2nd Annual High Performance Computing User Symposium

Louisiana State University, Baton Rouge

June 12 - 13, 2013

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Table of Contents

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 2^{nd} Annual 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. In addition to the workshops immediately preceeding and following this Symposium, we offer a wide variety of training targeted towards both new and advanced users. Examples of advanced training topics include programming/scripting languages, developmental and debugging tools, and various scientific application topics and software tools. All our weekly training is webcast using Adobe Connect and users have a choice of joining the webcast, attend in person at LSU or access recordings and training material on our website.

LONI, LSU ITS and LSU CCT have collaborated to organize the 2^{nd} Annual High Performance Computing User Symposium.

The purpose of the User Symposium is threefold:

1. to introduce LSU and LONI HPC users to each other in the hope that they will find ways to collaborate and enrich their research scope;
2. to facilitate the sharing of experiences using HPC resources in order to learn from 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.

Introduced in 2012, this Symposium was 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 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, and Xavier University of Louisiana. Special thanks to Robert R. Twilley and the School of the Coast & Environment (venue), Randy Duran (tables) and John I. Quebedeaux Jr (poster boards) for providing resources for the Symposium. I would also like to thank the Scientific Advisory Committee, staff at CCT and ITS for their efforts in making this Symposium a success.

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

This 2^{nd} 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,

It is with great pleasure that we welcome you to the 2^{nd} Annual HPC User Symposium. What better way to meet and collaborate with local professionals that have a desire to do what you do? Namely, the desire to perform research in so many critical scientific areas and to share tips and tricks with each other on how to utilize the tools and resources that are available.

With the recent introduction of SuperMike II and the continued support of LSU and LONI High Performance Systems, we are continuing to establish ourselves as a critical player in the role of HPC. Please take the time to learn, share, and express your thoughts on ways we can all get better at what we do.

Best wishes for a successful experience.

Ric Simmons,
Deputy Chief Information Officer
Louisiana State University

On behalf of LSU's Center for Computation & Technology (CCT), I am pleased to welcome you to this 2^{nd} Annual 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,

On behalf of Xavier University of Louisiana, I would like to welcome you to the 2^{nd} Annual High Performance Computing User Symposium at LSU. Xavier recently became the newest LONI institution through a $1.2 million grant from the National Science Foundation EPSCoR program and we are excited to help sponsor this event. In addition to providing funding to support fiber construction for Xavier's physical connection to LONI, NSF funding has supported research and educational programming to develop high performance computing expertise for Xavier's faculty and students. Over the past two years, Xavier faculty and students have begun to forge active research relationships with computational researchers throughout the State in bioinformatics, physics, mathematics, and materials science research. Our investigators are excited to take part in this Symposium and look forward to connecting with the HPC user community to build future collaborations.

Sincerly,
Gene D'Amour,
Senior Vice President for Resource Development
Xavier University of Louisiana

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 12th, 2013	Rotunda Lobby, Energy, Coast & Environment Building
6:00 pm - 8:00 pm	Registration and Poster Session
June 13th, 2013	Dalton J. Woods Auditorium, Energy, Coast & Environment Building
8:00 am - 8:20 am	Registration
8:30 am - 8:40 am	Welcome
Session I	Chair: Don Liu, Louisiana Tech University
8:40 am - 9:00 am	*XSEDE* James A. Lupo Center for Computation & Technology, Louisiana State University
9:00 am - 9:30 am	*Computational Chemistry using LONI, from small ab initio calculations to large scale simulations for molecular systems* Collin D. Wick Department of Chemistry, Louisiana Tech University
9:30 am - 10:00 am	*Teaching and Mentoring HPC in High School* J. Bradford Burkman Department of Mathematics, Louisiana School for Math, Science, and the Arts
10:00 am - 10:15 am	Break
Session II	Chair: Rachel Vincent-Finley, Southern University
10:15 am - 10:45 am	*Comparative and evolutionary genomics of halophytic (salt-loving) plants* Dong-Ha Oh Department of Biological Sciences, Louisiana State University
10:45 am - 11:15 am	*Molecular Simulation of Electric Double-Layer Capacitors Based on Carbon Nanotube Forests* Lawrence R. Pratt Department of Chemical & Biomolecular Engineering, Tulane University
11:15 am - 11:45 am	*Numerical Modeling of Sediment Transport on the Texas-Louisiana Shelf* Kehui Xu Department of Oceanography and Coastal Sciences, Louisiana State University
11:45 am - 12:00 pm	*Selected Graduate Student Oral Presentation* Ahmed S. Elshall Louisiana State University
12:00 pm - 1:00 pm	Lunch (provided)

