



HPCNano workshop 2006

The Second IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology (HPCNano06)

(www.hpcnano.org/HPCNano06/)

Nov. 13, 2006, Tampa, Florida, USA, in conjunction with IEEE/ACM Supercomputin 2006 (SC06)

Nanotechnology is an exciting field with many potential applications. Its impact is already being felt in materials, engineering, electronics, medicine, and other disciplines. Current research in nanotechnology requires multi-disciplinary knowledge, not only in sciences and engineering but also in high performance computing (HPC) technology. Many nano-science explorations rely on mature, efficient HPC and computational algorithms, practical and reliable numerical methods, and large-scale computing systems. This workshop offers academic researchers, developers, and practitioners an opportunity to discuss various aspects of HPC-related computational methods and problem solving techniques for nano-science and technology research.

The first workshop, HPCNano05, was a successful event hold in conjunction with IEEE/ACM SC05. HPCNano06 is the second workshop that will be conducted in conjunction with IEEE/ACM Supercomputing 2006 (SC06). The workshop will be guided by the SC2006's Workshop Committee and planned and executed by the workshop program committee. We hope to attract people from diverse science and engineering disciplines, nationally and internationally, to attend the workshop, present their research results, share their experiences and ideas, and plan future collaborations.

HPCNano06 invites authors to submit original and unpublished work (also not submitted elsewhere for review) reporting solid and innovative results in any aspect of high performance computing in nano-science and technology. The accepted papers will be published by either the IEEE Computer Society Press as a post-conference proceeding. Papers should not exceed 8 single-spaced pages of text using 10-point size type on 8.5 x 11 inch paper (see IEEE author instructions, a LaTeX style sheet and Word format is available, too). All bibliographical references, tables, and figures must be included in these 8 pages. Submissions that exceed the 8-page limit will not be reviewed. Authors should submit a PDF file that will print on a PostScript printer. Electronic submission is required. The site for submissions is <http://www.sc-submissions.org/>. Submission implies the willingness of at least one of the authors to register and present the paper.

Proceedings: All papers selected for this workshop are peer-reviewed and published as a separate post-conference proceeding by IEEE Computer Society Press. The papers will also be published in the IEEE Xplore, IEEE IEL, IEEE CS digital library (CSDL), and indexed by distinguished indexing services such as ISI, DBLP, etc. For author instructions see <http://www.computer.org/cspress/instruct.htm>

Special Issue: The best 6 to 8 papers from the workshop will be selected for journal length extension and their publication in a special issue of International Journal of High Performance Computing and Networking (IJHPCN).

HPCNano06's topics of interest (in no particular order) include, but are not limited to:

- Cyberinfrastructure-based cooperative computing in nanotechnology large scale computing in multi-scale modeling and simulation of nanoscale materials
- Petascale computing for computational nanotechnology
- Parallel algorithms, domain decompositions, and computational methods in nano-materials processing, characteristics, and statistical analysis
- Nano-material fabrication, synthesis, and processing simulations
- Microscopy nanostructures materials databases
- Large-scale molecular methods and simulations in nano-science and technology
- Nano-science -related data and image processing
- HPC-based modeling and simulation for Nano electromechanical systems
- High performance computing in Fourier transform infrared nano-surface
- Modeling and simulation of organic nanostructure materials and biomaterial processing
- HPC-based multi-scale spectroscopy data and image processing
- High performance data processing in microwave spectroscopy on quantum dots
- High performance computing in atomic-scale friction
- Large scale computing systems for nano-science (computational and network systems)
- Grid computing in nano science and technology
- High performance computing in bionanotechnology/nanobiotechnology

Further information can be found in the workshop's Web site at <http://www.hpcnano.org/HPCNano06/>

Organizers and Sponsors:

Organization: IEEE/Computer Society, ACM
National Research Agencies: NCSA, NASA
Industrial Partners: SGI, TeamHPC
Universities: University of Tennessee, Univ. of Iowa.



