



The Faculty of IT and the Monash e-Research Centre are proud to present the following seminar - part of the High Definition interactive video links of MURPA Seminar Series 2010

## Workflows for Computer Aided Drug Discovery: New Twitter for the Old Problem Presented by Dr Wilfred Li

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The Computer-aided drug discovery (CADD) is becoming more accessible with the availability of personal supercomputers, especially given the recent advancement in GPU computing. The cloud computing infrastructure represented by Amazon EC2 offers an attractive solution for those who only require intermittent access to computing resources on demand.

We have continued to use the Avian Flu Grid infrastructure to study inhibitor development for influenza pandemics. The associated research and development effort from NBCR, PRAGMA projects explores the deployment of scientific applications as services, and the use of 'workflow tools' such as Vision, Kepler, Nimrod/K and Vistrails to support the service mashups often required to support the CADD process. The central toolkit that provides a Web Service based simple protocol for these different workflow clients is the Opal toolkit, an open source software available at [sourceforge.net](http://sourceforge.net). Our effort has resulted in a prototype CADD workflow software based upon Vision, but the underlying services are accessible from a number of other clients.

The availability of these scientific application services advances the cyberinfrastructure for biomedical research and generates more requirements for focussed, user friendly scientific research and collaboration environments (including ways to build and/or leverage the social networks like Facebook, Twitter, LinkedIn and Google Wave for scientists.)

**Date:** Friday 30 April

**Time:** 10am-11am

**Location:** Seminar Room 135, Building 26,  
Clayton campus

**Registration:** [Debra.Truin@adm.monash.edu.au](mailto:Debra.Truin@adm.monash.edu.au)

### MURPA Seminar Series 2010

Monash Undergraduate Research Projects Abroad (MURPA) supports a unique summer mode placement in a leading research group overseas. It not only provides a research experience at the undergraduate level, but does this in an international context. Students are placed for a period of eight weeks allowing them to integrate into the research groups as team members.

MURPA also involves an advanced seminar scheme, in which students can attend seminars given by world leading experts before they leave. The seminar scheme is novel, because it uses a cutting edge High Definition interactive video links with the University of California - and often simultaneous links to Japan - making it feasible to attract some of the world's best researchers "virtually" to Monash. These seminars also allow students to "meet" potential UCSD mentors and obtain information about possible projects.

<https://messagelab.monash.edu.au/MURPA/MURPA2010>