Symposium Program

June 13th, 2013	
Session III	Chair: Frank R. Wesselmann, Xavier University of Louisiana
1:00 pm - 1:30 pm	*Symmetry Adapted & HPC Enabled Nuclear Structure Studies* Jerry P. Draayer Department of Physics & Astronomy, Louisiana State University
1:30 pm - 2:00 pm	*The effects of charge transfer on the properties of liquids* Steven W. Rick Department of Chemistry, University of New Orleans
2:00 pm - 2:30 pm	*Hybrid Parallel Computing of Minimum Action Method* Xiaoliang Wan Department of Mathematics, Louisiana State University
2:30 pm - 2:45 pm	*Selected Graduate Student Oral Presentation* Yifan Wang Louisiana Tech University
2:45 pm - 3:00 pm	Break
Session IV	Chair: Le Yan, Louisiana State University
3:00 pm - 3:30 pm	*Using HPC to Develop Branch Protection Estimators* David M. Koppelman Division of Electrical & Computer Engineering, Louisiana State University
3:30 pm - 4:00 pm	*Research Projects of HPC Group at Southern University* Liuxi Tan Department of Computer Science, Southern University
4:00 pm - 4:30 pm	*Fluid Flow and Heat Transfer in Polygonal Micro Heat Pipes* Harris Wong Department of Mechanical and Industrial Engineering, Louisiana State University
4:30 pm - 4:45 pm	*Selected Graduate Student Oral Presentation* Niladri Sengupta Louisiana State University
4:45 pm - 5:00 pm	*Selected Undergraduate Student Oral Presentation* Caleb Deluane Southeastern Louisiana University
5:00 pm - 5:10 pm	Closing Remarks

List of Posters

WEDNESDAY, JUNE 12TH, 2013 (ROTUNDA LOBBY, ENERGY, COAST & ENVIRONMENT BUILDING)

1 Molecular Dynamics Simulation of VECAR molecules

Caleb Delaune
Department of Chemistry and Physics, Southeastern Louisiana University

2 Genomic ultraconserved elements resolve the comparative phlyogeography of five Neotropical birds

Michael G. Harvey
Museum of Natural Science and Department of Biological Sciences, Louisiana State University

3 Mathematical Model of Metal Hydrogen Desorption and Inverse Problem

Fei Han
Department of Mathematics and Statistics, Louisiana Tech University

4 Comparison of different models of electron and nuclear couplings in biomolecules and clusters: High Performance Computing (HPC) at LSU

Kresimir Rupnik
Department of Chemistry, Louisiana State University

5 Parallel Covariance Matrix Adaptation-Evolution Strategy for Modeling of Complex Groundwater Systems

Ahmed S. Elshall
Department of Civil and Environmental Engineering, Louisiana State University

6 High Performance Computing for Region-Scale Groundwater Recharge Estimation in Southeastern Louisiana and Southwestern Mississippi

Ehsan Beigi
Department of Civil and Environmental Engineering, Louisiana State University

7 GPU Enabled Simulation of Free Boundary Flow using Smoothed Particle Hydrodynamics

Yifan Wang
Department of Mathematics and Statistics, Louisiana Tech University

8 Parallel Simulation of Particulate Flow with Virtual Identity Particles and Spectral Modal Element Method

Don Liu
Department of Mathematics and Statistics, Louisiana Tech University

9 Applications of a finite volume immersed boundary method for complex geometries in river environments.

Getnet Agegnehu
Department of Civil and Environmental Engineering, Louisiana State University

10 Parallel Computation of a Finite Volume Coastal Ocean Model

Yi Du
Department of Oceanography and Coastal Sciences, Louisiana State University

