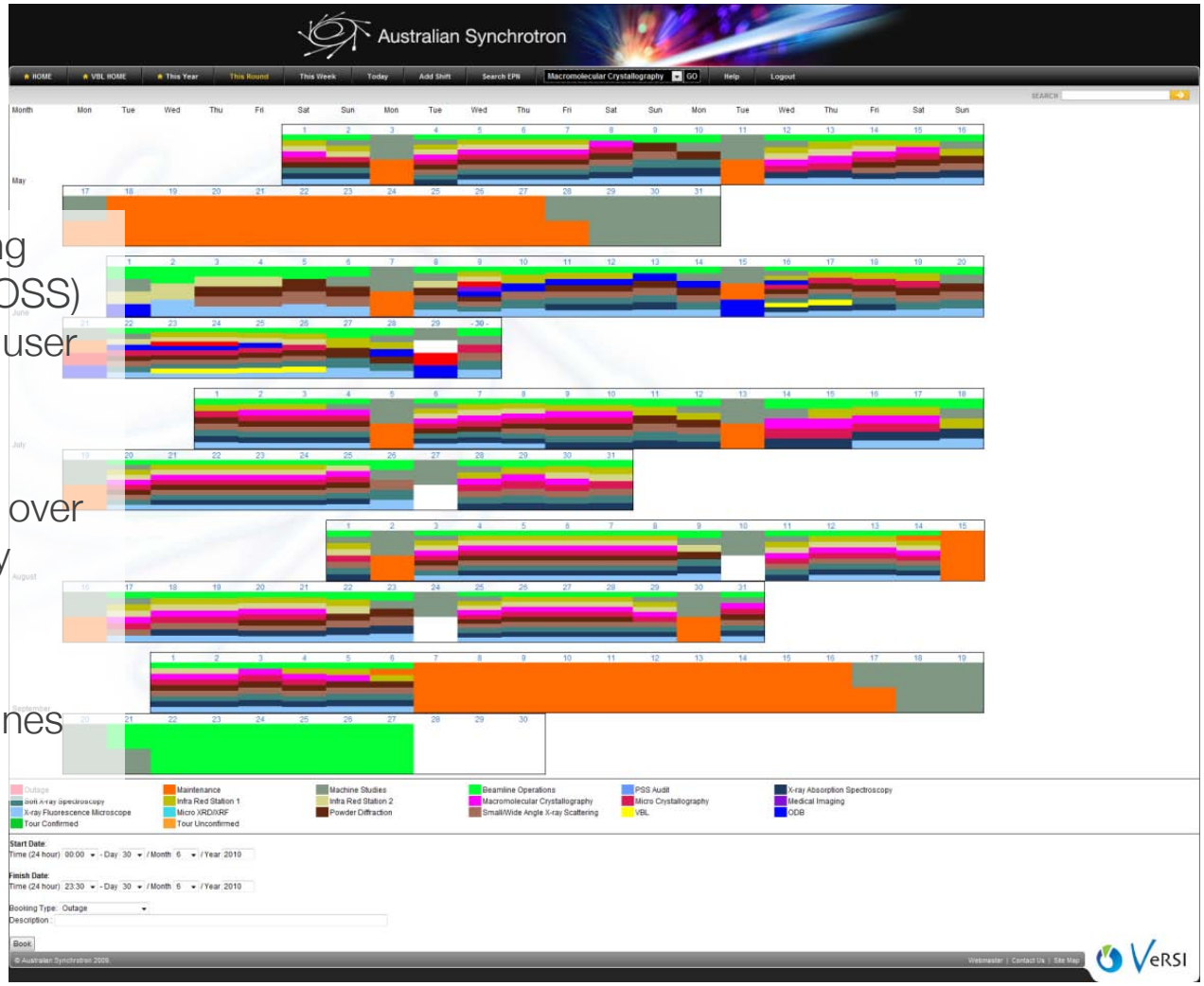
    - External users connect to server (“bridge”) using NX NoMachine (Linux X-windows)

