



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

# Multiscale Modeling of Proteins Presented by Dr Robert Konecny

Computing Systems Management, Computer Science Researcher,  
Center for Theoretical Biological Physics, UCSD  
Biography: <http://www.messagelab.monash.edu.au/KonecnyMURPA2010>

The biological activity within living cells encompasses the interaction of molecules from nano to macroscale, both in length and time. To gain a comprehensive insight into these interactions it is necessary to use tools which can span multiple length and time scales.

The talk will cover our research into large scale motions of viral capsid particles (Cowpea Chlorotic Mottle Virus, CCMV) upon maturation and the role of electrostatics in this process. To investigate long time scale interactions techniques like Brownian dynamics are used. We have employed this approach to perform long time scale simulations of an important enzyme, protein kinase A (PKA).

All these methods rely heavily on state of the art computational technology and sophisticated programming algorithms, including massive parallel schemes. An outline of how we are using these methods in our applications will also be presented.

**Date:** Friday 16 April  
**Time:** 10am-11am  
**Location:** Seminar Room 135, Building 26,  
Clayton campus

**Registration by 15 April:** [Rob.Gray@infotech.monash.edu.au](mailto:Rob.Gray@infotech.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>