11 Clutter Reduction in Visualization of Atomic Trajectories with Position Merging

Bidur Bohara
School of Electrical Engineering and Computer Science, Louisiana State University

12 First principles calculations of grain boundaries in Mg_2SiO_4 at high pressure

Dipta B. Ghosh
Division of Computer Science and Engineering, Louisiana State University

13 Toward tangible genomic user interfaces for enhancing mobile element research and education engaging multi-genome sequencing data

Shantanu Thatte
Center for Computation & Technology and School of Electrical Engineering and Computer Science, Louisiana State University

14 Effective Thermal Control Techniques for Liquid-Cooled 3D Multi-Core Processors

Yue Hu
Division of Electrical and Computer Engineering, Louisiana State University

15 Inferring the Expression Variability of Human Transposable Element-Derived Exons by Linear Model Analysis of Deep RNA Sequencing Data

Kun Zhang
Department of Computer Science, Xavier University of Louisiana

16 Alu Distribution and Mutation Types of Cancer Genes

Kun Zhang
Department of Computer Science, Xavier University of Louisiana

17 miRNA-Mediated Relationships between Cis-SNP Genotypes and Transcript Intensities in Lymphocyte Cell Lines

Kun Zhang
Department of Computer Science, Xavier University of Louisiana

18 *e*RefSite: Local Structure Refinement of Ligand Binding Sites in Protein Models

Wei Feinstein
Department of Biological Sciences, Louisiana State University

19 Developing Large-scale Scientific Application in Life Sciences Using High Performance Computing (HPC) and Cloud Computing

Joohyun Kim
Center for Computation & Technology, Louisiana State University

20 First-Principles Identification of Nitrogen-Doped Fullerene as Potential Cathode Catalyst for Hydrogen Fuel Cells

Feng Gao
Department of Physics, Southern University

21 GPU-accelerated ligand docking

Yun Ding
Department of Physics and Astronomy, Louisiana State University

22 A density functional study of the reactions of 2-chlorophenol, 1,2-Dichlorobenzene, Chlorobenzene with CuO - Cu_8O_8 clusters

Lucy Kiruri
Department of Chemistry, Louisiana State University

23 Synthetic libraries of drug-target complexes for structure-based drug design

Misagh Naderi
Department of Biological Sciences, Louisiana State University

24 *Ab-initio* Calculations of Accurate Electronic Properties of ZnS

Bethuel Khamala
Department of Physics, Southern University

25 Validation and Application of LES Modeling of Unidirectional and Wave Flow through Submerged Vegetation

Agnimitro Chakrabarti
Department of Civil and Environmental Engineering
Louisiana State University

26 GPU Implementation of a Variational Monte Carlo Study

Niladri Sengupta
Department of Physics and Astronomy, Louisiana State University

27 Quantum Cosmology with High Performance Computers

Brajesh Gupt
Department of Physics and Astronomy, Louisiana State University

28 Replica Exchange Dynamic Molecular simulations of Cyclic and Linear Amphiphilic Homopolymer

Lixin Liu
Department of Chemical and Biomolecular Engineering, Tulane University

29 Monte Carlo Simulations of Surface Induced Nucleation

Troy Loeffler
Department of Chemistry, Louisiana State University

Abstracts

Computational Chemistry using LONI, from small *ab initio* calculations to large scale simulations for molecular systems

Collin Wick

Department of Chemistry, Louisiana Tech University, Ruston, LA 71272

Abstract

Computational chemistry spans a large array of potential applications, offering tools to examine multiscale and multiphysics applications. Different tools are designed to investigate the physical properties of large systems, while others can be used to investigate chemical reactivity and specific environments. Monte Carlo simulations targeted towards polymeric systems will be described, including how unique attributes of these types of simulations allows the sampling of materials that cannot be sampled with traditional methods. Then, methods used to investigate reactivity in moderately large systems, including how the inclusion of additional physics allows an improved description of particular systems. Finally, investigations with efficient ab initio calculations will be described related to oxidation and reduction reactions relevant for battery electrodes. Overall, ways to enhance the capabilities of traditional molecular simulations methods will be described, that allows them to be expanded to more complicated physics and larger systems. Also, cases where computational methods can provide unique insight to an experiment and provide a unique interpretation of their results will be presented.

