PRISM Seminar Series – Spring 2012

PRISM
NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems

PURDUE UNIVERSITY Discovery Park

"Modeling Batteries and Quantum Dots"

Thursday February 23, 2012
9:00 am, Birck 1001

Richard Muller
Computational Chemist
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Abstract: This talk will cover two very different areas where computational modeling can help guide experiment. The first concerns Li-ion batteries, which are increasingly used as a way to reduce the carbon footprint associated with transportation, but which can, under abusive conditions, pose a safety hazard. I will discuss efforts at Sandia to develop a predictive modeling capability for battery safety, starting with atomic-scale density functional theory and connecting through the mesoscale to continuum-level cell simulations.

The second area concerns electrostatically-gated quantum dots in Si, which we pursue at Sandia as candidate qubits for quantum computing. We have developed a CAD capability that targets the specific issues related to simulating low-temperature, few-electron quantum dots as a way to accelerate experimental development of these devices. This capability can be used for Poisson and Schrodinger-Poisson simulations of quantum dots, and can also output external potentials for use with Purdue's NEMO program. I will discuss what the code does, and opportunities for collaboration with Purdue researchers.

Bio: Rick Muller (rmuller@sandia.gov) is a computational chemist whose research interests involve using linear algebra techniques to make electronic structure calculations faster and more accurate. He has a Ph.D. from the California Institute of Technology, where he applied pseudospectral techniques to accelerate quantum chemistry calculations, and used subspace techniques to accelerate wave function convergence. Since then he has focused on approaches to speed the eigenproblem in these calculations, and especially on techniques that use the density-matrix.

He is the lead of the PyQuante project that implements quantum chemistry algorithms in the Python programming language to make them easier to learn, understand, and improve. Many of the phenomena he has described above involve too many atoms or occur for too much time to describe purely with quantum chemical methods. His work of late has increasingly been interested with developing techniques in multiscale modeling to coarse-grain information from atomistic techniques so that it might faithfully be represented in mesoscale and continuum techniques. His graduate work developed faster algorithms for two-electron integrals in electronic structure algorithms using pseudospectral approaches, as well as faster convergence techniques, work that is currently released in Schrodinger's Jaguar program. As a postdoc, he investigated QM/MM methods for enzyme catalysis. he has also considered some improved methods for QMC simulations.

Refreshments will be served. For further information please contact Prof. Alina Alexeenko, alexeenk@purdue.edu
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