Inaugural High Performance Computing User Symposium

Louisiana State University, Baton Rouge

June 6 - 7, 2012

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Louisiana State University, Baton Rouge, LA 70803
June 6-7, 2012

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Foreword

On behalf of High Performance Computing at Louisiana State University (HPC@LSU) and the Louisiana Optical Network Initiative (LONI), I welcome everyone to the Inaugural High Performance Computing User Symposium. Over the last few years, HPC@LSU has provided administration and user support of LONI and LSU HPC resources to users of the HPC community within the state of Louisiana. We offer a wide variety of training geared towards both new users and advanced users. Examples of advanced training topics include programming/scripting languages, developmental and debugging tools, and various scientific application topics and software tools. Training classes can be attended either in person or via Adobe Connect for users from outside LSU. All of our training materials, slides and recordings are available on our website for review at all times. Immediately preceding this Symposium, we conducted a Parallel Programming Workshop which was a follow up to the Fortran Programming Workshop in February.

LONI, LSU ITS and LSU CCT have collaborated to organize this Inaugural HPC User Symposium. The purpose of the User Symposium is threefold:

1. to introduce LSU and LONI HPC users to each other in the hopes that they will find ways to collaborate and enrich their research scope;
2. to facilitate a chance for users to share their experiences using HPC resources and learn from those of others; and
3. to allow face-to-face interaction between the HPC user support team and the HPC users so that better user support services can be provided in the future.

This Symposium is the first of its kind for both LONI and LSU and we hope that it will become an annual event to connect researchers in the state. This Symposium is a little over one day and consists of poster contributions from our HPC user community and a series of invited talks by researchers. Participants are encouraged to take this opportunity to discuss their research activities with others and foster greater collaboration with other users. Members of the HPC User Support team and the HPC Enablement group within CCT will be available for the duration of the Symposium to answer any questions that you might have.

This symposium has been made possible due to generous support from the Board of Regents, LONI, LONI Institute and LA-SiGMA. I would also like to thank the staff at CCT and ITS for their efforts in making this Symposium a success.

Samuel P. White,
Director
High Performance Computing
Louisiana State University

On behalf of LSU's Center for Computation & Technology (CCT), I am pleased to welcome you to this Inaugural LSU HPC User Symposium. Please take this opportunity to meet your fellow researchers and exchange ideas and experiences gained on the wide range of HPC resources available through LSU and LONI. Terminology may differ between fields, but in many cases the underlying techniques are identical. This is also your chance to talk to a CCT representative and give your opinion on available services and any needs you feel are not being met. Please mingle, ask questions, interact with your colleages. I hope that you will find collaborators here to enrich your future research, and that you run across ideas to fire your imagination.

Joel Tohline,
Director
Center for Computation & Technology
Louisiana State University

Dear Colleagues,

Welcome to Louisiana State University and to the inaugural HPC User Symposium. It is an honor and a pleasure to serve as your hosts for the next several days.

During the past decade, researchers throughout Louisiana have established themselves as leaders in a number of fields of research that rely heavily on very high performance, non-commodity computational resources - collectively known as High Performance Computing (HPC) resources – to solve complex problems across multiple disciplines including physics, chemistry, engineering, astronomy, and more recently, computational biology. HPC resources are critical in developing hurricane forecasts and, during actual hurricanes, in delivering real-time hurricane models to state and federal emergency officials. The level of funding and technical support for HPC has allowed LSU to participate in the Louisiana Optical Network Initiative (LONI) as both resource provider and consumer. The demonstration of dedicated HPC capital and human resources has also facilitated numerous grants including those from Teragrid and NSF, a prerequisite which has become increasingly significant as the level of national funding has become increasingly constrained.

During the week you will hear from peers representing a wide range of disciplines and scholarly endeavor. Sessions will include both oral presentations and poster sessions, as well as numerous opportunities for conversation, engagement, and exchange.

This inaugural HPC User Symposium emphasizes bringing together communities to facilitate information exchange, discussions and new collaborations for research and education related to innovative high performance computing applications and advancing scientific discovery and scholarship. The User Symposium sponsors and staff welcome you to participate in the breadth of symposium offerings, and above all, to enjoy your week!

On behalf of High-Peformance Computing @ LSU,

Melody Childs,
Deputy Chief Information Officer
Louisiana State University

This Inaugural High Performance Computing User Symposium represents exactly the kind of community engagement and development that the LONI network seeks to encourage among its participants - opportunities for the users of the tools and resources available throughout the network to further develop their skills and knowledge so that our researchers become more productive.

I am pleased to have LONI serve as a supporter and sponsor of this event, and I know that this will be a valuable and rewarding investment for our research community.

Donald J. Vandal,
Executive Director
Louisiana Optical Network Initiative (LONI)

Dear Colleagues,

On behalf of the LONI Institute and the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA), I would like to welcome you to the inaugural HPC User Symposium. Both LA-SiGMA and the LONI Institute are state wide virtual organizations for research and education in the computational sciences. We are proud to help sponsor the attendance of our members so that they may participate in this forum which is critical to our mission. I hope that you will all enjoy the occasion to share and learn new research ideas and take the opportunity to build lasting new research collaborations.

Mark Jarrell,
Principal Investigator
LONI Institute and LA-SiGMA

Welcome to the LONI HPC Workshop and Symposium

On behalf of Louisiana EPSCoR, and the Board of Regents, I would like to welcome you to the LONI HPC Workshop and Symposium. This is a great opportunity for faculty, staff, and students to learn about the high performance computing resources that LONI offers. The Symposium and Workshop will provide an opportunity for face-to-face interactions among LONI HPC resource users and encourage collaboration that will promote research competitiveness.

Thank you for participating, and I wish you all a productive and enjoyable meeting.

Michael Khonsari,
Louisiana EPSCoR Project Director and
Associate Commissioner for Sponsored Programs R&D, Louisiana Board of Regents

Symposium Program

June 6th, 2012	
6:00 pm - 8:00 pm	Registration and Poster Session opens at Life Sciences Annex
June 7th, 2012	
8:00 am - 8:20 am	Registration
8:20 am - 8:30 am	Welcome
Session I	Chair: Le Yan, Louisiana State University
8:30 am - 9:10 am	*High Performance Computing for Proton Radiation Therapy*
	Dr. Wayne Newhauser
	Louisiana State University and Mary Bird Perkins Cancer Center
9:10 am - 9:50 am	*Classical Molecular Dynamics Simulations of Biologically Relevant Molecules*
	Dr. Brian Novak
	Louisiana State University
9:50 am - 10:00 am	Break
Session II	Chair: Cheri McFerrin, Louisiana State University
10:00 am - 10:40 am	*Simulations of Strongly Correlated Systems*
	Dr. Juana Moreno
	Louisiana State University
10:40 am - 11:20 am	*eThread: a highly optimized machine learning-based approach to meta-threading and the modeling of protein tertiary structures*
	Dr. Michal Brylinski
	Louisiana State University
11:20 am - 12:00 pm	*Data Visualization: Workflow, Software, and Case Study*
	Dr. Jinghua Ge
	Louisiana State University
12:00 pm - 1:00 pm	Lunch (provided)

Symposium Program

June 7th, 2012	
Session III	Chair: Brad Burkman, Louisiana School for Math, Science and Arts
1:00 pm - 1:30 pm	*Phylogenetics enters the genomic era: from HIV to turtles* Dr. Jeremy Brown Louisiana State University
1:30 pm - 2:10 pm	*Computational challenges for pore-scale image-based modeling* Dr. Karsten Thompson Louisiana State University
2:10 pm - 2:40 pm	*Cluster Typical Medium Theory Approach for Disordered Systems* Hanna Terletska Louisiana State University
2:40 pm - 2:50 pm	Break
Session IV	Chair: James A. Lupo, Louisiana State University
2:50 pm - 3:30 pm	*Parallel Computation of Turbulent Flows using Large Eddy Simulations* Mr. Prasad Kalghatgi, Louisiana State University
3:30 pm - 4:00 pm	*"ManyJobs" on Distributed Cyberinfrastructure* Dr. Hideki Fujioka Tulane University
4:00 pm - 4:30 pm	*Estrogenic Potential of Bisphenol A and Nitrated and Chlorinated Metabolites of Bisphenol A - Molecular Docking Studies* Mr. Sainath Babu Southern University
4:30 pm - 5:00 pm	*Quantum Cosmology with High Performance Computers* Brajesh Gupt Louisiana State University
5:00 pm - 5:10 pm	Closing Remarks