Teaching and Mentoring HPC in High School

J. Bradford Burkman

Instructor in Mathematics, Louisiana School for Math, Science, and the Arts, 715 University Pkwy, Natchitoches, LA 71457
XSEDE Campus Champion, Louisiana Scholars College, Morrison Hall, Northwestern State University of Louisiana, Natchitoches, LA 71497

Abstract

The Louisiana School for Math, Science, and the Arts, the state boarding school for capable and motivated students in grades 10-12, is exploring how to interest students in HPC and give them the skills to explore this field that will open doors to them not only in the sciences but also in data-intensive humanities research. This talk with highlight developments in the past year, future plans, and ways university researchers can help in this effort.

Comparative and evolutionary genomics of halophytic (salt-loving) plants

Dong-Ha Oh and Maheshi Dassanayake

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

Abstract

Unlike the majority of plant species including most crops, halophytic plants can survive seawater-level salt concentrations in the soil solution. Using next-generation sequencing platforms, we assembled genomes of two halophytic species, *Thellungiella parvula* and *T. salsuginea*, that are closely related to the model plant *Arabidopsis thaliana*. Originating from the hyper-saline Lake Tuz of central Turkey and the sea coasts of northern China, the two *Thellungiella* species have adapted to extremely saline environments for estimated 8∼12 million years, after their divergence from *Arabidopsis*. Comparison of genomes and transcriptomes between *Thellungiella* and *Arabidopsis* provide insights into the mechanism of the adaptive evolution, as well as rich genomic resources for improving crop traits.

Molecular Simulation of Electric Double-Layer Capacitors Based on Carbon Nanotube Forests

Lawrence R. Pratt

Department of Chemical & Biomolecular Engineering, Tulane University, New Orleans, LA 70118

Abstract

Described here are the first simulations of electric double-layer capacitors based on carbon nanotube forests modeled fully at a molecular level. The computations determine single-electrode capacitances in the neighborhood of 80 F/g, in agreement with experimental capacitances of electric double- layer capacitors utilizing carbon nanotube forests or carbide-derived carbons as electrode material. The capacitance increases modestly with the decrease of the pore size through radii greater than 1 nm, which is consistent with recent experiments on carbide-derived carbon electrodes. Because the various factors included in these simulations are precisely defined, these simulation data will help to disentangle distinct physical chemical factors that contribute to the performance of these materials, e.g., pore geometry, variable filling of the pores, pseudocapacitance, and electronic characteristics of the nanotubes.

Numerical Modeling of Sediment Transport on the Texas-Louisiana Shelf

Kehui Xu

Department of Oceanography and Coastal Studies, Louisiana State University, Baton Rouge, LA 70803

Abstract

A three-dimensional coupled hydrodynamic-sediment transport model for the Texas-Louisiana continental shelf was developed using the Regional Ocean Modeling System (ROMS) and used to represent fluvial sediment transport and deposition for the year 1993. The model included water and sediment discharge from the Mississippi River and Atchafalaya Bay, seabed resuspension, and suspended transport by currents. Input wave properties were provided by the Simulating WAves Nearshore (SWAN) model so that ROMS could estimate wave-driven bed stresses, critical to shallow-water sediment suspension. The model used temporally-variable but spatially-uniform winds, spatially-variable seabed grain size distributions, and six sediment tracers from rivers and seabed. At the end of the year 1993, much of the modeled fluvial sediment accumulation was localized with deposition focused near sediment sources. Mississippi sediment remained within 20 to 40 km of the Mississippi Delta. Most Atchafalaya sediment remained landward of the 10-m isobath in the inner-most shelf south of Atchafalaya Bay.