      good long distance performance

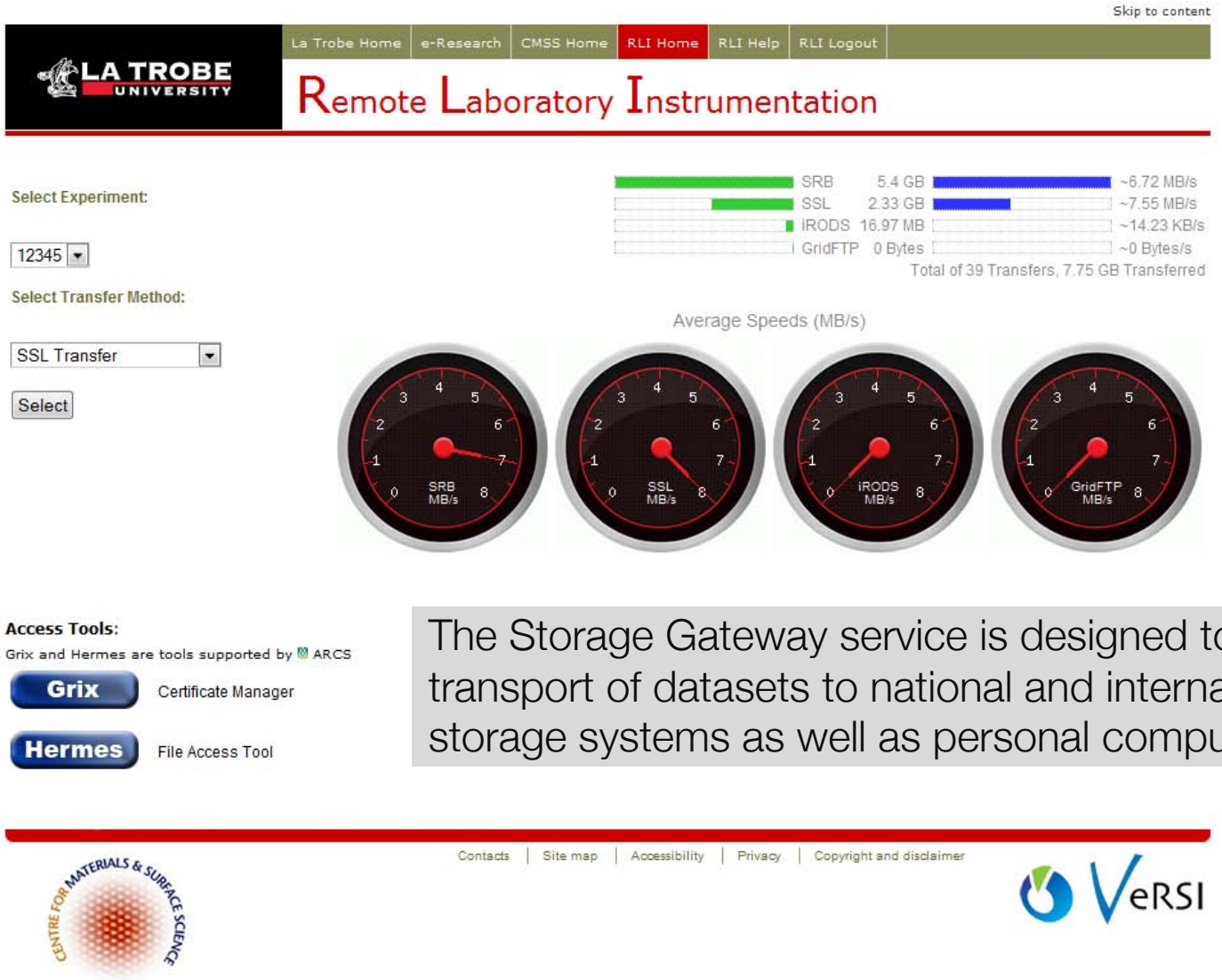
- Automatic deployment of NX NoMachine client

Beamline Operating Scheduling System (BOSS)

- The Beamline Operating Scheduling System (BOSS) is a tool for booking in user beamline activities.
- Now with user change over scripts for almost every beamline
- In use on all AS beamlines



Storage Gateway



The Storage Gateway service is designed to enables transport of datasets to national and international storage systems as well as personal computers

Video Collaboration

- Aethra Vega X7 H323 Video conferencing unit.
- 720p HD video images.
- Requires 4Mb bandwidth.
- enterprise reliability.
- VCBpro HD 12 port MCU deployed.
- VpointHD soft clients deployed and managed by MXM.

