



Nanoscience and High Performance Computing

High Performance Computing is used in nanoscience to investigate the relationship between the size, shape and structure of nanoscale materials (nanomorphology) and the thermal and chemical environment to which they are exposed. Through the use of VPAC's High Performance Computing facilities researchers at the Royal Melbourne Institute of Technology (RMIT) and the University of Melbourne were able to gain an insight into how these materials can be predicted, controlled and manipulated by varying physical parameters.

<<< Nanoscience in High Performance Computing

Winner of the 2008 L'Oreal Australia for Women in Science Fellowship and RMIT 2008 Alumnus of the Year, Dr Amanda Barnard has recently been awarded the International Union of Pure and Applied Physics (IUPAP) 2009 Young Scientist Prize in Computational Physics. This award is to be presented to Dr Barnard in December 2009 at the Conference on Computational Physics in Kaohsiung, Taiwan.

These recent awards acknowledge Dr Barnard's international contributions to nanoscience and nanomorphology - the study of the structures, shapes and crystal structures of materials at the nano scale.

While completing a Ph.D in Physics at RMIT in 2003 and as a Future Generation Fellow at the University of Melbourne in 2008, Dr Barnard used VPAC's supercomputing facilities to combine analytical theoretical modeling and high performance computer simulations to examine the structure, shape and phase of materials at the nanoscale and explore their stability with respect to their chemical environment.

The results of her research provided fundamental insight into how nanomorphology may be predicted, controlled and manipulated by varying physical parameters (such as temperature, composition, surface chemistry, defect density or agglomeration), allowing for the generation of predictive models of the stability of nanostructures when exposed to ecosystems. This provides a basis of a more systematic approach to the assessment of risk associated with possible nanohazards.

In an interview with ABC's Catalyst which was filmed within VPAC's High Performance Computing Facilities and premises on Thursday 9th July 2009, Dr Barnard noted in reference to nano images, that such modelling would not be possible if it were not for High Performance Computing facilities such as those at VPAC.

Since finishing her research at the University of Melbourne Dr Barnard has focused her attention as the Leader of CSIRO's Virtual Nanoscience Laboratory, which is part of the CSIRO Material Science and Engineering Division.

Further Information

For further information regarding this project or for information on VPAC's Advanced Computing solutions and services, please contact Systems at help@vpac.org or phone +61 3 9925 4410, or visit www.vpac.org.