Welcome Message

The workshop program committee and sponsors welcome you. This year's workshop is sponsored by IEEE/Computer Society, ACM, NASA, NCSA, University of Iowa, University of Tennessee, SGI, TeamHPC. The theme for this year's workshop is Unperceived Engagement between Petascale Computing and Microscale Modeling.

Nanotechnology is an exciting field with many potential applications. Its impact is already being felt in materials, engineering, electronics, medicine, and other disciplines. Current research in nanotechnology requires multi-disciplinary knowledge, not only in sciences and engineering but also in high performance computing (HPC) technology. Many nano-science explorations rely on mature, efficient HPC and computational algorithms, practical and reliable numerical methods, and large-scale computing systems.

The committee firmly believes that today's HPC infrastructure enables people to extend the capability of computation and simulations in exploratory nanotechnology. HPC will play an important role in future multi-scale models and large-scale simulations of nanostructure materials synthesis, fabrication, and processing. HPC technology accelerates the innovation and creation of new nanostructure materials, nano-devices, and their promising applications.

This workshop offers academic researchers, developers, and practitioners an opportunity to discuss various aspects of HPC-related computational methods and problem solving techniques for nano-science and technology research. The workshop promotes future national and international collaborations in this multi-disciplinary domain. The workshop develops provide a great opportunity to initiate cyberinfrastructure-based perascale computing in nano-science and nanotechnology.

As with our previous workshops, we welcome and encourage your active engagement with our speakers from various multi-disciplinary communities. Your participation represents an important ingredient in our future collaboration to ensure that our HPC communities commit to develop cyberinfrastructure-based HPC resources and expertise needed for large-scale computations in nanotechnology.

We look forward to an exciting day of discussion and deliberation. Thank you for joining us.

Sincerely,

Dr. Thom Dunning, NCSA
Dr. Jack Dongarra, University of Tennessee Knoxville
Dr. Jun Ni, University of Iowa
Dr. Andrew Canning, LBNL, DOE



Workshop Organizers

General Co-Chairs

Thom Dunning, Director of National Center for Supercomputing Applications (NCSA), USA

Rupak Biswas, Director of NASA Advanced Supercomputing, NASA Ames, USA

Advisory Committee

Jack Dongarra, Director of ICL and CTR, University of Tennessee Knoxville, USA

Meyya Meyyappan, Director of Center for Nanotechnology, NASA Ames, USA

Yoshio Oyanagi, University of Tokyo, Japan

Deepak Srivastava, Center for Nanotechnology (CNT), NASA Ames Research Center, USA

Program Co-Chairs

Jun Ni, Research Scientist, Scientific Computing and HPC Manager, Information Technology Services, The University of Iowa, USA

Andrew Canning, Staff Scientist, Lawrence Berkeley National Laboratory (Berkeley Lab), DOE, Adjunct Professor, UCLA

Publicity Chair

Tom Balwin, Manager, IEEE Computer Society Press

Program Committee

Michael Stopa, Director, National Nanotechnology Infrastructure Network (NNIN)/Computation, Harvard University, USA

Dan Stanzione, Director, HPC Initiative, Arizona State University, USA

M. P. Anantram, Professor, Department of Electrical and Computer Engineering, University of Waterloo, Canada

Gang Chen, Professor, Department of Mechanical Engineering, MIT, USA

Derek Stewart, Manager, Modeling and Theory, Cornell Nanoscale Facility (CNF), Cornell University, USA

Hisashi Nakamura, Director, Research Organization for Information Science & Technology (RIST), Japan

Ray Bair, Project Director, Argonne Leadership Computing Facility, Argonne National Laboratory

Hamid R. Arabnia, Professor, Department of Computer Science, Univ. of Georgia, USA

Martina Bachlechner, Professor, Department of Physics, W. Virginia University, USA

Don Brenner, Director, Computational Materials Science (CMS), Department of Materials Science and Engineering, NCSU, USA

