The “21st century microscope” will not be a single instrument; rather it will be an orchestration of specialised imaging technologies, data storage facilities, and specialised data processing engines. Moreover, scientists increasingly require access to a wide range of imaging instruments, across multiple modalities and multiple scales, to characterize a scientific sample or perform an experiment. The NeCTAR-funded Characterisation Virtual Laboratory (CVL) is developing software infrastructure to make it easier for researchers to make good use of this new landscape by providing easier access to the tools and techniques that they require to capture, process, analyse and visualise multi-modal imaging data.

The CVL is focused on three scientific domains: 1. Neuroscience led by the University of Queensland; 2. Energy Materials Atom Probe techniques (EM-AtomProbe) led by University of Sydney and Energy Materials X-ray (EM-Xray) led by Australian National University; and 3. Structural Biology (SB) led by Monash University. The project is working closely with member of the National Characterisation Council: the Australian Microscopy and Microanalysis Research Facility (AMMRF), the National Imaging Facility (NIF), Australian Nuclear Science & Technology Organisation (ANSTO) and the Australian Synchrotron (AS).

The CVL software infrastructure has been designed in three layers (Figure 1):

1) A remote desktop environment configured for scientific computing that is accessible across Australia and can be applied to a broad range of research areas;
2) Specialised releases of the desktop (or workbenches) that provide a range of the most common tools to a three scientific domains relevant to a specific domain; and
3) Specialised workflows that will drive the fabric in specific research areas.

Fabric: The Fabric is a managed desktop environment for interactive analysis and visualisation of multi-modal and multi-scale data. This environment is being developed for the general purpose NeCTAR Cloud, and specialised systems such as the Multi-modal Australian ScienceS Imaging and Visualisation Environment (MASSIVE), as well as other computing and data storage facilities. A minimal-functionality prototype of this
service, called the MASSIVE Desktop, has been developed for the MASSIVE system, and has proved to be popular amongst a range of MASSIVE users, including those analysing images in neuroscience, geology, materials science, paleontology, and biological fluid dynamics.

**Workbenches:** The Workbenches are the primary method that researchers interact with the CVL – they are specialised configurations of the Characterisation VL Desktop that gather a collection of tools that are important to that community.

The workbenches also include services and tools to integrate key Australian instruments with Australian computing infrastructure, including the NeCTAR cloud and MASSIVE. Integrating instruments means that researchers are able to easily move data from an instrument to the cloud or a HPC facility for data management, processing, analysis or visualisation.

**Multi-modal Workflows.** The three specialised workflows developed will leverage the underlying Workbenches, including integrated data management, and the underlying fabric, and will address a specific, but reusable, integration challenge for multi-modal or large-scale imaging.

**Neuroimaging Workbench**

The Neuroimaging Workbench is an environment that will provide researchers with a range of standard neuroimaging tools and new mechanisms to retrieve data from neuroimaging data repositories, such as DaRIS. In addition, it is creating specialised Galaxy workflows for more complex analyses that currently require significant installation and configuration effort. These more complex workflows will allow a user to create a minimum deformation average model, restack and re-align histological imaging data into a contiguous 3D block and co-register MRI image data with restacked histology data. Data for the Neuroimaging Workbench will be sourced primarily from instruments at NIF sites. This includes multiple clinical and pre-clinical MRI systems, PET and CT instruments. DaRIS federation capability will be used as a means to access data from remote DaRIS repositories at NIF nodes.

**Energy Materials – Atom Probe and X-ray Micro Tomography Workbenches**

The Atom Probe (EM-AT) workbench is helping scientists exploit the power of atom probe tomography to capture information at the nanoscale – and ultimately, at atomic resolution. There are approximately 50 tools identified that will be installed into the EM-AP workbench to be made available to the community. The instruments being integrated are the AMMRF’s two Electrode Atom Probes: LEAP 3000 Si and LEAP4000X Si, currently housed at the University of Sydney. AMMRF’s Data Management System (DMS) is being integrated with this system to capture the data. Galaxy is being used as the platform for workflow management. The outcome of this workbench will be that scientists will be more easily able to collect and analyse data currently only available to AMMRF researchers, students and visitors.

The X-ray workbench is gathering existing software, algorithms and recent research results for the analysis of energy materials tomographic data. The workbench is focused on the analysis of materials from X-ray micro-tomography, although in practice any 3D structural data can be processed. This workbench will allow researchers access to the ANU Research School of Physical Sciences and Engineering Department of Applied Mathematics’ extensive suite of tomographic analysis and data processing tools. Data processed by the workbench is sourced from the ANU Micro-CT (tomography) instruments and data capture tools.

**Structural Biology Workbench**

The Structural Biology workbench provides researchers with access to a number of interactive tools for processing protein crystallography and electron microscopy data. The project is integrating a number of instruments, including: a range of light and electron microscopes available at Monash University, and the Walter and Eliza Hall Institute of Medical Research; and in the future, instruments associated with the Victorian Clive and Vera Ramaciotti Centre for Structural Cryo-Electron Microscopy to be procured in mid 2013. In addition, the project integrates a number of further instruments by directly integrating the Tardis data management platform with the CVL – allowing researchers to export data from instruments such as Macromolecular Crystallography beamlines.

**Early Outcomes**

This presentation will outline early outcomes of the CVL. This includes:

- The successful uptake of the MASSIVE Desktop, a pre-cloud prototype of the CVL. The CVL work done on the MASSIVE Desktop has directly contributed to a strong over base of nearly 100 scientists from Australian Synchrotron, CSIRO, Monash University, and other research institutes across Australia.
- The development and uptake of the specialised Workbenches, a number of which are currently in user testing.
- The innovative technology that is being employed to develop this environment.