– Condensed Matter Nuclear Physics –
Symmetry Adapted & HPC Enabled Nuclear Structure Studies

Jerry P. Draayer, Tomáš Dytrych, and Kristina D. Launey
Department of Physics and Astronomy, Louisiana State University
Baton Rouge, LA 70803, USA

As the quark-gluon plasma – governed by strong interaction physics – cools, nucleon condensates form and cluster into nuclei that sit at the center of every atom, from hydrogen (single proton nucleus) to uranium (92 protons and 146 neutrons in its most abundant 238 isotope) and beyond. An *ab initio* symmetry-adapted no-core shell-model (SA-NCSM), with results that corroborate and are complementary to those first enabled within the framework of the no-core shell model (NCSM) [1], facilitates high performance computing (HPC) studies of the structure of atomic nuclei. Applications of the theory show that bound states of light nuclei are dominated by high-deformation and low-spin configurations [2]. The applicable symmetries, ferreted out using HPC tools, reveals the origin of collective modes – the emergence of symplicity within complexity – in such nuclei, and provide a framework for determining the nature of bound states of nuclei in terms of a relatively small fraction of the complete shell-model space.

While applications to p-shell and selected heavier nuclei [2, 3, 4, 5] illustrate the success of the *ab inito* approach, a simple algebraic interaction, which reduces to the Elliott SU(3) model [6] in the single-shell limit, augmented by the SU(3) symmetry breaking spin-orbit interaction, reproduces characteristic features of the low-lying 0^+ states in ^{12}C. This includes the elusive first excited 0_2^+ state, known as the Hoyle state [7] that was predicted based on observed abundances of heavy elements in the universe, and which has attracted much recent attention [8, 9, 10, 11]. An implication of the latter is that efforts to reproduce the structure of ^{12}C using a 'bottom up' *ab inito* effective interaction theory may benefit from 'top down' algebraic considerations that serve to expose emergent properties in terms of simple interaction forms that seem to dominate the structure of deformed nuclei, especially the 0^+ states of ^{12}C.

Enabling support of HPC resources from LONI (Louisiana Optical Network Initiative) and the DOE (SciDAC) along with complementary theoretical support from the DOE (EPSCoR), NSF (PetaApps) and SURA (Southeastern Universities Research Association) is acknowledged.

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The effects of charge transfer on the properties of liquids

Steven W. Rick

Department of Chemistry, University of New Orleans, New Orleans, LA 70148

Abstract

Non-covalent interactions include a significant charge transfer component, which leads to he transfer of small amounts of charge from one particle to another. The transfer of charge changes both short- and long-ranged interactions. Most force fields do not treat charge transfer, and treat molecules as neutral or ions as having integer charges. It is more physical to assign charges based on the electron density, resulting in molecular or ionic charges which depend on their environment. We have recently developed a simple and efficient method for treating charge transfer in molecular simulations, which will be presented. Application of the model to water, water interfaces, and aqueous salvation of ions will also be presented.

Hybrid Parallel Computing of Minimum Action Method

Xiaoliang Wan

Department of Mathematics, Louisiana State University, Baton Rouge, LA 70803

Abstract

In this work, we report a hybrid (MPI/OpenMP) parallelization strategy for the minimum action method. For nonlinear dynamical systems, the minimum action method is a useful numerical tool to study the transition behavior induced by small noise and the structure of the phase space. The crucial part of the minimum action method is to minimize the Freidlin-Wentzell action functional. Due to the fact that the corresponding Euler-Lagrange equation is, in general, highly nonlinear and of high order, we solve the optimization problem directly instead of discretizing the Euler-Lagrange equation to provide a general but equivalent numerical framework. To enhance the efficiency of the minimum action method for general dynamical systems we consider parallel computing. In particular, we present a hybrid parallelization strategy based on MPI and OpenMP. Numerical results are presented to demonstrate the efficiency of the proposed parallelization strategy.

Using HPC to Develop Branch Protection Estimators

David M. Koppelman

Division of Electrical and Computer Engineering, Louisiana State University, Baton Rouge, LA 70803

Abstract

Modern CPUs are designed for, among other things, workloads that contain branches that are difficult to predict. For some workloads considerable performance is lost due to mispredicted branches. Using HPC and visualization techniques new CPU features have been developed that avoid some of that performance loss by using a *protection estimator* to identify branches that are good candidates for *protection*. Much less work is discarded when a protected branch is mispredicted.