Charlie Catlett, Director of NSF TeraGrid Project, ANL, USA

Jack Dongarra, Director of ICL and CTR, University of Tennessee Knoxville, USA

Xianfang Xu, Professor, Department of Mechanical Engineering, Purdue University, USA

William A. Goddard, Professor, Department of Chemistry, CalTech, USA

Won-jong Kim, Professor, Mechanical Engineering, Texas A&M University, USA

Stanimire Tomov, Senior Research Associate, DOE Nano project, University of Tennessee, USA

Gerhard Klimeck, Professor, Technical Director of Network for Computational Nanotechnology (NCN), Purdue University, USA

Jerry Jenkin, CFD Research Corporation, USA

Kenji Tsuruta, Dept. of Electrical & Electronic Engineering, Okayama University, Japan

Watson Layne, Professor, Department of Computer Science and Mathematics, Virginia Tech., USA

Meyya Meyyappan, Director, Center for Nanotechnology, NASA Ames, USA

Aiichiro Nakano, Professor, Department of Computer Science, USC, USA

Jun Ni, Research Scientist and Manager of, Scientific Computing, Information Technology Service, Director, HPC Nanotechnology Research Lab (HPC NRL), and Director, Medical Imaging HPC Lab (MIHPC), The University of Iowa, USA

Padma Raghvan, Professor, Department of Computer Science, Penn State University, USA

Craig Stewart, Director of Research & Academic Computing, UITS, Indianan University, USA

John Savage, Professor, Department of Computer Science, Brown University, USA

Shaowen Wang, Research Scientist, GROW Project Leader, Information Technology Services, The University of Iowa, USA

Barbara A. Kucera, Deputy Director, Center for Computational Sciences, University of Kentucky

Deepak Srivastava, Scientist, Center for Nanotechnology (CNT), NASA Ames Research Center, USA

Bret Stouder, Vice President, TeamHPC, USA

Priya Vashishta, Professor, Department of Materials Science, USC, USA

Matthew Wolf, Professor, College of Computing at Georgia Tech., USA

Laurence T. Yang, Professor, Department of Computer Science, Francis Xavier University, Canada

Shaoping Xiao, Professor, Director, Nano-Sci. Tech Research Lab (NanoSTRes Lab), Department of Mechanical Engineering, The University of Iowa, USA

Minyi Guo, Professor, Shanghai Jiao Tong University, China; and Performance Evaluation Lab, School of Computer Science and Engineering, The University of Aizu, Japan.

Stan Posey, SGI Mountain View, CA, USA



Workshop Program

Nov. 13, 2006

Location: Room Salon J (Marriott)

8:00AM-8:10AM

Opening

Thom Dunning, NCSA

8:10AM-8:20AM

Workshop Introduction to HPC for Nanotechnology

Jun Ni and Jack Dongarra, The University of Iowa and University of Tennessee, USA

8:20AM-8:40AM

Linear Scaling NanoScience Simulations for Petascale Computing

Zhengji Zhao, Lin-Wang Wang and Juan Meza (Lawrence Berkeley National Laboratory (Berkeley Lab), Department of Energy, USA)

Abstract. There are many large-scale nanoscience problems that require ab initio accuracy electronic structure total energy calculations and atomic relaxations. Unfortunately, the traditional direct ab initio method scales as $O(N^3)$, where N is the number of atoms in the system, and most of the $O(N)$ methods studied in the last decade have various numerical convergence problems and computer parallelization issues. In this talk, we present an alternative $O(N)$ method which divides the whole system into small fragments. By combining the fragments in an ingenious pattern, the artificial boundary effects of the spatial division can be cancelled out. As a result, the numerical accuracy of this method compared with the direct ab initio calculation is very high, comparable to the chemical accuracy needed for most material science studies. In this method, the electronic wavefunctions for each fragment is solved by an ab initio method using a small group of processors, and there is no communication needed between the groups. As a result, the parallelization of the algorithm is straight forward, and the method scales linearly to the number of processors. We have used this method to calculate nanostructures (e.g, Si quantum dots passivated with H atoms) with more than ten thousand atoms using thousands of processors under the conventional planewave pseudopotential approach. The charge selfconsistency is done with conventional charge mixing scheme. We will show the scaling of this method to the number of atoms of the system, and to the number of processors used. We will demonstrate that this approach provides a practical way for future petascale computation in material/nano-material science.

