

## **Seminar Outline: e-Xemplar: Protein Structure - Grid Computing in Structural Biology**

Determining the 3D structure of a protein using the technique of X-ray crystallography can be computationally intensive. My lab has developed methods that speed up this process by a significant factor by utilizing existing computing power in the laboratory, on campus, and even across the globe. Protein Crystallography generates a large amount of raw diffraction data, which must be annotated and archived. However the large size of a dataset (typically >30 Gb) presents challenges. We are addressing this in Australia using a federated database approach, representing the first real repository solution for the protein crystallography community.

### **Biography: Associate Professor Ashley Buckle**

A/Prof Ashley Buckle completed his PhD in 1994 in the lab of Prof Sir Alan Fersht at Cambridge University, where he focused his research on the structure determination of ribonuclease-DNA and protein-protein complexes. As a postdoctoral then staff scientist at the MRC Centre Cambridge he made contributions to the understanding of protein stability, molecular recognition and the action of molecular chaperones. He relocated to Monash in 2003 and is currently a NHMRC Senior Research Fellow. His current research is split between structural studies of a variety of interesting biological systems (using protein crystallography), crystallographic method development, and bioinformatics."