The protection estimator was developed using HPC facilities and visualization tools. As is typical in research of this sort a simulator is used which estimates the performance of a proposed computer design running a chosen program (or *benchmark*). The simulator used in this work, RSIML, is a heavily modified version of RSIM, developed at Rice university. For the work reported here the simulator was modified to simulate the protection estimator and the branch protection mechanism. The simulator output is a *dataset file* which contains details of the execution of the benchmark. The dataset file is read by an LSU-developed visualization program, PSE, which is used to analyze the results of execution. Simulations detailed enough for data collection typically run thousands of times slower than a real system, performing detailed simulation only over selected samples can keep run times to within a few hours.

Following computer architecture research practice, multiple variations of proposed designs are simulated on a set of benchmarks, on systems of different sizes, etc. Even with some restraint, an experiment can include hundreds of configurations. Experiments are run on HPC computing clusters, including those at LSU and those available via LONI. A simulation experiment is orchestrated by a perlscript which distributes simulation runs to cores, and collects results.

A large fraction of fetched instructions in modern general-purpose dynamically scheduled processors are later squashed, a consequence of the delay between the time a branch is fetched and its outcome resolved. It has long been noted that many of those squashed instructions are subsequently refetched, motivating the design of processors that in some way preserve rather than squash the control-independent instructions that would otherwise be squashed. A branch is said to be *protected* if its recovery does not squash control independent instructions. Doing so effectively is tricky because of the overhead of preserving control independent instructions and because preserving them does not guarantee performance improvement even with zero overhead.

An execution model has been developed that can be used to easily quantify the expected reduction in execution time when protecting a branch. Based on the model a low-cost protection estimator has been developed and integrated with a control-independence processor. The system dynamically discovers control independence and dynamically estimates reduction; protection decisions are made based on the estimated reduction and on recent branch behavior. The technique not only improves performance on some benchmarks, but more importantly for others it yields speedup where an oblivious scheme suffers slowdown. Overall speedup averages 15% for the SPECcpu2006 integer benchmarks and selected SPECcpu2000 benchmarks.

Research Projects of HPC Group at Southern University

Liuxi Tan[1], Shizhong Yang[1], Jialin Lei[1], Cheng Guo[1], Michael Jackson[1], Shengmin Guo[2], and Ebrahim Khosravi[1]

[1]Department of Computer Science, Southern University, Baton Rouge, LA 70813
[2]Department of Mechanical Engineering, Louisiana State University, Baton Rouge, LA 70803

Abstract

The HPC simulation has been the third pillar besides theoretical and experimental research in the recent decade. In Southern University, our HPC group has been performing HPC simulation in following research topics: (1). Novel efficient *ab initio* molecular dynamics method development; (2). Accurate band structure GW method calculation on novel superconductors and nano materials; (3). High temperature Cr and Nb based alloy oxidation and thermal barrier coating (TBC) simulation; (4). Oxide dispersion strengthened (ODS) alloy and dislocation creep simulation; (5). High temperature high entropy alloy simulation and experiment validation; (6). Nickel metal sulfur embrittle simulation and experimental validation; (7). Nitrogen doped C_{60} as fuel cell catalyst simulation; (8). Ligand/protein and protein/protein docking and MD simulation and data analysis. The interesting state-of-the-art results will be introduced and briefly discussed and LONI HPC simulation will be introduced.

Fluid Flow and Heat Transfer in Polygonal Micro Heat Pipes

Sai Sashankh Rao, and Harris Wong

Department of Mechanical and Industrial Engineering, Louisiana State Univeristy, Baton Rouge, LA 70803

