MARRYING A HIGH PERFORMANCE COMPUTER WITH SYNCHROTRON BEAMLINES

R. Farnsworth, Australian Synchrotron (ASCO), Melbourne, Victoria, Australia

Abstract

A high performance computing facility is being established to service the imaging needs of beamlines at the Australian Synchrotron. It is planned to schedule the high performance together with the experimental procedures in order to provide a near real time imaging response to experimental data collection. In this way significantly greater efficiency in the use of experimental facilities can be achieved. It is also intended to utilise the non scheduled beam time to provide a centre of high performance imaging excellence for other scientific imaging needs in the geographic region. A Petabyte data store, fast links to the researchers home institutes, an optiportal, 3d imaging resources, grid portals are also provided to researchers.

INTRODUCTION

The Australian Synchrotron is a major Australian national research facility that strives to provide equitable opportunity for engagement and involvement to as wide a community of stakeholders and scientists as possible.

The Australian Synchrotron Company has entered into a Grant Agreement with the Victorian government that will provide part funding for a high performance computer and imaging facility. This grant was by the Department of Industry Innovation and Regional Development based on a business case[1] presented by the Australian Synchrotron.

The Australian Synchrotron now plans to enter into collaborative venture with Monash University and the CSIRO[*] to create a combined national imaging and visualisation facility that will be known as MASSIVE. Funding for the collaboration additional to that proposed in the Australian Synchrotron business case will be provided by CSIRO, Monash University and the National Computational Infrastructure. MASSIVE will be governed by the three collaborating partners, and will jointly operate separate but interconnected High Performance Computer facilities, one located at the Australian Synchrotron and known as MASSIVE1, and the second located at Monash University and known as MASSIVE2.

USE CASES

The Australian Synchrotron has the following needs for an HPC facility:
- a state-of-the-art computation, imaging and visualisation centre at the Australian Synchrotron

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[*] Australia's *Commonwealth Scientific and Industrial Research Organisation*

designed to meet the exacting needs of scientists engaged in experiments at the synchrotron;
- a Supporting Program with elements of collaborative research engagement, support and training and outreach.

The science programs include
- Experimental work, including real-time image reconstruction, at the Imaging and Medical Therapies, Macromolecular Crystallography, Microspectroscopy, and the Small and Wide Angle Scattering beamlines
- Post-processing of images and data from these and other beamlines
- Software development work developing new parallel algorithms for reconstructing 3D phase contrast Computer Tomography (CT) images.

These needs will be satisfied by the MASSIVE collaboration, alongside a range of other imaging and visualisation applications put forward by Monash, CSIRO and the national community channelled through the NCI Specialised Facility program, using the interconnected MASSIVE1 and MASSIVE2 high performance computer facilities.

HARDWARE

Hardware will be purchased "off the shelf" from standard vendors in this space. It will be an approximately five Teraflop multiprocessor computer with a mix of conventional and non-conventional processors, a tightly-coupled disk storage system and an imaging resource. It will be available in early Autumn[†] of 2010.

SUPPORT

Operating and systems support will be provided by the Victoria Partnership for Advanced Computing and others under service level agreements.

Dedicated staff and other parties will provide specific user, coding and application support.

APPLICATIONS

A number of applications are planned for at the start of operations. Further applications are also being planned. The initial application software will include:

CTAS (For Medical Imaging)

This suite of applications is under continuing development and support by the Australian Synchrotron: CTAS package is a set of tools for the Computed Tomography (CT) and Tomothynsesis (TS) reconstruction for the parallel beam geometry as usually

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[†] The Southern Hemisphere Autumn of course

available at the synchrotron sources. It also contains additional tools for the various X-ray contrast manipulations such as Diffraction Enhanced Imaging etc.

X-TRACT (For Medical Imaging)

Computed Tomography Reconstruction reconstruction software under Continuing Development and support by CSIRO. It is an image analysis and processing application with functionality targeting researchers working in imaging science and technology fields, especially in optical, electron and X-ray microscopy and astronomy.