List of Posters

WEDNESDAY, JUNE 6TH, 2012 (LIFE SCIENCES ANNEX LOBBY)

1 Chemora - A Multilevel Code Generation and Optimization Framework for Heterogenous Systems

Jian Tao
Center for Computation & Technology, Louisiana State University

2 3D Mass Diffusion-Reaction System Modeling in the Neuromuscular Junstion

Abdul Khaliq
Institute for Micromanufacturing, Louisiana Tech University

3 Spin Glass Simulation with Parallel Tempering on GPU

Ye Fang
Department of Electrical & Computer Engineering, Louisiana State University

4 Computational Network Biology for Systems-Level Functional Annotation of Proteins and Proteomes

Daswanth Lingam
Department of Electrical and Computer Engineering, Louisiana State University

5 Introducing Students to HPC

Brad Burkman
Department of Mathematics, Louisiana School for Math, Science and Arts

6 Optimal Microarchitectural Design Configuration Selection for Processor Hard-Error Reliability

Lu Peng
Department of Electrical and Computer Engineering, Louisiana State University

7 SAGA-Bliss and BigJob: Scaling Research to Support Production Science

Ole Weidner
Center for Computationa & Technology, Louisiana State University

8 Dynamical embedding of the dual fermion dynamical cluster approach for strongly correlated systems

Zi. Y. Meng
Department of Physics & Astronomy, Louisiana State University

9 Ferromagnetic Semiconductors: Prospect and Future

Ryky Nelson
Department of Physics & Astronomy, Louisiana State University

10 Adsorption of atmospherically relevant gases on bare and surfactant coated ice films

Thilanga P. Liyana-Arachchi
Cain Department of Chemical Engineering, Louisiana State University

11 Hirsch-Fye Quantum Monte Carlo on GPUs

Sameer AbuAsal
Department of Electrical & Computer Engineering, Louisiana State University

12 Numerical Model System for Ecosystem Restoration and Flood Risks Reduction (ERFRR) in the Northen Gulf Coast

Kelin Hu
Department of Civil & Environmental Engineering, Louisiana State University

13 Meso-Scale Analysis of Deformation Induced Heating of Metalized Explosive

Sunada Chakravarthy
Louisiana State University

14 Development of a Non-Hydrostatic Model for Simulation of Nonlinear Waves over Submerged Vegetation

Ling Zhu
Louisiana State University

15 Simulation of Wave Attenuation by Fluid Mud Using a Finite-Volume Navier-Stokes Model

Qi Fan
Department of Civil & Environmental Engineering, Louisiana State University

16 Numerical modeling of nonlinear triad interaction of shallow water

Qian Zhang
Department of Civil & Environmental Engineering, Louisiana State University

17 Role of the van Hove Singularity in the Quantum Criticality of the Hubbard Model

Kuang-Shing Chen
Department of Physics & Astronomy, Louisiana State University

18 Ab-Initio Study of Iron Oxide Clusters and their Reactions with Phenol, 2-Chlorophenol and 4-Chlorophenol

Cheri McFerrin
Department of Chemistry, Louisiana State University

19 Computational Studies of the Hydrogen Storage Capabilities of $KMgH_3$

Brandon Borill
Department of Chemistry, Louisiana State University

20 Monte Carlo Simulations of Nucleation in 2d Systems

Troy Loeffler
Department of Chemistry, Lousiana State University

Abstracts

High Performance Computing for Proton Radiation Therapy

Wayne Newhauser

Medical Physics Program, Louisiana State University, Baton Rouge, LA 70803
Chair of Physics, Mary Bird Perkins Cancer Center, Baton Rouge, LA 70809

Abstract

Predictions of exposure to charged particle radiation are commonly performed for patients receiving radiotherapy. This presentation will review the physical and computational approaches to predict radiogenic toxicity in these patients. The discussion will include a brief overview of the sources of radiation exposure and how these vary with host and treatment factors. Modeling approaches discussed will including algorithms to predict radiation dose and radiogenic risk for the development of second cancers, including the application of Monte Carlo methods and supercomputing techniques. The review will conclude with a brief summary of currently available dose computing capabilities, unmet needs, and possible directions for future research.

Note: Material in the seminar will be presented at an introductory level. No prior knowledge of radiotherapy is necessary.

Biosketch: Dr. Newhauser's research focuses on heavy particle dosimetry calculations and measurements. After receiving degrees in nuclear engineering and medical physics at the University of Wisconsin, he worked as a post-doctoral fellow and staff scientist at the German National Standards Laboratory (PTB, Braunschweig), an assistant professor at Harvard Medical School and Massachusetts General Hospital, and a tenured associate professor of radiation physics at The University of Texas M. D. Anderson Cancer Center. Currently, Prof. Newhauser serves as director of the graduate program in medical physics at Louisiana State University and Chief of Physics at the Mary Bird Perkins Cancer Center, both in Baton Rouge. In his current position, he teaches and leads a research group that investigates advanced radiotherapies, radiation effects, and cancer survivorship. Dr. Newhauser is also a board certified, licensed, and practicing medical physicist. He is active in several professional and scientific societies and serves in leadership roles in the American Association of Physicists in Medicine and the American Nuclear Society.

Classical molecular dynamics simulations of biologically relevant molecules

Brian Novak

Department of Mechanical Engineering, Louisiana State University, Baton Rouge, LA 70803

Abstract

I will present work on molecular dynamics simulations of biological systems, including the motion of one of the domains of the enzyme biotin carboxylase which undergoes a large (45°) conformational change upon binding ATP, DNA sequencing based on time-of-flight measurements in nanochannels, self-assembly of surfactant molecules including the nonionic span-80 and ionic bile salts, and interaction of DMSO, α-tocopherol (vitamin E), and PLGA nanoparticles with lipid bilayers. Due to the limitations and strengths of existing molecular dynamics packages, different ones were used for different problems. The NAnoscale Molecular Dynamics (NAMD), Groningen Machine for Chemical Simulations (GROMACS), and Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) packages have been used.

Simulations of Strongly Correlated Systems

Juana Moreno

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803

Abstract

The field of strongly correlated systems is one of the most active areas in condensed matter physics. This interest is motivated, in part, by a variety of complex emergent phenomena, including high-temperature superconductivity, quantum criticality and complex phases induced by electron-phonon couplings. The recent very rapid development of high performance heterogeneous computer platforms together with a similar emergence of highly accurate many-body algorithms allow the treatment and modeling of complex correlated material systems which were intractable just a few years ago. Important progress has been made by the development of finite size methods, including exact diagonalization and Quantum Monte Carlo (QMC) techniques. However, due to the minus sign problem, these methods are limited to small lattice sizes. Another successful approach is the dynamical mean field approximation and its cluster extensions, which treat the local or short-ranged dynamical correlations exactly and non-local or long-ranged correlations in a mean field approximation. Due to the effective medium, the Fermion minus sign problem is much milder than that found in finite sized simulations. However, it is still the primary limitation of these methods. To address this problem, multiscale approaches are used which treat only the correlations at the shortest length scales with exact cluster solvers, intermediate length scales are treated using a diagrammatic approach, such as the parquet equations or the dual-fermion formalism and, the longest length scales are captured by the mean field. I will discuss how these new algorithms impact a few model systems including our understanding of quantum criticality in the Hubbard model, new phases in ultracold quantum gases, and spintronics materials. I will conclude discussing recent algorithm redesign motivated by the evolution towards hybrid multicore architectures employing graphical processing unit (GPU).

eThread: a highly optimized machine learning-based approach to meta-threading and the modeling of protein tertiary structures

