

**4th International Workshop on  
High Performance Computing for  
Nanoscience and Technology**



# **HPCNano|08**

**In Conjunction with IEEE/ACM SC|08,  
Austin Convention Center, Austin, Texas  
Nov. 21, 2008  
Room 13 A/B**

**Sponsored by NSF-CISE, DOE-LBNL, UIUC-NCSA,  
University of Iowa**



# Technical Program

**Session Chair: Osni Marques**

**8:30AM-8:40AM**

**Opening (Welcome Message) from Workshop Chairs**

Andrew Canning, Lin-Wang Wang (Lawrence Berkeley National Laboratory),  
Jun Ni (University of Iowa)

**8:40AM-9:00AM**

**The View from Washington: DOE SciDAC and INCITE Programs in Computational Nanoscience**

Lali Chatterjee, Program Manager, Computational Science Research and Partnerships (SciDAC) Division - Office of Advanced Scientific and Computing Research  
U.S. Department of Energy

**9:00AM-9:30AM**

**Quantum Algorithms for Modeling the Properties of Nanocrystals, Nanofilms and Nanowires**

James R. Chelikowsky, Center for Computational Materials, Institute for Computational Engineering and Sciences Departments of Physics and Chemical Engineering, University of Texas, Austin Texas

**Abstract:** One of the most challenging issues in materials physics is to predict the properties of matter at the nanoscale. In this size regime, new structural and electronic properties exist that resemble neither the atomic, nor the solid state. By changing the size of the system inherently intensive properties become extensive-like properties, which can be strongly altered from the macroscopic limit. Such properties can have profound technological implications, e.g. at small length scales a poor optical material like silicon can be converted to an optically active one. Unfortunately, the development of theoretical methods to predict the properties of these systems is a formidable challenge. Nanoscale systems may contain numerous electronic and nuclear degrees of freedom, and often possess little symmetry. My presentation will center on recent advances in this area based on new algorithms, which are designed to exploit high performance computational platforms. I will apply these algorithms to nanoscale systems containing over ten thousand atoms, and present predictions for the structural and electronic properties of semiconductor nanofilms, nanowires, and nanocrystals. I will also illustrate a new scheme to simulate non-contact atomic force microscopy (AFM) images by using first-principles self-consistent potential from the sample without explicit modeling of the AFM tip.

# Technical Program

**9:30AM-10:00AM**

**Full-Band Simulation of Realistic Nanoelectronic Devices at the Atomic Scale**

Mathieu Luisier (Purdue University) and Gerhard Klimeck, Associate Director for Technology, Network for Computational Nanotechnology (NCN)

**Abstract:**

The size of electronic devices has been aggressively scaled down so that the success or the failure of any physical operation relies on a countable number of atoms. A variation of the atomic ordering from a given design may profoundly affect the current characteristics of nanowire transistors, the emission wavelength of quantum dot lasers, or the behavior of doping impurities. Armed with our full-band eigenstate solver NEMO3D and quantum transport simulator OMEN we are able to investigate a wide range of nanoelectronic devices based on single to multi-million atom structures. Good agreement with experimental data has been demonstrated in various applications. Parallelization and high-performance computers are essential to enable such intensive studies. NEMO3D and OMEN scale almost perfectly up to 8,192 and 32,768 cores, respectively. The increasing availability of Peta-scale compute platforms will therefore help to move hero-simulation-experiments to day-to-day device design and engineering.

**10:00AM-10:30AM Break**

**Session chair: Andrew Canning**

**10:30AM-11:00AM**

**Time-dependent quantum transport model for carbon nanotube based on tight-binding molecular dynamics**

Satoshi Nakamura[1], Mikio Iizuka[1], Syogo Tejima[1], Yoshihisa Shizawa[1], David Tomaneck[2], and Hisashi Nakamura[1]

[1] Research Organization for Information Science and Technology, 2-2-54, Nakameguro, Meguro-ku, Tokyo, 153-0061, Japan

[2] Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824-1116, USA

**Abstract:**

We consider time dependent quantum transport phenomena of a molecular clamped between macroscopic leads in a current-carrying state at finite voltage. Our approach is based on the non-equilibrium Green's function technique and the tight-binding molecular dynamics simulation. We apply this method to study quantum transport for carbon nanotubes.