8:40AM-9:00AM

Open-architecture Implementation of Fragment Molecular Orbital Method for Peta-scale Computing

Toshiya Takami, Jun Maki, Junichi Ooba, Yuichi Inadomi, Hiroaki Honda, Taizo Kobayashi, Rie Nogita, and Mutsumi Aoyagi (Computing and Communications Center, Kyushu University, and PSI Project Laboratory, Kyushu University, Japan)

Abstract. We present our perspective and goals on high-performance computing for nanoscience in accordance with the global trend toward "peta-scale computing." After reviewing our results obtained through the grid-enabled version of the fragment molecular orbital method (FMO) on the grid testbed by the Japanese Grid Project, National Research Grid Initiative (NAREGI), we show that FMO is one of the best candidates for peta-scale applications by predicting its effective

performance in peta-scale computers. Finally, we introduce our new project constructing a peta-scale application in an open-architecture implementation of FMO in order to realize both goals of high-performance in peta-scale computers and extendibility to multi-physics simulations.

9:00AM-9:20AM

NSF TeraGrid Project and its Supercomputing Resources for Solving National Challenge Problems in Sciences and Engineering Disciplines

Charlie Catlett, Director, NSF TeraGrid Project, University of Chicago and Argonne National Laboratory, USA

9:20AM-9:40AM

nanoHUB.org – A fully operational Science Gateway for the nano Science Community

Gerhard Klimeck¹, Rick Kennel², Michael McLennan², Stephen Clark², Clemens Heitzinger¹,

Shaikh S. Ahmed¹, Wei Qiao¹, David Ebert¹, Sebastien Goasguen², Krishna Madhavan²

¹Network for Computational Nanotechnology, Purdue University, W. Lafayette, IN 47907

²Rosen Center for Advanced Computing, Purdue University, W. Lafayette, IN 47907

Abstract. The Network for Computational Nanotechnology (NCN) is a multi-university, NSF-funded initiative with a mission to lead in nanotechnology research and education as well as outreach to students and professionals by offering a set of cyber services. These services are at the core of a unique web-based infrastructure tailored to serve the nation's National Nanotechnology Initiative. The primary NCN outreach vehicle is the nanoHUB (<http://www.nanoHUB.org>), which currently provides interactive online simulation and educational resources such as tutorials, seminars, and online courses packaged using e-learning standards. In the past 12 months, the educational and outreach services were accessed by over 16,200 users. More than 3,500 users performed over 94,000 online simulations thanks to the middleware supporting the nanoHUB. Over 30 applications are available online ranging from toy models to sophisticated simulation engines. The NCN provides the resources for modeling, simulating and computing without any software installation to users with access to a web browser. All the NCN services are freely open to the public. The NCN represents a community-based, service-oriented, science architecture that leads the way for new cyberinfrastructure-enabled science.

At the core, the NCN research mission is based on four research themes: nanoelectronics, nanoelectromechanics, nanobio, and high performance computation (HPC). One facet of the NCN goals is the development of new “community codes” that provide the nanoscience research community with new capabilities and that lay a foundation for a new generation of CAD tools that will pave the way to ground breaking nanotechnology devices. The HPC theme is charged with “grand challenges” to enable the three nanotechnology research themes to study realistically complex systems that have previously been computationally impossible or too expensive to explore. The development of numerical techniques and their packaging into portable software, capable of a variety of high accuracy simulations of nano-electronic, nano-biological, and nano-mechanical systems is the overarching goal of this research theme. Several codes that stem from NCN research supported efforts have now been deployed or are in the last steps before deployment on the nanoHUB as parallel applications.