Michal Brylinski

Center for Computational and Technology, Louisiana State University, Baton Rouge, LA 70803

Abstract

Template-based modeling that employs various meta-threading techniques is currently the most accurate, and consequently the most commonly used, approach for protein structure prediction. Despite the evident progress in this important field, accurate structure models cannot be constructed for a significant fraction of gene products, thus the development of new algorithms is required. Here, we describe the development, optimization and large-scale benchmarking of eThread, a highly accurate meta-threading procedure for the identification of structural templates and the construction of corresponding target-to-template alignments. To carry out fully automated template-based protein structure modeling, eThread integrates 10 state-of-the-art threading/fold recognition algorithms in a local environment and extensively uses various machine learning techniques. Tertiary structure prediction employs two protocols based on widely used modeling algorithms: Modeller and TASSER-Lite. As a part of eThread, we also developed eContact, which is a Bayesian classifier for the prediction of inter-residue contacts and eRank, which effectively ranks generated multiple protein models and provides reliable confidence estimates for structure quality assessment. Excluding closely related templates from the modeling process, eThread generates models, which are correct at the fold level, for $> 80\%$ of the targets; $40 - 50\%$ of the constructed models are of a very high quality, which would be considered accurate at the family level. Furthermore, in large-scale benchmarking, we compare the performance of eThread to several alternative methods commonly used in protein structure prediction. Finally, we estimate the upper bound for this type of approaches and discuss the directions towards further improvements.

Data Visualization : Workflow, Software, and Case Study

Jinghua Ge

Center for Computation and Technology, Louisiana State University, Baton Rouge, LA 70803

Abstract

This talk reviews scientific visualization activities at LSU either directly using HPC resource, or handles data produced from HPC resources. A visualization process usually starts from picking a proper visualization software with desired features you are looking for, and matching your data with the visualization softwares data loading mechanism. For a parallel visualization process on HPC, data format is especially important so visualization algorithms can be applied to the datasets in a parallel manner.

This talk also discusses visualization as a complete process which involves data storage, data processing, numerical data analysis, parallel computing, and 3D modeling, animation, and rendering pipeline. Although some visualization software strive to provide as many functions as possible, many other tools will be introduced for specific tasks. Other aspects, such as batch rendering, software integration, provenance management, will also be introduced.

Phylogenetics enters the genomic era: from HIV to turtles

Jeremy M. Brown

Department of Biological Sciences, Louisiana State University, Baton Rouge, LA 70803

Abstract

Unraveling the Tree of Life, an accurate depiction of the relationships between all living things, has been one of the foremost goals of biologists since Darwin. The Tree is important not only because it provides a framework on which to hang our understanding of how all living things have evolved, it also has immediate practical implications for medicine, forensics, agriculture, and conservation. Massive genomic datasets generated by new, high-throughput DNA sequencing techniques present an unprecedented wealth of information for inferring phylogenies. I will discuss two ongoing projects in my lab that use genome-scale data to address phylogenetic questions. The first project involves sequencing the genomes of HIV samples taken from individuals in small transmission clusters in order to reconstruct patterns of transmission. This work has implications for forensics and epidemiology. The other project attempts to filter genomic data to identify those genes that provide the most reliable phylogenetic information. As genome-wide data have begun to be used for phylogenetic reconstruction, strong incongruences in signal across genes have become apparent. However, very little work has been done to develop methods for identifying the reliability of inferences from different parts of the genome.

Computational challenges for pore-scale image-based modeling

Karsten E. Thompson

Craft & Hawkins Department of Petroleum Engineering, Louisiana State University, Baton Rouge, LA 70803

Abstract

Fluid transport in porous media is relevant to processes ranging from energy production to environmental transport to advanced materials manufacturing. A long-standing problem faced by engineers working in these areas are linking the fundamental physics that occur at the pore scale to the empirical design equations that must be used in practice. Over the past two decades, the development x-ray microtomography and similar 3D imaging techniques has led to a new area of computational modeling, which we refer to as image-based modeling. Using these techniques, simulation of pore-scale transport processes is performed directly on microtomography images (as opposed to idealized structures as in the more traditional approach).

High-performance computing is relevant to this area of research because of the large computational problems that are generated from small physical structures (often millimeters in scale at the largest). This talk will use 3D microtomography images to introduce three interesting physical problems that are of interest to scientists and engineers, and then show novel computational methods that are being developed to simulate fundamental physics at the pore scale.

Title: **Cluster Typical Medium Theory Approach for Disordered Systems**

Authors: C. E. Ekuma[1], Z. Y. Meng[1], H. Terletska[1], K. M. Tam[1], J. Moreno[1], M. Jarrell[1], and V. Dobrosavljević

[1] Department of Physics & Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA
[2] Department of Physics, Florida State University, Tallahassee, FL 32301, USA

Abstract:

Disorder (due to doping, impurities, structural defects) is a common feature of many materials, and may play a key role in many technologies and interesting behaviors. A prominent example of such a disorder effect is Anderson localization [1], where electrons can become localized at sufficient disorder strength.

Theoretical methods commonly used to study disordered systems, including the coherent potential approximation (CPA) and its cluster extensions (dynamical cluster approximation (DCA) [2]), fail to describe localization. Such mean-field like theories treat correlations exactly on short length scales by sampling disorder configurations within a cluster and long length scales with a mean field, which is ultimately metallic. To address this problem, the typical medium theory (TMT) replaces the (algebraic) average medium with a (geometric) typical medium. This method has been successfully applied within the CPA with a single impurity as a cluster solver.

We have recently extended this method to employ a finite size periodic cluster instead of the impurity as a cluster solver. As a result, our cluster typical medium theory (CTMT) approach incorporates systematic non-local corrections to the local TMT approximation. We performed a systematic study of localization in different cluster size systems and dimensions. Our analysis demonstrates consistent behavior with known established results. We also believe that our CTMT method opens an new avenue to study localization both in model and in real materials.

1. P. W. Anderson, Phys. Rev. 109, 1492 (1958).
2. M. Jarrell and H. R. Krishnamurthy, Phys. Rev. B. 63, 125102 (2001).
3. V. Dobrosavljević, A. A. Pastor, and B. K. Nikolić, Europhys. Lett. 62, 76 (2003).

Parallel Computation of Turbulent Flows using Large Eddy Simulations

Prasad Kalghatgi
Phd Student (Graduate Advisor—Prof. Sumanta Acharya)
Department of Mechanical Engineering, LSU

Abstract

Time and Space resolved turbulent simulations are extremely computation intensive simulations. Among them fully resolved Navier Stokes solutions (DNS) and Large Eddy Simulation are at the frontiers and provide accurate representation of turbulent flows with out or very less ad-hoc modeling. DNS being prohibitively expensive for industrial scale turbulent flows, we use Large Eddy Simulation technique with a dynamic sub-grid stress model for accurate cost-effective representation of high Reynolds number flow in complex geometries. An in-house developed parallel multi-block chemically reacting compressible flow code for generalized curvilinear coordinates, CHEM3D, is used. For incompressible flows, low Mach number preconditioning is used (Weiss and Smith, 1995). A second order backward 3-point physical time differencing is used for the temporal derivatives. Second order low diffusion flux-splitting algorithm is used for convective terms (Edwards, 1997). Second order central differences are used for the viscous terms. An incomplete Lower-Upper (ILU) matrix decomposition solver is used. Domain decomposition and load balancing are accomplished using a family of programs for partitioning unstructured graphs and hypergraphs and computing fill-reducing ordering of sparse matrices, METIS. The message communication in distributed computing environment is achieved using Message Passing Interface, MPI (Gropp et al., 1999). All the multi-block structured curvilinear grids presented in this paper are generated using commercial grid generation software GridPro^{TM} and ANSYS-ICEM CFD.

Among applications investigated by a present and past researchers are, (i) thickened flame modeling of turbulent combustion, (ii) immersed boundary method for (turbulent flows in stirred tanks), (iii) Film cooling of gas turbine blades (iv) large eddy simulation of countercurrent shear flows and their stability studies. The author is involved in the LES of countercurrent flows and Film cooling of gas turbine blades.