GEOpixie (For Microspectscopy)

This software is based on IDL and for quantitative and non-destructive Particle- Induced X-ray Emission (PIXE) analysis and imaging. It needs to be parallelized.

Fluorescence Tomography (For Microspectscopy)

To be developed in house, similar in concept to CT, giving cross-sectional information about a sample) but based on fluorescence measurement and requires an additional dimension of processing.

MASSIVE USAGES BREAKDOWN

Figure 1 shows the anticipated percentage use by activity. It is anticipated the other applications will arise over time.
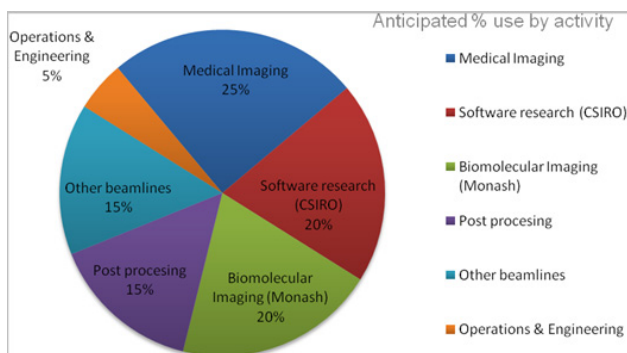

Figure 1: Usage breakdown pie chart.

In order to control the data collection and optimise the experimental conditions on the Imaging and Medical Beamline (IMB) scientists have to be able to visualise the data in near real-time, or, the experiment is in progress. The images captured by detectors at the IMB are very large and necessitate the movement of data sets in the terabyte range. These constraints dictate that significant computing power is available "on demand" and that the computer is tightly coupled – physically and electronically – to the detectors on the experimental rig.

The facility will position scientists using the IMB at the forefront of real-time 3D imaging of synchrotron data. Research in the area of phase contrast computer tomography being undertaken by CSIRO and Monash University, in conjunction with the Australian Synchrotron, will lead to new and powerful software tools for generating exquisitely detailed 3D images. CSIRO is a

world leader in the development of algorithms for reconstructing phase contrast CT images (tomography is imaging by sections or sectioning) that are optimized for parallel architectures such as the proposed MASSIVE computer.

It is anticipated that scientists using the IMB will generate 25% of the MASSIVE1 computing load. A further 20% of the machine time will be devoted to CSIRO for imaging software development and 20% to Monash University for use by the planned Imaging Consortium Facility. It is anticipated that both CSIRO and Monash will provide in-kind support for the centre by providing staff to MASSIVE and both parties have indicated as such.

PETABYTE DATA STORE

A multi Petabyte data store is being procured to provide long term storage for the data one processed and curated.

It is anticipated that this store will be one of a number of national co-operative data silos that contain either the raw experimental data set or the processed experimental data. Efforts are being made though national initiatives to provide Storage brokers to index the data both stored at the Synchrotrons and at other research institutes. One such collaborative venture, used for Raw X-ray diffraction images is the TARDIS ventures. [2]

NETWORKS

The Australian Synchrotron has dedicated connections in to Victorian Education and Research Network (VERN) [5]. This optical fibre will link almost 120 research and tertiary education sites across metropolitan and regional Victoria. Three institutes are actively connected.

The Australian Synchrotron is also linked to Australia's Academic and Research Network (AARNET) for general access to the rest of the country.

OPTIPORTAL AND VISUALISATION

An Optiportal is a tiled display, that is, many displays capable of acting as one or many virtual displays. Used in a wide variety of visualization approaches; viewing high definition static images, video, or in streaming mode. Experiments are currently being undertaken to determine best applications at the Australian Synchrotron. A relatively modest 0.369 Gigapixel optiportal is in operation and has been used to:

- Host remote lectures
- Promote collaborative research
- Display Protein and other Crystal structures in enormous detail
- As a display tool.

Currently the 3d imaging experiments have not proven enormously useful.

REFERENCES

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[5] http://www.vernet.net.au.