Large-scale usage of such parallel applications will be through a new TeraGrid initiative called “Science Gateway”. The nanoHUB and the TeraGrid are now partnering to provide state-of-the-art computing resources to the nanoHUB users. With the TeraGrid entering a new phase after its construction, the nanoHUB is getting connected to the TeraGrid to make TeraGrid resources available to nanoHUB users as transparent compute backends. Computationally intensive nanoHUB applications that solve problems across multiple computational scales are being deployed on TeraGrid resources, and NCN partners will be able to access these resources for their own research. Science Gateways represent a shift from the

traditional high performance computing use by enabling entire communities of users associated with a common scientific goal to use the national resources through a common interface. Science Gateways are enabled by a community allocation whose goal is to delegate account management, accounting, certificates management and user support to the gateway developers.

Finally, the NCN recognizes that scientific codes are really only accessible to a community if they are truly usable. We are developing a framework that enables rapid deployment of legacy applications with appealing graphical user interfaces (GUIs). This framework, called Rappture, lets developers forego the creation of their own I/O routines, and it generates user friendly GUIs automatically. The nanoHUB middleware serves these GUI based applications through the user's browsers and makes the connection to the compute backends through virtualization technology. A visualization server has been developed to deliver interactive data analysis to at least 100 users simultaneously with hardware accelerated graphics delivered to the end user without any local hardware.

In this talk, we will present the NCN, the nanoHUB middleware and its capabilities as well as the educational technology supporting our teaching strategy. Finally, we will show how the nanoHUB infrastructure leads to state-of-the-art research in nanotechnology by showing concrete examples of deployed tools.

9:40AM-10:00AM

Large Scale Simulations for Composite nano Carbon Materials

S. Tejima(1), H. Nakamura(1), T. Fututa(2) and D. Tomanek(3) and M. Endo(4)

(1)Research Organization for Information Science & Technology, 2-2-54, Naka-Meguro, Meguro-ku, Tokyo, 153-0061, Japan; (2) Honda R&D Co. Ltd., Wako Research Center, 1-4-1 Chuo, Wako-shi, Saitama, 351-0193 Japan; (3)Physics and Astronomy Department, Michigan State University, East Lansing, MI 48824, USA; (4)Faculty of Engineering Shinsyu University, Department of Electrical and Electronic, 4-17-1, Wakasato, Nagano, 380-8553, Japan

Abstract. In nanoscience and technology, the process development of synthesizing real materials is one of important steps for industrial application, as well as the finding of novel properties of nanostructures. Large-scale simulations have been carried out so far for obtaining mechanical properties of carbon nanotubes ranged from simple nanotubes to the structured composite material, by using the tight-binding molecular dynamics on the Earth Simulator. As fundamental researches, elastic properties as stretching, compressing, bending and buckling have been investigated on single-walled, double-walled carbon nanotubes and compound ones, 'peapod.' Expanding the simulation of fundamental properties, we have also developed a process-simulation that enables us to design and build up carbon-nanotube complex with new applicability for increasing mechanical strength, transporting energy and transmitting information. Through large-scale simulation on bundling and welding carbon nanotubes without additive molecule, we have reached new carbon-nanotube complex structures that consist of sp^2 and sp^3 orbital interaction and are expected to be super tough materials with high conductivity and flexibility. Our research indicates that large-scale simulation is a quite effective methodology for nano-material design and its application.

10:00AM-10:20 Coffee Break

10:20AM-10:40AM

Parallel scaling of Teter's minimization for Ab Initio calculations

Torsten Hoefler, Wolfgang Rehm and Rebecca Janisch, Technical University of Chemnitz, Germany

Abstract. We propose a parallelization scheme for the conjugate gradient method by Teter et. al. and report a detailed analysis of its scalability. We use MPI collective operations exclusively to take advantage of optimized collective implementations with possible hardware support. Our parallel conjugate gradient calculation can be applied in addition to the already implemented parallelism in the application ABINIT. We propose distribution schemes for the band vectors and

the 3D-FFT, and provide both a detailed runtime and scalability analysis and a model for the used collective operations. We use this model of collective communication to predict the parallel scaling and to show that the scalability is mostly limited by the communication. Our codes scales up to 52 processors for a small 43 atom system and up to 120 processors for a larger 86 atom system for a single k-point on our test cluster. Our results suggest that non blocking collective communication could be used to enhance the application running time especially for cluster computers.