"ManyJobs" on Distributed Cyberinfrastructure

Hideki Fujioka[1], Rajib Mukherjee[2], Abhinav Thota[3], Shantenu Jha[4] and Thomas C Bishop[2]
[1]Center for Computational Science, Tulane University, New Orleans, LA 70118
[2]Department of Physics and Chemistry, Louisiana Tech University, Ruston, LA 71272
[3]Indiana University, Bloomington, IN 47408
[4]Rutgers University, Piscataway, NJ 08854

Introduction

The simulation approach presently used by many scientific groups severely limits their ability to use multiple resources in an efficient manner. The most common method used to run a large number of jobs is to use a single computing resource and submit each job to the queuing system. Even if the queue dependency options are utilized, the researcher spends significant time for intervening manually and must contend with potentially long queue waiting times or move data to another resource. To overcome these obstacles, we have developed a pilot-job based tool called ManyJobs for efficient utilization of distributed resources. At the beginning of a run, ManyJobs submits job requests to the queue manager of all computing resources listed by the user. The requests are issued from a central ManyJobs database, which could be hosted on a local workstation or one of the computing resources. Once a queued job starts, ManyJobs assigns it a task. Upon job completion the task status is registered with the ManyJobs database and submits another job request to keep the workflow active. The process repeats until all computational tasks in the database are finished. The ManyJobs database is capable of managing task dependencies such that multiple simulation threads can run concurrently. ManyJobs is written in Python and utilizes 'ssh' for the communication between the ManyJobs database server and the head/computing nodes of the cluster resources.

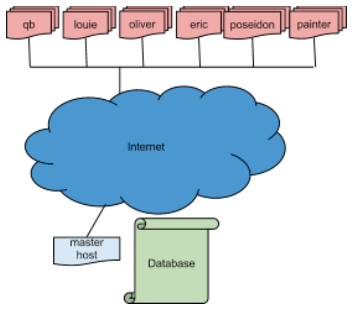

Fig.1: An example of ManyJobs system schematic

Experiments and Results

We ran ManyJobs using five LONI resources. The simulation consists of four independent task-threads. Each thread consists of approximately 500 dependent tasks. Each task took about 2.5 hours with 128 cores. Fig.2 shows the throughput for first 24 hours of ManyJobs run. The vertical axis indicates the number of concurrent tasks run on each LONI resource; Painter (LaTech), Poseidon (UNO), Eric (LSU), Oliver (ULL), and Louie (Tulane). Each colored-bar represents time for task started and completed, and which resource task ran. Bars of same color belong to same thread. Tasks in same thread cannot run concurrently. After a task is completed, the following task began running almost immediately on the same resource or a different resource. Arrows indicate transfers of tasks in same thread across the resources. For example, the task that began running on Poseidon (red) at time=0.03(hr) finished at time=1.98(hr), then next task began running on Louie at time=2.03(hr) and finished at time=3.98(hr). The third task in this thread ran on the same resource, the fourth task ran on Oliver and fifth task and later ran on Louie. Within 24 hours, Eric, Oliver and Louie took maximum two concurrent tasks, Poseidon took one task in the beginning then no tasks ran, and Painter didn't take any tasks.

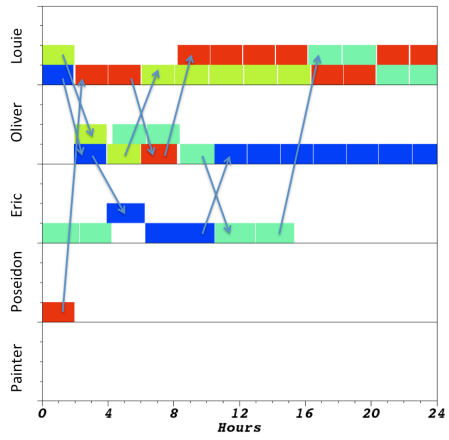

Fig.2: ManyJobs throughput over 5 LONI

Acknowledgments

Hideki Fujioka is funded by LONI institute support. Bishop, Mukherjee and Jha are funded by the NSF EPSCoR LASiGMA project under award #EPS-1003897 for the computational effort. Scientific part of the project is supported by NIH(R01GM076356) to T. C. Bishop.

Estrogenic Potential of Bisphenol A and Nitrated and Chlorinated Metabolites of Bisphenol A - Molecular Docking Studies

Sainath Babu,[1] Nadeem. A. Vellore,[2] Venkata A. Kasibotla,[1] Harlan. J. Dwayne,[3] Michael. A. Stubblefield,[3] & Rao. M Uppu[1]

Departments of [1] Environmental Toxicology and [3] Mechanical Engineering, Southern University and A & M College, Baton Rouge, LA; [2] Department of Medicinal Chemistry, University of Utah, Salt Lake City, UT

ABSTRACT

Bisphenol A (BPA), an endocrine disruptor, is a key ingredient in the manufacturing of polycarbonate plastics. Factors such as dose, site of action, biotransformation (mainly phase II conjugation), and the individual susceptibility are known to influence the toxicity of BPA. Studies have shown that nearly 25% of BPA can undergo oxidative transformation by cellular oxidants such as peroxynitrite and hypochlrous acid. Unlike the metabolites of phase II metabolism which are rapidly eliminated, the metabolites of BPA formed in non-enzymatic reactions bio-accumulate and thus mediate BPA toxicity. Since BPA binds the estrogen-related receptor-gamma (ERRγ) with much higher affinity than that observed with the conventional estrogen receptor (ER), we performed molecular docking of BPA along with four of its putative metabolites using Autodock 4.2. We compared their binding energies with those of estradiol which is the natural ligand for the receptor. Based on the Lamarckian genetic algorithm, the three best conformations were selected and averaged for each ligand and a detailed analysis of molecular interactions based on the free energies of binding was computed. The order of binding energies were BPA > monochloro-BPA > mononitro-BPA > dichloro-BPA > dinitro-BPA > estradiol. These results suggested that oxidative metabolites of BPA retained their estrogenic activity. They appeared as potent as BPA and would possibly act as agonists for estradiol through competitive binding with ERRγ. Further investigations on the molecular dynamic simulations are currently underway to establish the interactions of BPA and its metabolites with ERRγ at the atomic level.

Quantum Cosmology with High Performance Computers

Brajesh Gupt,[1] Peter Diener,[1,2] and Parampreet Singh[1]

[1]*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803*
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One of the main problems in theoretical physics is the issue of cosmological singularities. Classically, singularit are found e.g. at the center of black holes and at the Big Bang. It has been hoped that quantum gravity will resolve t cosmological singularities and provide answers to the fundamental question related to the origin of the universe. T objective of this research is to explore these issues using the state of the art numerical techniques on high performar computers (HPC) and GPU based supercomputers [1].

Loop quantum gravity (LQG) is a theory of quantum gravity according to which the spacetime has discrete quantu geometry at its fundamental level. Loop quantum cosmology (LQC) applies LQG in a cosmological setting. Due the underlying quantum geometric effects, LQC resolves all the physical singularities in a homogeneous and isotro universe by replacing the Big Bang by a Big Bounce bridging two disparate phases of the universe, namely t expanding and contracting phases which were otherwise disjoint in the classical theory[2–4]. The evolution equati of LQC is a difference equation endowed with underlying discreteness in the spatial geometry unlike the Wheel DeWitt (WDW) evolution equation which is a partial differential equation based on the continuum description spacetime. The evolution given by the WDW equation follows the classical trajectory and ends up in a Big Ba singularity, while the LQC evolution bounces. However, they both agree extremely well in the semiclassical limit, i the LQC difference equation can be very well approximated by the WDW equation when the volume is very lar compared to the planck volume and the energy density is less than a percent of the planck density (i.e low curvatu of the spacetime geometry).

