

MURPA Seminar Friday 3rd September 2010 at 9am (please note earlier time - from Illinois)

Venue: Seminar Room 135, Building 26 Monash Clayton

Subject: Using Virtual Machines to accommodate Computational Chemistry in courses and classrooms.

Speakers: Dr Edee Wiziecki, Cybereducation Lead National Center for Supercomputing Applications(NCSA), at University of Illinois and R. Jay Mashl, Research Scientist and Lead ICLCS Instructor

#### Abstract

The Institute for Chemistry Literacy through Computational Science (ICLCS) is a 5-year NSF-funded project to bring research-level computational chemistry tools to pre-college and college classrooms. Over the past 4 years, we have collected data from standardized tests that show we are positively impacting pre-college student achievement by enhancing the content knowledge and pedagogy of their teachers (ICLCS Fellows). And, we have growing numbers of undergraduate students at Illinois utilizing our resources in their chemistry courses.

One of the computational tools used by our program's Fellows and their high-school students is WebMO, a web-based interface to quantum chemistry software, such as Gaussian and GAMESS that empowers users to construct and visualize molecules and to obtain various properties. The primary advantage of the web interface is that inputs are generated and output files are parsed automatically, helping to hide the complexities of handling data, thereby enabling the users to focus on the chemistry content and enhancing the learning experience. In order to meet the computational demand imposed by potentially thousands of students and other users simultaneously, a number of design challenges in service availability, throughput, and scalability where needed to be solved. The result was the development of a highly scalable, high-performance computing prototype configuration utilizing virtual machine technology for hosting a modified version of WebMO. In this talk we will present some of the details of the underlying architecture and also ways in which it has been used at workshops and in classrooms.

#### Bios:

Edee Norman Wiziecki

Edee Norman Wiziecki, co-Principal Investigator and Project Director of the Institute for Chemistry Literacy through Computational Science, directs the education program for the National Center for Supercomputing Applications on the campus of the University of Illinois at Urbana-Champaign. She leads the team whose mission is to bridge the gap between research and education. The team conducts a wide variety of activities and programs including those that disseminate advanced information and communication technologies to new and established communities. For the past 15 years, Ms Wiziecki has directed the Girls Engaged in Math and Science Program to encourage girls to enter STEM careers, and has developed numerous programs using virtual communities for teaching and learning.

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R. Jay Mashl

Jay Masl is a Research Scientist at the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign. As an author of several scientific publications in modeling and computer simulation, he brings a researcher's perspective to using computational tools in education. He is a co-developer of a computational prototype of a virtualized version of WebMO, a popular web interface to computational chemistry software. He is also an instructor in computational tools at the Institute for Chemistry Literacy through Computational Science (ICLCS) program.

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