10:40AM-11:00AM

Linear Scaling Ab-initio Method for Nanoscience

Yang Wang, G.M. Stocks, Aurelian Rusanu, D.M.C. Nicholson, and Markus Eisenbach, and J.S. Faulkner (Pittsburgh Supercomputing Center, Oak Ridge National Laboratory, Florida Atlantic University, USA)

Abstract. Nano-structured materials present substantial theoretical challenges due to the need to treat the electronic interactions quantum mechanically whilst dealing with a large number of atoms. Interestingly, recent advances in the locally self-consistent multiple scattering (LSMS) method, a first principles order-N scaling technique specifically implemented to exploit massively parallel computing, are making the direct quantum simulation of nano-structures possible. The LSMS method is an order-N approach to first principles electronic structure calculation. It is highly scalable on massively parallel processing supercomputers, and is suited for performing large unit cell simulations to study the electronic and magnetic properties of materials with complex structure. In this presentation, we show that the LSMS method essentially accomplishes the first step towards understanding the electronic and magnetic structure of nano-structured materials with dimension size close to 10 nanometers (nm). As an example, we describe a 14,400 atom calculation of the electronic and magnetic structure calculated for an iron-platinum nanoparticle in L10 structure embedded in iron-platinum random alloy.

11:00AM-11:20AM

Ultra-fast phenomena in nano-scaled materials with the aid of supercomputer

Yoshiyuki Miyamoto, Fundamental and Environmental Research Laboratories, NEC Corporation, 34 Miyukigaoka, Tsukuba, 305-8501, Japan

Abstract. In this talk, I will represent application of parallel processors for simulating very fast phenomena in materials like carbon nanotubes. In this simulation, real-time dynamics of electron and ions are simultaneously treated by solving the time-dependent Schrödinger equation for electron wave functions, and by solving the classical Newton's equation for ions. These simulations can be done without any adjustable parameters on the basis of the Time-Dependent Density Functional Theory (TDDFT) within the Ehrenfest scheme for the molecular dynamics (MD) simulation. In the initial condition of the TDDFT-MD simulation, we can prepare solution of the time-independent Kohn-Sham equation with either ground state or (mimicked) excited state. In this presentation, I'll show more detailed technique for the numerical simulation. I will also show some examples in nanotubes and nano-graphite; (1) fast relaxation of photo-induced hot-carriers in nanotubes, and (2) collision of highly charged Ar ion on multiple graphene layers and subsequent structural deformations. These simulations give understanding and predictions for performance of nano-scale device and for structure formations. All of the presented calculations are performed by using the Earth Simulator under collaboration with Profs. A. Rubio and D. Tománek. The author is also supported from Research organization for Information Science and Technology (RIST) in Tokyo.

11:20AM-11:40AM

Failure of Nanoscale Interfaces: Large-scale Molecular-Dynamics Simulations

Martina E. Bachlechner, Robert H. Leonard, Eli T. Owens, and Wm. Trevor Swan III, Physics Department, West Virginia University, USA

Abstract. Large-scale molecular-dynamics (MD) simulations are an excellent technique to study failure of nanoscale interfaces at the atomistic scale. Strain rates for externally applied tensile strain and impactor velocities for hypervelocity impact change the failure response of the interface not only quantitatively but also qualitatively. Additionally, the long-range nature of stress and strain fields necessitates the study of system size effects on the severity of the damage. Frequent writing of configurations for detailed analyses during long simulation runs requires efficient strategies for the handling of large and numerous data sets.