In this work we numerically evolve semiclassical states (representing the wavefunction of the universe) correspondi to specified initial data, using the LQC evolution equation. For a typical evolution of a 1+1 dimensional (one spat and one time dimension) widely spread state, which corresponds to a quantum universe, the total run time, the LQC difference equations, can be estimated to be of the the order of 10^{10} years on a single CPU core. To around this issue we propose the *"Chimera"* scheme which utilizes the fact that the LQC difference equation can approximated very well by the WDW equation at large volume. Thus we can split the domain in 2 pieces where t LQC equation is solved on the inner domain and the WDW equation on the outer domain. Since the WDW is a PI with a continuum limit we can reduce the computational cost by applying a coordinate transformation on the ou domain. Using the Chimera scheme the evolution of a widely spread state can be brought down to less than an ho on a single CPU core using a total memory of 11Mb.

We plan to develop 2+1 (two spatial and one time dimension) and 3+1 dimensional implementations of t "Chimera" scheme, for which HPC is definitely needed. The number of grid points scales as n^d in higher dim sions, where n is the number of grid points in one dimension and d is the number of spatial dimensions. We c estimate that the simulation of a similar (as discussed above) widely spread state would require of the order of 10,0 core hours and 600 Gb memory for a 2+1 dimensional evolution. If the interface between the inner and outer dom is moved to twice the volume (the "Chimera" equivalent of a convergence test) it would take about 100,000 core hou and 2.4 Tb of memory for the entire simulation. These simulations can thus be achieved on a 1000 core machine a day (for lower resolution) and in a week (for higher resolution). For 3+1 dimensions, the requirements for a wid spread state well exceed the capability of the currently available HPC systems. A subset of parameters, correspondi to sharply peaked states can however be run at current HPC system at a reasonable cost. In this project we pl to implement the Chimera scheme in 2+1 and 3+1 dimensions within the Cactus framework. This allows us to ta advantage of the work being done in the "Chemura" project at LSU on supporting GPU computing in Cactus.

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Chemora - A Multilevel Code Generation And Optimization Framework For Heteregenous Systems

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(Dated: May 10, 2012)

The Chemora framework takes a high level set of mathematical equations describing a Cauchy problem on a complex patchwork of curvilinear grids and generates a solution optimized to make full use of CPU's (paying attention to thread, cache and vectorization issues), GPU's (paying attention to register use, warp occupancy issues, etc.), and the MPI message passing infrastructure that connects them.

Chemora leverages and extends the Cactus component framework for for orchestrating the computation, moving data between processors or between the CPU and GPU, and adds a dynamic layer capable of generating or regenerating complex code at runtime (both CUDA and OpenCL) to achieve the highest performance. A built-in analysis module provides feedback on GPU performance and advises a running calculation or informs decisions for subsequent computations.

We use the system to solve the Einstein equations to simulate the final coalescence of binary black hole systems, which are leading candidates as sources of gravitational waves detectable by detectors, such as Advanced LIGO (Laser Interferometer Gravitational-wave Observatories). While the Einstein equations are compact when written in tensor notation, the expanded form required for computation contains hundreds of variables with right hand sides containing hundreds of terms. This code provides an acid test, requiring careful balancing of registers and shared memory as well as analysis of both the data and instruction cache.

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3D Mass Diffusion-Reaction System Modeling in the Neuromuscular Junction

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Abstract

A full 3D model of acetylcholine and acetylcholine receptor dynamics in the neuromuscular junction under conditions of inactivated enzyme has been developed. An improved Crank–Nicolson finite difference scheme is employed for solving the 3D model with Neumann boundary condition in cylindrical coordinates. In particular, a new, stable and accurate finite difference scheme is developed for the Neumann boundary condition. The simulation analysis agrees well with experimental measurements of end-plate current, and duplicates the open receptor results of earlier investigations. Sensitivity of the open receptor dynamics to the changes in the diffusion parameters has been studied. It presents the first simulation of asymmetric emission of acetylcholine in the synaptic cleft and an analysis of the subsequent effects on open receptor population as a function of time. Results show that the population of open receptors decreases as acetylcholine is emitted closer to the edge of the NMJ. Future investigations will focus in-depth study of anisotropic diffusion in the cleft, asymmetric distribution of vesicles in the pre-synaptic membrane, and completing the chemical reaction processes with the addition of acetylcholinesterase to the chemical kinetics of the NMJ.

Spin Glass Simulation with Parallel Tempering on GPU

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Abstract

This report presents our optimization efforts and tuning methods for spin glass simulation on nVidia GPUs. We discuss the choice and integration from various design alternatives, such as data layouts; memory transaction / arithmetic operation conversion; kernel granularities; parallel tempering swap frequency; tiling; and loop unrolling. We also explain our innovational binary data format named CMSC (Compact Multispin Coding) as a variation of AMSC (Asynchronous Multispin Coding) [1]. Our evaluation reveals a speedup of 18% when switching from AMSC to CMSC. The overall design outperforms former GPU implementations [234] by a factor of 5, and reaches 83% of the fastest system which is based on customized hardware [5].

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Names: Daswanth Lingam, Michal Brylinski

Title: Computational Network Biology for systems-level functional annotation of proteins and proteomes

Abstract:

Computational Systems Biology aims to develop and apply efficient algorithms to address critical scientific questions through computer simulations and theoretical modeling. The system-wide level modeling is particularly relevant in modern biological sciences, where the key challenge has shifted from the study of single molecules to the exhaustive exploration of molecular interactions and biological processes at the level of complete proteomes. Understanding how complex living systems work can help find treatments for disorders of poorly understood etiology, such as cancer and neurodegenerative disorders. The major focus of our group is the design and development of novel tools for the modeling and analysis of biological networks using Computational Systems Biology. We are interested in applying various Computational Systems Biology tools to study the evolution and organization of pathways into biological networks with the primary application in modern drug discovery and design.

Introducing Students to HPC
Abstract for HPC User Symposium 2012 Poster

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At the Louisiana School for Math, Science, and the Arts, we have struggled to get students interested in HPC, and in computing in general. Especially since the state revoked the computer-science high-school graduation requirement, the students who were already interested in computing are still taking our programming courses, but we have trouble enticing students to explore computing.

There are four pernicious problems we face. The worst that most students have no idea how to navigate file systems and have a low tolerance for being uncertain of what they're doing. Another is that even our best coders do not understand the canonical examples, because they are taking Data Structures before Linear Algebra. Third, our good coders spend so much time coding that they are failing at least one course. Finally, many faculty do not recognize the power and influence of computing in their disciplines.

We have had several successes.

In November, we took seven students to SCALA'12, Scientific Computing Around Louisiana, here at LSU.

This month we had a week-long course in parallel programming, using OpenMP and MPI. Four of the six students have requested LONI accounts to continue their explorations.

In November, we became the first high school to receive a LittleFe teaching cluster. I will spend the summer, in an NSF RET through LA-SiGMA, to develop applications relevant to our students.

This fall, I will personally mentor three of our best coders, to make sure they are doing their other academic work as well as programming.

We have a Computational Thinking Program that hosts evening workshops and speakers. This year we will start with introductory topics in Excel, Google Docs, MathType, GeoGebra, and Sage. For students we succeed in interesting in computing, we will offer smaller sessions on visualization, mathematical and scientific applications, and parallelization.

In the spring, I will teach a Numerical Methods course. Prerequisites are Calc I and a semester of either `C++` or Python.

There are many challenges to introducing students to HPC, but many opportunities for the students who develop interest and skills.

Optimal Microarchitectural Design Configuration Selection for Processor Hard-Error Reliability

Ying Zhang, Lide Duan, Bin Li, Lu Peng

Abstract: traditional design space exploration mainly focuses on performance and power consumption. However, as one of the first-class constraints for modern processor design, the relationship between hard-error reliability and processor configurations has not been well studied. In this paper, we investigate this relationship by exploring a large processor design space. We employ a rule search strategy, i.e. Patient Rule Induction Method, to generate a set of rules which choose optimal configurations for processor hard-error reliability and its tradeoff with performance and power consumption.