# Technical Program

**11:00AM-11:30AM**

## **Large-Scale First-Principles Molecular Dynamics for Nanoscience Applications**

Francois Gygi, University of California Davis, Davis CA 95616

**Abstract:** The availability of petascale platforms is expected to dramatically extend the scale and accuracy of first-principles simulations for nanoscience applications. This will however require adapting and sometimes redesigning, numerical algorithms in order to achieve good scalability. We present recent progress in the development of parallel algorithms and implementations of First-Principles Molecular Dynamics (FPMD) for operations on parallel platforms including over 10,000 CPUs. Applications to nanoscience problems are used to illustrate the challenges encountered when running large-scale FPMD simulations. Supported by NSF under grant OCI PetaApps 0749217

**11:30AM-12:00PM**

## **Nanoscale Materials Applications using NWChem on the ORNL Cray XT**

Edoardo Aprà, Computer Science and Mathematics Division Oak Ridge National Laboratory

**Abstract:** In the first part of the talk we will discuss the porting effort of the computational chemistry package NWChem to the CRAY XT hardware. In the second part of the talk we will report recent results of electronic structure calculations of nanoscale materials on the ORNL Cray XT. Research supported by the Office of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy, under Contract No. DE-AC05-00OR22725 with UT-Battelle, LLC.

**12:00 PM-12:30PM**

## **QMCPACK: A Quantum Monte Carlo package for petascale computers**

Jeongnim Kim, National Center for Supercomputing Applications and Materials Computation Center at University of Illinois Urbana-Champaign

**Abstract:** With advances in algorithms and the changing landscape of high performance computers (HPC), the quantum Monte Carlo method has become a leading contender for high accuracy calculations for the electronic structure of realistic systems. QMC, being statistical, is naturally scalable to a large number of processors. There are several different and independent ways to parallelize a QMC calculation: over different random walkers, through computation of wavefunction pieces, over boundary conditions. QMCPACK is developed to take advantage of modern hardware and software environments. It aims to provide robust computing infrastructure for the QMC methods to effectively use massively parallel, HPC systems of current and future generations. We discuss the design and implementation details of QMCPACK and analyze its performances on current HPC systems. We present an overview of applications enabled by QMCPACK and conclude with the outlook of the QMC algorithms for the current and next generations of petascale computers and our plans for emerging computing architectures.

Supported by the NSF under grant no. DMR-03 25939 ITR and a part of the QMC Endstation project supported by the U.S. -DOE under Contract No. DOE-DE-FG05-08OR23336. This research used resources of National Center for Supercomputing Applications at University of Illinois Urbana-Champaign and the National Center for Computational Sciences and the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory. In collaborations with D. M. Ceperley and K. Esler at University of Illinois Urbana-Champaign.

# Technical Program

**12:30-2:00 PM Lunch**

**Session Chair: Lin-Wang Wang**

**2:00 PM-2:30PM**

## **First-principles computational spectroscopy at the Molecular Foundry**

David Prendergast (Theory Group, Molecular Foundry, LBNL)

**Abstract:** Making a robust link between measured spectra and electronic or atomistic structural models is vital for novel nanoscale materials. Typically, the information provided by spectroscopy is useful only in comparison with an established database of spectra for well understood systems. The Theory Facility at the Molecular Foundry is bridging this gap in interpretation by developing computational approaches to predicting the spectroscopy of nanostructures. Even for simple systems, first-principles (parameter-free) approaches are computationally demanding. For our planewave implementations, these calculations involve frequent distributed fourier transforms and dense distributed matrix algebra. We highlight recent work on predicting and interpreting the core-level spectra of a range of systems, from molecular solids and liquids to biologically relevant organic species, and we focus on the development of a robust computational framework and efficient methods to accurately predict these spectra from first principles.