12:00PM-1:20PM Lunch

1:20PM-1:40PM

Electronic Structure Calculations for large Nanosystems on High Performance Computers

Andrew Canning, Computational Research Division, Lawrence Berkeley National Laboratory and Dept. of Applied Science, UC-Davis, USA

Abstract. Electronic Structure calculations based on the density functional theory approach have become one of the biggest consumers of cycles on high performance computers around the world. This is due to the accurate representation of the underlying physics as well as the computational efficiency of this approach. In this talk I will discuss this approach, as used in nanoscience applications on high performance computers as well as new methods that go beyond density functional theory and allow us to simulate larger systems with first principles accuracy. Performance of these methods on high performance computers such as the IBM BGL, Cray XT3, NEC Earth Simulator and PC clusters will also be discussed. I will discuss some applications of these methods to nanosystems and detector materials.

1:40PM-2:00PM

A bulk-based preconditioner and its efficiency in accelerating eigensolvers for electronic nano-structure calculations

Christof Voemel, S. Tomov, O. Marques, L-W. Wang, and J. Dongarra

1Cyclotron Road, MS 50F-1650, Computational Research Division, Lawrence Berkeley National Lab, Berkeley, CA 94720
2CL andCITR, University of Tennessee, USA

Abstract. The focus of this work is to accelerate the parallel computation of interior eigenstates for large Hermitian matrices arising from plane-wave discretization of effective single-particle Schrodinger equations. Of interest is solving for a small number of interior eigenstates around the band gap of colloidal quantum dots (these eigenstates model electronic and optical properties of the system at hand). We developed a bulk-based technique that uses the eigenstates from the bulk materials constituent for the quantum dot to design an improved preconditioner (compared to diagonal) and a better starting vector choice (compared to random). For large quantum dots this led to about a factor of 4 decrease in the number of iterations until convergence compared to previous calculations. In this talk I will describe the mathematical problem at hand, explain the proposed acceleration techniques, and give results on their scalability, efficiency as compared to previous calculations (diagonal preconditioning with random starting vector), and as a comparison when used in combination with different eigensolvers.

2:00PM-2:20PM

HPC Technology Considerations for Computational Nanoscience Applications

Stan Posey and Michael Brown, SGI Mountain View, CA, USA

Abstract. Industry and research organizations continue to increase their investments in nano-science and related applications, such that the growing numbers of computational scientists continue to demand more from computer system environments. These application workflow demands typically include rapid single simulation job turnaround and multi-job throughput capability for users with diverse application requirements in a high-performance computing (HPC) system infrastructure. Additional complexity arises from the need for many nanoscience simulations to coexist in an HPC environment with other scientific research software and multi-scale applications, that all compete for the same HPC resources. For today's economics of HPC, these resources such as CPU cycles, memory, system bandwidth and scalability, storage and I/O, and file and data management – must deliver the highest levels of user productivity and HPC reliability that is possible from a commercial HPC platform. This presentation examines application-driven HPC workflow efficiencies for relevant applications in computational nanoscience. Modeling parameters such as model size, solution schemes, range of scales (and coupled scales), and a variety of simulation conditions can produce a wide range of computational behavior and large-scale data management requirements, such that careful consideration should be given to how HPC resources are configured and balanced to satisfy increasing user requirements.

2:20PM-2:40PM

Evolutionary Photonics

Alexander Gondarenko, Stefan Preble, Hod Lipson, Michal Lipson, Cornell University, USA

Abstract. We use an evolutionary process for designing novel photonic structures for the confinement of light. We show emergence of periodicity and 2 dimensional structures with previously unseen shapes. The evolved structure has sub diffraction limit light confinement and demonstrates periodicity as the principal condition for effective control of distribution of light. We discuss use of evolutionary algorithms and their scaling on large architectures and their application for inverse problems in photonics.