Presenters: Ole Weidner, Shantenu Jha, Andre Merzky, Andre Luckow

SAGA-Bliss and BigJob: Scaling Research to Support Production Science

An increasing number of computational scienctists require the concurrent use of multiple distributed compute and storage resources in order to scale their applications along both the data and compute axis. However, inhomogeneous access methods, software stacks and middleware services still present a major barrier to cross-resource scalability and interoperability.
To address these fundamental and persistent challenges, we have developed SAGA-Bliss and BigJob. SAGA-Bliss is a distributed computing package for Python; BigJob is a pilot-job framework implemented using SAGA-Bliss. We show how SAGA-Bliss and BigJob can be used in two different modes: (A) to implement novel application architectures, abstractions and frameworks and (B) to distribute and run large number of jobs and their associated data concurrently across multiple HPC resources.
SAGA-Bliss and BigJob are both production-grade tools for scalable science, as well as a platform for research into applied distributed computing in heterogeneous environments.

SAGA-Bliss (http://saga-project.github.com/bliss/):

SAGA-Bliss is a light-weight Python package that implements parts of the OGF GFD.90 SAGA interface specification and provides plug-ins for different distributed middleware systems and services. SAGA-Bliss implements the most commonly used features of GFD.90 based upon extensive use-case analysis, usability and simple deployment in real-world heterogeneous distributed computing environments and application scenarios.
Currently, SAGA-Bliss implements the job and the file management core APIs as well as the resource management API extension. SAGA-Bliss provides a plug-in mechanism to connect with different middleware systems and back-ends. The latest version of SAGA-Bliss provides job and file management plug-ins for SSH, SFTP, the HPC scheduling systems PBS, Torque and SGE (locally and remotely - tunneled via SSH), as well as a resource management plug-in for Eucalyptus (EC2) clouds. SAGA-Bliss can be used to access distributed cyberinfrastructure like XSEDE, LONI and FutureGrid, as well as clouds and local clusters.

BigJob (https://github.com/saga-project/BigJob):

BigJob is a Python pilot-job framework implemented on top of SAGA. Pilot-jobs provide a flexible and dynamic execution model by decoupling workload submission from resource assignment, which allows the distributed scale-out of applications on multiple, potentially heterogeneous resources. Another important advantage of this approach is that aggregated queue waiting times, which often contribute significantly to the overall time-to-completion of many-job workloads, can be severely reduced.
BigJob supports a wide range of application types and can be used over a broad range of infrastructures, including XSEDE, OSG, FutureGrid, EGI and LONI. BigJob supports multiple types and granularity of concurrency, e.g., large MPI jobs as well as single node/core jobs equally well. BigJob has been used to support Molecular Biophysics, Computational Chemistry, Statistical Physics and Computer Science research, on XSEDE, FutureGrid, OSG and other distributed infrastructures.

Dynamical embedding of the dual fermion dynamical cluster approach for strongly correlated systems

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Abstract

We extend the recently developed dual fermion dynamical cluster approach[1] with a further embedding of the dual fermion lattice into a larger, third length scale. The resulting approach is a complete multi-scale many-body technique for strongly correlated electron systems. It treats the short length scales explicitly by the dynamical cluster approach[2], intermediate length scales diagrammatically with the dual fermion technique[3], and the largest length scales approximately at a dynamical mean-field level. This technique iterates to self-consistency on all the three length scales, and the embedding scheme preserves the causality. The transformation from real fermion to dual fermion is exact, and the dual fermion diagrammatical perturbation has a small parameter such that each n-body insertion scales as $1/\mathrm{Lc}^n$, where Lc is linear cluster size in the short length scale. To illustrate the implementation and applicability of this method, we test it with the one and two dimensional Falikov-Kimball model and Hubbard model. Our preliminary results show a faster convergence in our multi-scale method compared with previous two-length-scale approach. Besides all the other advantages, the multi-scale many-body technique will give us the necessary momentum resolution to address the fundamental questions such as the formation of hole-pocket and the nature of pseudogap state in the underdoped high-temperature copper oxide superconductors.

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Ferromagnetic Semiconductors: Prospect and Future

R. Nelson, A.-M. Nili, J. Moreno, W. Ku, M. Jarrell, N. Ranjitkar, A. Paudyal, G. Joseph, P.A. Derosa, B. R. Ramachandran

Abstract

This project will extend to magnetic and conductive organic materials, ongoing research on semiconductors. Existing efforts are focused on the study of ferromagnetic semiconductors using combination of Wannier functions-based ab-initio and many-body methods. The pure and doped Hamiltonian of the (Ga,Mn)As and (Ga,Mn)N are ab-initio calculated and dowfolded. The subtraction of these two Hamiltonians tells about the influence strength of the impurity (Mn). Dynamical mean-field approximation is applied to examine the effect of the Mn impurities into the magnetic and electrical properties of (GaMn)As and (Ga,Mn)N. Results are compared with experiments and prior results on (Ga,Mn)As. This work will be expanded to other systems, in particular, a similar approach will be used to study the electrical and magnetic properties of metallo porphyrins.

Adsorption of atmospherically relevant gases on bare and surfactant coated ice films

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Polycyclic aromatic hydrocarbons (PAHs) consist of two or more carbon-hydrogen ring compounds in which at least one ring has an aromatic structure. PAHs are known to have important carcinogenic and mutagenic effects. Furthermore, these compounds can undergo photo chemically induced oxidation and nitration reactions with reactive oxygen species (ROSs) [e.g., ozone (O_3) and radicals such as singlet oxygen, hydroperoxy (HO_2), hydroxyl (OH) and nitrate (NO_3)]. Reactions of PAHs with ROSs produce oxy- and nitro-PAHs that are even more toxic than PAHs. PAHs can be adsorbed at the surfaces of water droplets, atmospheric aerosols, fog and mist, and ice and snow. This process consists of adsorption to the interface and dissolution in the bulk water and quasi-liquid layer (QLL). The processes taking place at atmospheric air/ice therefore have a profound impact on the fate and transport of PAHs and other trace gases in the atmosphere.

However, and despite their relevance, a fundamental understanding of the adsorption and heterogeneous reactions of aromatic hydrocarbons and reactive oxygen species at air/ice interface is still lacking. Here we report a molecular simulation study where we attempt to elucidate molecular-level details of the adsorption mechanism of gas-phase naphthalene and ozone species onto air/ice interfaces coated with different surfactant species (1-octanol, 1-hexadecanol, or 1-octanal). The surface adsorption of both naphthalene and ozone onto surfactant-coated air/ice interfaces is enhanced when compared to bare air/ice interface. Both naphthalene and ozone tend to stay dissolved in the surfactant layer present at the air/ice interface rather than adsorbing on top of the surfactant molecules.

Hirsch-Fye Quantum Monte Carlo on GPUs

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Abstract

In Dynamical Mean Field Theory and its cluster extensions, such as the Dynamic Cluster Algorithm, the bottleneck of the algorithm is solving the self-consistency equations with an impurity solver. Hirsch-Fye Quantum Monte Carlo is one of the most commonly used impurity and cluster solvers. This work implements optimizations of the algorithm, such as enabling large data re-use, suitable for the Graphics Processing Unit (GPU) architecture. The GPU's sheer number of concurrent parallel computations and large bandwidth to many shared memories takes advantage of the inherent parallelism in the Green function update and measurement routines, and can substantially improve the efficiency of the Hirsch-Fye impurity solver.

POSTER

Numerical Model System for Ecosystem Restoration and Flood Risks Reduction (ERFRR) in the Northern Gulf Coast

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The Northern Gulf Coast constitutes one of the most culturally and ecologically rich coastal ecosystems in the world. These ecosystems are a buffer against storm damage and a nursery and foraging area for fish and crustaceans. Restoration of important coastal features such as wetlands and barrier islands is a critical strategy that will provide the 'natural infrastructure' to protect coastal communities. Numerical experiments are being developed to quantify the flood risks reduction by predicting the effect of future landscape features created by potential restoration projects. Several models will be used to compare and contrast storm surge and wave reduction before and after ecosystem restoration. The model system and results during historical hurricane events in the Northern Gulf Coast are presented in this poster. The study has been supported by the NSF Northern Gulf Coastal Hazards Collaboratory (Award number 1010640) and NGI (09-NGI-08). Computational resources were provided by LONI and LSU.