**2:30PM-3:00PM**

## **Title: Hybrid quantum simulations for solvated biomolecules**

M. Hodak,<sup>1</sup> W. Lu<sup>1,2</sup> and J. Bernholc,<sup>1,2</sup> 1) Center for High Performance Simulation and Dept. of Physics, NC State U., Raleigh. 2) CSMD, Oak Ridge Nat. Lab., TN

**Abstract:** Quantum biosimulations are among the largest attempted on current high-performance computers, because the relevant fragments of biomolecules are usually quite large and they must be solvated in water for simulations to be realistic. Most often, the quantum description of the solvent dominates the computational time. We have developed a hybrid method which allows for explicit quantum treatment of the solvent at a low computational cost. In our method, Kohn-Sham (KS) density functional theory (DFT) is combined with orbital-free (OF) DFT. The KS DFT is used to describe the biomolecule and its first solvation shells, while the OF DFT is employed for the rest of the solvent. The flow of solvent molecules across the KS/OF interface is allowed and the total energy is conserved. This method has been implemented in a highly parallel real-space quantum molecular dynamics code and has already been applied to understand the role of copper in prion and Parkinson's diseases.

# Technical Program

**3:00PM-3:30PM**

## **Nanocar simulations by utilizing resources of SKIF supercomputers**

A. V. Nemukhin<sup>1,2</sup>, A.V. Akimov<sup>1,3</sup>, A.A. Moskovsky<sup>1,2,4</sup>, Kupchenko I.V.<sup>1</sup>, Konyukhov S.S.<sup>1</sup>, Anatoly B. Kolomeisky<sup>3</sup>.(1) - Department of Chemistry, M.V. Lomonosov Moscow State University (2) - N.M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences (3) - Department of Chemistry, Rice University(4) – Program Systems Institute, Russian Academy of Sciences

**Abstract.** Nanocars are synthetic molecules, that mimic shape of real cars on nano-scale: they have four spherical “wheels” made of fullerene, bond together chemically by planar chassis (see figure). Such species have been recently synthesized and characterized experimentally on metal gold surface. We have undertaken first theoretical simulations of thermally-induced movements of nanocar particles, adsorbed on metal surface. Molecular dynamics simulations were able to reproduce qualitative features of the experimentally observed migration of nanocars on gold crystals. Future work will include simulations of nanocars with C70 “wheels” and carborane-based nanocars on glass surface.

The work was supported in part by SKIF-GRID supercomputing project. The SKIF-MSU supercomputer has been installed in early 2008, with 60 TFlops of peak performance, and is the most powerful supercomputer in the Russia and Eastern Europe. Access to high-end computational facility opens the door to first-principle molecular dynamics and thorough verification of fullerene-surface potential via first-principle calculations.

**3:30 PM-4:00PM**

## **Non-local Density Functional Calculations using Large Scale Computing Facilities; Application of Screened-Exchange Density Functional Method**

Byoung Hak Lee (Texas State University) and Lin-Wang Wang (Lawrence Berkeley National Laboratory)

**Abstract.** We present screened-exchange density functional method calculations that utilize large-scale parallel computing facilities. Most of beyond-local density functional approximation (LDA) methods that attempt to overcome the well-known band gap problem have non-local potentials. The calculation of non-local potentials increases the computational complexity from  $N^3$  to  $N^5$ , compared with LDA calculations. We demonstrate that this can be overcome by parallelizing the non-local potential evaluation. We show that our screened-exchange density functional method which includes the correlation effect within the non-local screened Coulomb exchange interaction can predict the band gap of various semiconductor systems with remarkable agreement with experiments.

# Technical Program

**4:00 PM-4:30PM**

**Ultra-fast response of nano-carbons under dynamical strong electric field.**

Yoshiyuki Miyamoto, Nano Electronics Research Laboratories, NEC

**Abstract.** In this presentation, I will give applications of the time-dependent density functional theory on simulating ultra-fast dynamics of nano-carbons under strong optical field. Irradiation with strong laser field causes unexpected structural changes of graphite and modification of optical field inside carbon nanotubes. I will demonstrate rapid exfoliation of surface grapheme mono-layer from AB-stacked graphite by irradiation of strong laser pulse and enhancement of the dielectric field inside semiconducting carbon nanotubes by irradiation of light with resonance frequency. These simulations were performed by combination of real-time propagation of electrons wavefnctions and molecular dynamics under strong external field. The numerical stability of these simulations were checked by the energy conservation rule [Miyamoto and Zhang, PRB (2008)]. Large scale calculations were feasible with the aid of computational power provided by the Earth Simulator

**Workshop Close (see you at HPCNano09)**

**[www.hpcnano.org/hpcnano09/](http://www.hpcnano.org/hpcnano09/)**