2:40PM-3:00PM

Nanomaterials Simulation using High Performance Computing: From Greenhouse Gases to High-Tech Materials

Andrew Chizmeshya Center for Solid State Science, Arizona State University, USA

Dan Stanzione, Center of Fulton School High Performance Computing, Arizona State University, USA

Abstract. Nanotechnology, and particularly the design of materials at the nanoscale, is increasingly dependent on High Performance Computing. In this talk, we will discuss some specific areas of nanoscale materials research at ASU that provide computational challenges, the techniques used to address them, and the challenges that remain in applying HPC to this research. In particular, the following three problems will be examined:

- The carbon sequestration group at ASU is developing advanced chemical and materials concepts to permanently bind the CO₂ produced by stationary source fossil fuel combustion (e.g., power generation from coal). Common magnesium rich minerals are decomposed and carbonated in an aqueous high pressure CO₂ process to produce a final mineral carbonate which is benign and stable on geological time scales. Recent research has established that a rate limiting step in this process is the formation of a glass-like protective layer on the dissolving mineral feedstock, which hinders the

extraction of magnesium. The application of HPC to carry out large scale quantum and classical simulations of this passivating layer's structure and properties has led to important new insights. The performance and scaling of various dynamic liquid/solid process simulations will be discussed in the context of this problem.

- The quantitative simulation of chemical vapor deposition (CVD) processes used to grow new semiconductor systems requires a realistic treatment of gas-gas and gas-solid interactions. The use of new gas phase sources drives growth conditions into unfamiliar regimes, making the insight from simulation invaluable. We will describe large scale quantum molecular dynamics simulations aimed at elucidating the gas-surface interactions in the new poly-silyl-germane system, including hydrogen desorption, decomposition and clustering reactions. HPC requirements for simulation scale-up will be discussed. While many HPC-enabled codes exist for nanoscale simulation, each code works only in specific regimes. Misapplication of these codes is an increasing problem. A short survey will be presented detailing both the scaling properties and the capabilities of several of the primary first principles and classical simulation codes used in nanomaterials research.

3:00PM-3:20PM Coffee Break

3:20PM-3:40PM

Multiscale simulations of impurity segregation in nanostructured materials

Kenji Tsuruta, Department of Electrical and Electronic Engineering, Okayama University, 3-1-1 Tsushima-naka, Okayama 700-8530, Japan

Abstract. We present some attempts to simulate nanoscale phenomena, which involve different length-scales and time-scales, using multiscale molecular-dynamics approaches. To simulate realistically an impurity-segregated nanostructure, we have developed the hybrid quantum/classical approach, which has been implemented on our grid-enabled pc clusters. We apply the method to analyses on hydrogen-defect interactions in Si and on Ni segregation in diamond defects. We have also developed the stochastic-difference-equation (SDE) based method for simulating long-time processes in nanostructured systems. The method bridges the states separated by high-energy barriers in a configuration space by optimizing the action, defined as an error accumulation in discretizing atomic pathways. We show some applications, including a wetting phenomenon and a surface segregation, to demonstrate the effectiveness of the SDE method.

3:40PM-4:00PM

Multi-scale modeling of transport phenomena during process of nanostructured composite materials and metal alloys for petascale simulation

Jun Ni, Shaoping Xiao, Shaowen Wang, The University of Iowa, USA

Abstract. This presentation addresses the basic multi-scale model of transport phenomena during the processing of nanostructured composite materials and metal alloys. The model depicts many physical phenomena on microscopic and macroscopic scales. It accounts the mechanism of microscopic-level nucleation, micro-meso-level nano-particle movement, nanocrystal growth with associated kinetics, and macroscopic materials formation, liquid-state segregation, convection and diffusion, and the final property distributions (physical, chemical and mechanical) and defects. The model begins with molecular dynamics to account for origin of nucleation, meso-scale kinetic evolution and dynamic interactions of phases during phase change, thermal and species equilibriums and conservation's, as well as particle interactions. The model is designed for future large-scale simulations on petascale computing systems. The infrastructure of model implementation is briefly addressed by decompose loosely-coupled tasks on large-scale distributed computing systems, such as Grid recourses like TeraGrid.