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Meso-Scale Analysis of Deformation Induced Heating of Metalized Explosive

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ABSTRACT

The heterogeneous meso-structure associated with solid explosives lead to high frequency fluctuations in temperature fields which give rise to the formation of **hot-spots**. The hot-spots are difficult to experimentally resolve, and are influenced by the material's meso-structure. In this study a combined Lagrangian finite element-discrete element technique is used to computationally examine the deformation induced heating in granular metal (Al)-explosive (HMX) mixtures due to piston supported uniaxial waves. Emphasis is placed on characterizing the effects of particle-size, metal mass fraction and porosity on hot-spot distribution and bulk thermo-mechanical fields.

Sponsors: Defense Threat Reduction Agency (DTRA-WMD), U.S. Air Force Research Laboratory (AFRL-RWME)

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Development of a Non-Hydrostatic Model for Simulation of Nonlinear Waves over Submerged Vegetation

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Accurate prediction of nonlinear surface waves is very important in coastal and ocean engineering. Rapid advances in computational technology allow directly solving the Euler equations or Navier-Stokes equations for non-hydrostatic free surface flows for practical applications. This paper presents a numerical model for simulating the propagation of fully dispersive, nonlinear water waves in coastal areas. Finite difference method on an unconventional grid is used to solve the governing equations with the free-surface boundary conditions. The sigma coordinate transformation helps map the irregular physical domain with the wavy free surface and uneven bottom to the regular computation domain. An improved technique for the vertical discretization is utilized to optimize the model performance to simulate fully dispersive waves with a minimum number of vertical layers for the sake of reducing the computational cost.

A first order forward difference for time and a second order central difference for space in combination with a semi-implicit scheme are utilized to discretize the governing equations. The algorithm is split into hydrostatic and non-hydrostatic phases. An efficient large-scale linear system equations solver, HYPRE (High Performance Pre-conditioners) is employed to solve the discrete Poisson equation for pressure correction in the non-hydrostatic phase. The effectiveness of the optimized sigma transformation approach for the treatment of the free surface is tested against analytical solutions. One application of this model is to reproduce the process of nonlinear wave propagation over submerged vegetation. By incorporating drag forces in the momentum equations, we are able to simulate wave attenuation by saltmarsh vegetation. The model is being tested against available laboratory and field data. Detailed results will be presented with form of a poster.

Simulation of Wave Attenuation by Fluid Mud Using a Finite-Volume Navier-Stokes Model

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Louisiana State University

Water wave motion is one of the key factors that cause the change of coastline Therefore, an accurate model for near-shore wave simulation is critical to the protectio and restoration of the Louisiana coast. Most of the existing wave models focus on wav propagation over an impermeable rigid bed. However, cohesive sediment and fluid mu are common along the Louisiana coast. A wave model that is capable of modeling wav attenuation by fluid mud is needed.

The poster presents a numerical model solving the three-dimensional Navier-Stoke equations for simulating fully-nonlinear and fully dispersive water waves over flui mud. A finite volume method on a modified staggered grid is employed. This new gri enables the modeling of dispersive waves with much fewer layers and thus improves th efficiency. In this model, the computational domain is treated as a two-layer viscou fluid system with the water layer on the top and the fluid mud layer at the bottom. A dual-mesh grid structure is designed for the two layer water-mud system. The sam numerical schemes are used for these two fluid layers that accommodate differences i fluid properties and boundary conditions.

Because the model is not limited to shallow water waves, the non-hydrostatic pressur needs to be properly considered. A pressure correction method that divides the tim integration into the hydrostatic step and non-hydrostatic step is employed. An efficient scalable solver for a large system of linear equations, HYPRE (High Performance Pre conditioners), is used to solve the Poisson equation that comes from the non-hydrostati pressure correction. The scalability of HYPRE makes it possible to model non-linea waves in a large domain for practical applications using massive-processor, high performance computers. The model is tested against analytical solutions as well a available laboratory and field measurements. Details will be presented at th Symposium.

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Numerical modeling of nonlinear triad interaction of shallow water waves

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When waves propagate in shallow water, nonlinear interactions of wave components result in energy transfer and the mismatch between bound and free waves governs the beat length. Triad interaction of water waves in shallow water is important for a number of physical processes and to explain the energy transfer between low and high frequency parts of the wave spectra during wave propagation.

The evolution equations based on the Boussinesq-type equations were derived using the multi-scale perturbation analysis and then were solved to simulate nonlinear triad interaction of shallow water waves by three approaches plus a fourth-order Runge-Kutta (RK4) scheme. On the other hand, two numerical models of FUNWAVE-TVD (Fully Nonlinear Boussinesq Wave Model with TVD Solver) developed by Fengyan Shi et al. (2011) and FUNWAVE 1.0 1-D (1998) by Kirby et al. are used to simulate pure three wave interaction as well as wave shoaling on cluster Queen Bee of LONI (the Louisiana Optical Network Initiative). Comparison of different numerical models in both examples will be shown.

Role of the van Hove singularity in the Quantum Criticality of the Hubbard Model

K.-S. Chen, S. Pathak, S.-X. Yang, S.-Q. Su, D. Galanakis,
K. Mikelsons, M. Jarrell and J. Moreno

June 4, 2012

A quantum critical point is found in the phase diagram of the two-dimensional Hubbard model [Vidhyadhiraja et al., Phys. Rev. Lett. **102**, 206407 (2009)]. It is due to the vanishing of the critical temperature associated with a phase separation transition, and it separates the non-Fermi liquid region from the Fermi liquid. Near the quantum critical point, the pairing is enhanced since the real part of the bare d-wave pairing susceptibility exhibits an algebraic divergence with decreasing temperature, replacing the logarithmic divergence found in a Fermi liquid [Yang et al., Phys. Rev. Lett. **106**, 047004 (2011)]. In this paper we explore the single-particle and transport properties near the quantum critical point using high quality estimates of the self energy obtained by *direct* analytic continuation of the self energy from Continuous-Time Quantum Monte Carlo. We focus mainly on a van Hove singularity coming from the relatively flat dispersion that crosses the Fermi level near the quantum critical filling. The flat part of the dispersion orthogonal to the antinodal direction remains pinned near the Fermi level for a range of doping that increases when we include a negative next-near-neighbor hopping t' in the model. For comparison, we calculate the bare d-wave pairing susceptibility for non-interacting models with the usual two-dimensional tight binding dispersion and a hypothetical quartic dispersion. We find that neither model yields a van Hove singularity that completely describes the critical algebraic behavior of the bare d-wave pairing susceptibility found in the numerical data. The resistivity, thermal conductivity, thermopower, and the Wiedemann-Franz Law are examined in the Fermi liquid, marginal Fermi liquid, and pseudo-gap doping regions. A negative next-near-neighbor hopping t' increases the doping region with marginal Fermi liquid character. Both T and negativet' are relevant variables for the quantum critical point, and both the transport and the displacement of the van Hove singularity with filling suggest that they are qualitatively similar in their effect.

Ab-Initio Study of Iron Oxide Clusters and Their Reactions with Phenol, 2-Chlorophenol, and 4-Chlorophenol

Lucy W. Kiruri, Cheri A. McFerrin, Barry Dellinger, and Randall W. Hall
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Copper and iron oxide nanostructured particles have been identified to be particularly effective catalysts for the formation of polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/F) and other pollutants during combustion processes. Environmentally persistent free radicals form over combustion-produced copper and iron-oxide containing nanoparticles, and these radicals have been shown to be intermediates in the formation of PCDD/F and be a possible cause of the observed health impacts of airborne fine particles. It is thought metal atoms in the metal oxide clusters facilitate the formation of radicals via electron transfer from a physisorbed molecular precursor to the metal atom in a metal oxide cluster. For this reason, we are studying the structure and reactivities of metal oxide clusters. This involves accurate density functional calculations and the development of force fields capable of allowing calculations involving metal oxide clusters containing tens to hundreds of metal atoms. LA-SiGMA's focus on accurate density functionals and force fields is a critical component of understanding the mechanism for metal oxide catalysis of PCDD/Fs.