Video Collaboration

- Full web control integration.
- Displays Call Status.
- Allows camera selection local and remote
- Pan tilt functionality local and remote.
- Dual video.

VeRSI

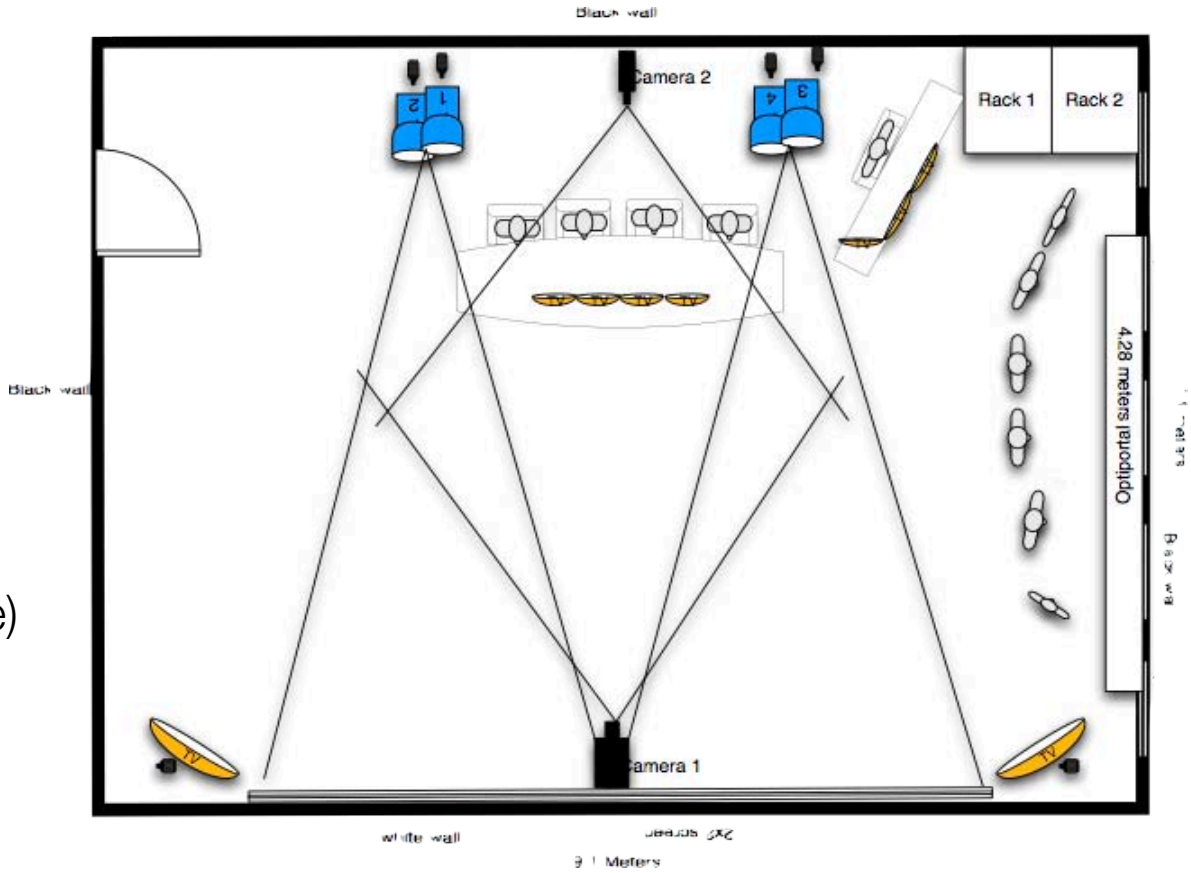
Australian Synchrotron
lighting the path to innovation