Computational Studies of the Hydrogen Storage Capabilities of $KMgH_3$

Brandon Borill[1], Randall Hall[1], Daniela Mainardi[2], Fernando Soto[2]
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The study of metal hydrides as hydrogen storage materials is driven by the desire to further understand potential alternative energy applications. Numerous studies are investigating the properties of complex metal hydrides. Potassium magnesium hydride ($KMgH_3$) is one such hydride. Other complex metal hydrides such as lanthanum nickel hydride ($LaNi_5H_6$) and sodium magnesium hydride have been studied and are continuing to be researched.

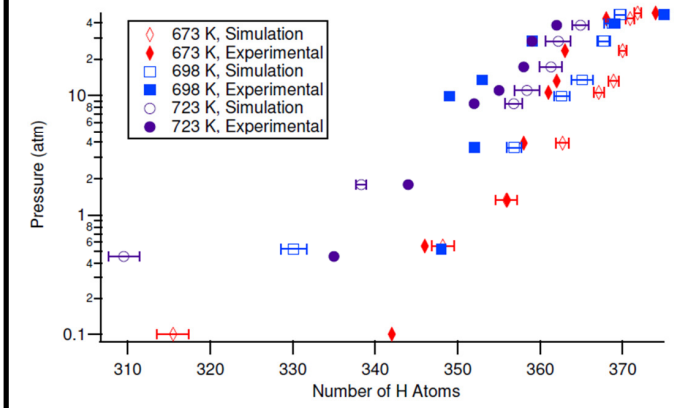

Figure 1: A PCT (pressure-composition-temperature) plot comparing the experimental data to the simulations

Monte Carlo simulations have been performed to determine the number of metal atoms at various temperatures and pressures for $KMgH_3$. Experimental research performed by Komiya *et al.* involved the investigation of the percent hydrogen in $KMgH_3$ samples at 673 K, 698 K, and 723 K at varying pressures [1]. The results from our Monte Carlo simulations revealed statistically similar results to their experiments (Figure 1). It is important to note the interpretation of the experimental data is derived from a digitized plot of the data from Komiya *et al*.

[1] Komiya, K., Morisaku, N., Rong, R., Takahashi, Y., Shinzato, Y., Yukawa, H., Morinaga, M. *J. Alloys Compd., 453*, 157 (2008).

Monte Carlo Simulations of Nucleation in 2d systems

Troy Loeffler and Bin Chen

The physical phenomenon of Nucleation is a major step in phase transitions where a supersaturated vapor phase begins condensing into microscopic clusters of the new stable phase. By understanding the conditions of this formation it is possible to understand the resulting macroscopic structures form. Historically experimental data has been difficult to obtain and often for complex systems there are too many variables to account for. As a result simulations have provided an avenue to examine nucleation and explain the inner workings of the process.

Our research makes use of previously developed techniques such as Volume Bias Aggregation, Umbrella Sampling, and other simulation methods in order to create a free energy profile as a function of the cluster size. We compare our results to the predominant nucleation theory know as Classical Nucleation Theory (CNT) to investigate how ideally a system behaves. Our research group makes use of the LSU HPC and LONI computing centers to generate large data sets to obtain fast and accurate convergence of our data.

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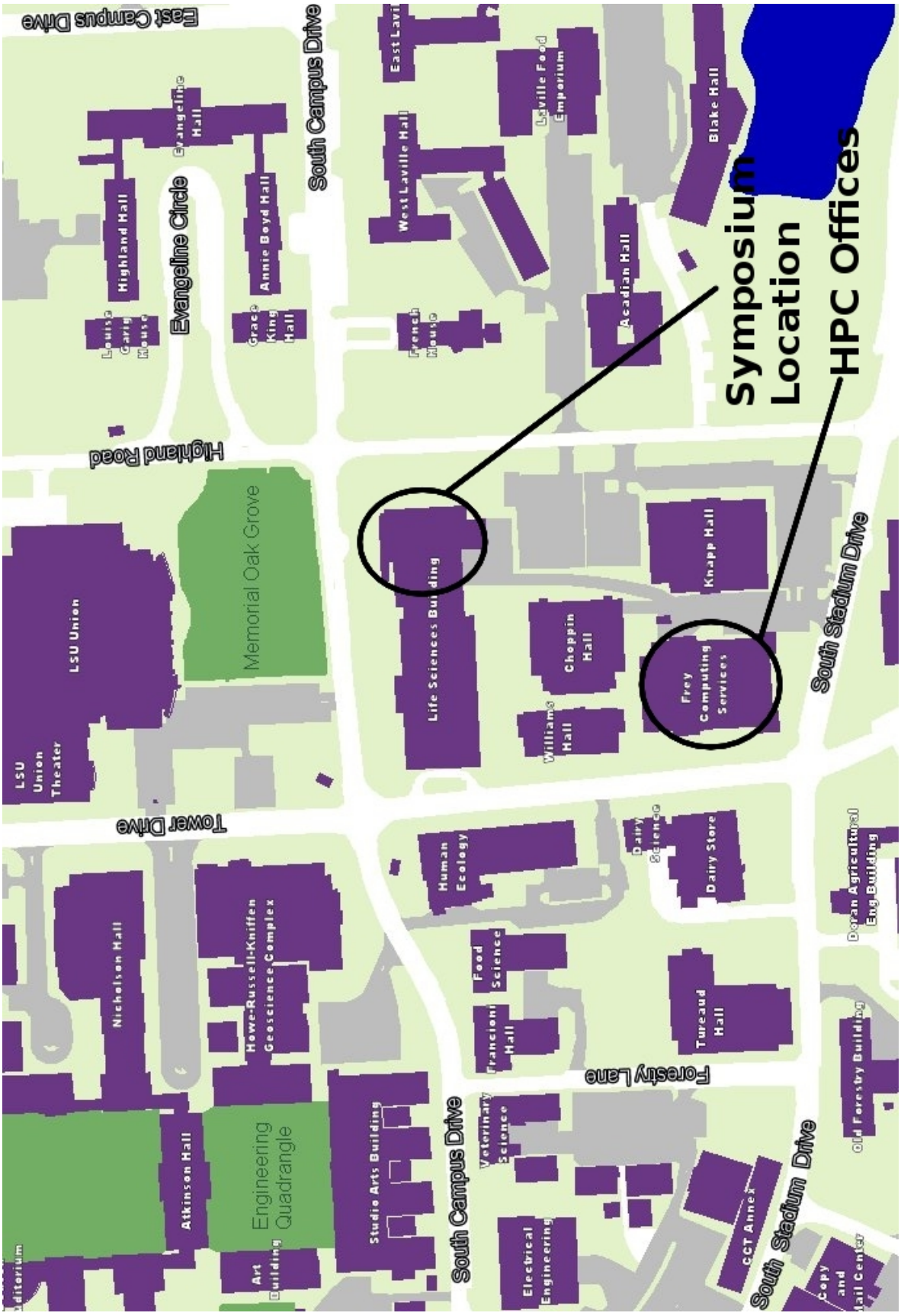
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Grace King Hall
Louisa Garig House
French House
East Lavi
West Laville Hall
Laville Food Emporium
Blake Hall
Acadian Hall
LSU Union
LSU Union Theater
Life Sciences Building
Knapp Hall
Choppin Hall
William Hall
Frey Computing Services
Human Ecology
Dairy Science
Dairy Store
Dolan Agricultural Eng Building
Food Science
Francioni Hall
Tureaud Hall
Old Forestry Building
Nicholson Hall
Howe-Russell-Kniffen Geoscience Complex
Atkinson Hall
Studio Arts Building
Art Building
Veterinary Science
Electrical Engineering
CCT Annex
Copy and Mail Center

Life Science Annex Lobby Poster Setup