LA TROBE UNIVERSITY

Mission Control at La Trobe

Virtual Beam Line Lab

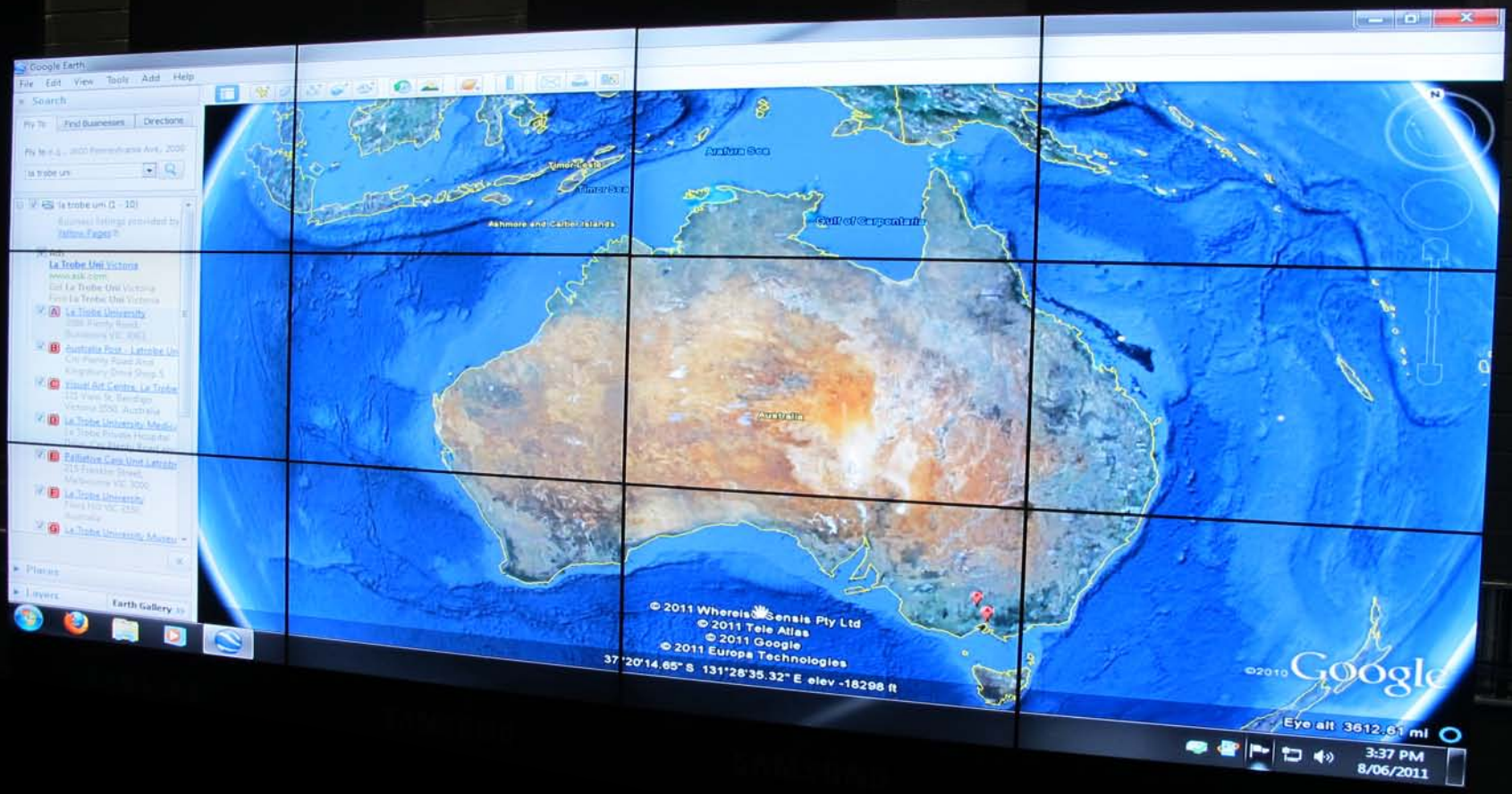
- Remote control suite
  - synchrotron beam lines
  - XPS instrument (RLI)
  - future remote access facilities
- Small groups (3-5 people)
- Class groups (~ 30 people)




XPS-Ultra Beamline Camera Views
XPS-Ultra Video Call

Data visualisation

- Display Wall
  - 12 HD displays tiled (4W x 3H)
  - 720p resolution *1280 x 720 pixels*
  - 2 mm bezel
  - Samsung display wall *integral mounting system*
- Data capacity
  - High spec Dell workstation with 2 graphics cards
  - Each screen individually addressable at HD
  - 11 million pixels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Australia
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Remote Teaching at La Trobe

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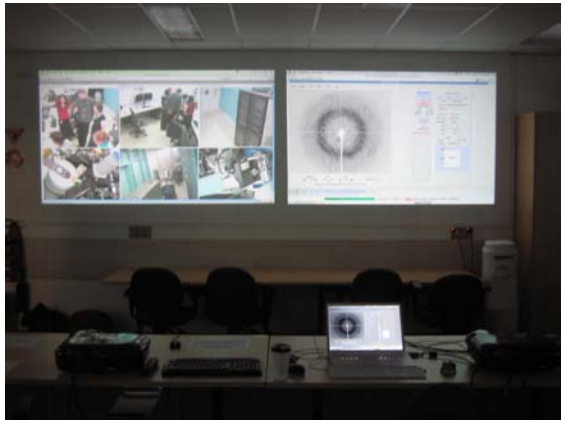
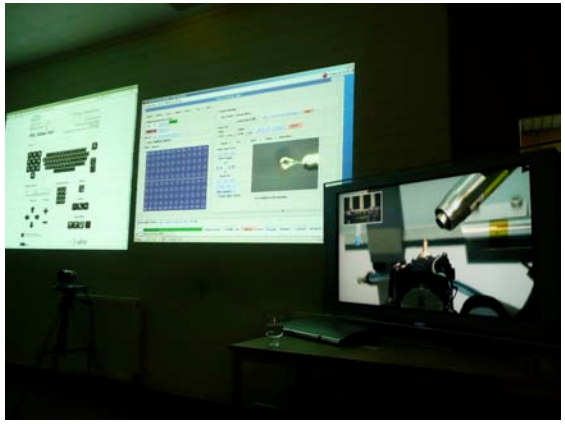
VeRSI



Australian Synchrotron
lighting the path to innovation



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Dealing with data

- There is a vast amount of it being produced …
- Obligations to store and publish original data
- Good data stewardship
- What are the obligations of the service provider?
- New opportunities for interrogating large datasets
  - Data mining
  - Open access databases (cf. mass spectrometry)
  - Multivariate analyses and similar

Building an integrated repository

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On-the-fly data capture

On-the-fly metadata capture

Integration with proprietary datasystems

Hierarchy of access

- Core group
- Institutional partners and clients
- Open access

Building an integrated repository

- Project funded by the
  Australian National Data Service (ANDS)

- Using a FEDORA repository

  - Originally developed at Cornell University
  - Open source international project
  - Very widely used for library and other data management internationally
  - Recognisable, robust and flexible solution

Harvesting and storing the data

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Data are collected by the ToF-SIMS instrument (for example)

Metadata is harvested from the data file and linked with user and project metadata

Data and metadata are passed to the repository using SWORD data deposit service

Data is stored in the native (proprietary) format or may be translated into an ISO standard-based format or specialist XML format

International standards for data

- *Surface Chemical Analysis Standard Data Transfer Format*
- Versailles Project on Advanced Materials and Standards (VAMAS)
- ISO 14976:1998
  Surface chemical analysis - Data transfer format

- This standard co-exists with a variety of proprietary data formats devised by instrument manufacturers

A next generation standard

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Current ISO standard

- Flexible and applicable to many analytical techniques
- Not constructed using a modern file format

A next generation standard

- XML-based
- Structured to allow easy database/repository integration
- Facilitate metadata search, and data mining

Potential applications

- Use the standard data format and repository to create large, open access data archives
- Use these for large scale multi-variate analyses
- Data sharing, better validation, better software tools

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Building a *Virtual Research Laboratory*

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Partners

- La Trobe University
- Australian Synchrotron
- ANSTO
- Deakin University + others
- International collaborators

Key tasks

- *Virtual Beam Line 2.0*
- Development of the integrated repository concept
- Roll out the remote access concept more broadly

Data

- Create an open access reference database as a pathfinder project
- Develop multi-variate analysis tools
- Support ISO and VAMAS standards modernisation

www.latrobe.edu.au/surface

www.versi.edu.au

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Providing nano and micro-fabrication facilities
for Australia's researchers