Abstract

Micro heat pipes have been used to cool microelectronic devices, but their heat transfer coefficients are low compared with those of conventional heat pipes. A typical micro heat pipe has a long and narrow cavity of polygonal cross section sealed at both ends. A long vapour bubble occupies the center of the cavity, while the liquid fills the corner regions. As one end of the pipe is heated, the liquid evaporates into the bubble and increases the vapour pressure. The higher pressure drives the vapour to the cold end where it condenses to regenerate the liquid and releases the latent heat. The condensate flows along the corner channels back to the hot end to complete the cycle. We study the steady operation of triangular, square, hexagonal, and rectangular micro heat pipes assuming a small temperature difference across the pipes. This leads to skew-symmetric fluid flow and temperature distribution along a pipe so that we focus only on the evaporative half of the pipe. Since the pipe is slender, flow fields vary slowly in the axial direction. Thus, the evaporative motion can be treated as two-dimensional at each cross-sectional plane. By incorporating proper evaporation kinetics, we find that evaporation occurs mainly near the vapour-liquid-solid contact line. An analytic expression is derived for the evaporation rate per unit contact-line length in the asymptotic limit of large Evaporation number. The axial vapour and liquid flows are treated as uni-directional, and are coupled at the interface. The coupled problem is solved in the asymptotic limit of zero viscosity ratio. Because the pipe is assumed insulated outside, heat can only transfer by vapour flow and conduction in the liquid and pipe wall. Analytic expressions are obtained for the pipe temperature, vapour pressure, and Nusselt number Nu. They depend on two dimensionless numbers: the heat-pipe number H_p, which is the ratio of heat transfer by vapour flow to conductive heat transfer in the liquid and pipe wall, and the resistance ratio R, which is the ratio of viscous resistance of vapour flow to evaporation resistance. In the limit $H_p \to 0$ or $R \to \infty$, conduction dominates. When $H_p \to \infty$ and $R \to 0$, vapour-flow heat transfer dominates and a thermal boundary layer appears near the hot end, the thickness of which scales as ${H_p}^{-1/2}L$, where L is the half-length of the pipe. A similar boundary layer exists at the cold end. Outside the boundary layers, the temperature is uniform. These regions correspond to the evaporating, adiabatic, and condensing regions commonly observed in conventional heat pipes. This is the first time that a single equation is derived for the pipe temperature that captures all three regions in polygonal micro heat pipes. We apply our model to four published micro-heat-pipe experiments and obtain good agreement for Nu. Three experiments have $R \gg 1$, leading to $Nu \sim 1$. For enhanced heat transfer, micro heat pipes should be designed with $H_p \gg 1$ and $R \ll 1$.

Molecular Dynamics Simulation of VECAR molecules

Caleb Delaune, Uddhab Tiwari and Hye-Young Kim

Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA 70402

Abstract

Molecular dynamics simulations are performed using GROMACS to study the properties of newly synthesized amphiphilic antioxidant molecules, Vecar [1], as a pure bulk material and as a solute in water. The chemical structure of the molecule is composed of a truncated vitamin E and a slightly modified Carnosine which are, respectively, linked to the opposite ends of a simple carbon chain of varying length. This new molecule is an amphiphilic surfactant molecule and its force field is generated from the Automatic Topology Builder. We will report the progress and results of our computer simulation study performed using LONI HPC resources. This research is supported by Louisiana BOR grant (LEQSF(2012-15)-RD-A-19) and by the Louisiana Optical Network Institute (LONI).

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Genomic ultraconserved elements resolve the comparative phylogeography of five Neotropical birds

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Advances in sequencing technology permit researchers to generate massive genomic datasets, but their application to phylogeographic studies has been limited by the difficulty of generating data from homologous loci across many individuals. Sequence capture of conserved portions of the genome now permits the generation of homologous data across individuals that can then be multiplexed on next-generation sequencing platforms. We evaluated a recently developed class of genomic markers known as ultraconserved elements (UCEs) to determine whether sufficient polymorphism exists in and around these loci to resolve intraspecific relationships and estimate population genetic parameters such as divergence time, effective population size, and migration rate. We apply this method to populations of five Neotropical passerine birds distributed in humid forest throughout the Neotropical lowlands. We successfully align sequences from between 776 and 1516 loci, 23-42% of which are polymorphic, in the five species. We analyze these alignments in a coalescent framework in order to obtain population genetic parameter estimates, construct species trees, delimit species, and model demographic history. Comparisons suggest that poorly dispersing taxa have lower effective population sizes and shallower divergences across barriers, and contain more species, than more vagile taxa. These results are consistent with results from independent datasets, but provide higher resolution of the histories of these populations than was possible previously. Since UCEs can be amplified across a wide array of taxa and can be generated rapidly at low cost, we conclude that they are promising markers for use in phylogeographic and comparative phylogeographic studies.

Keywords: phylogenomics, coalescent, demography, sequence capture, next-generation sequencing

Mathematical Model of Metal Hydrogen Desorption and Inverse Problem

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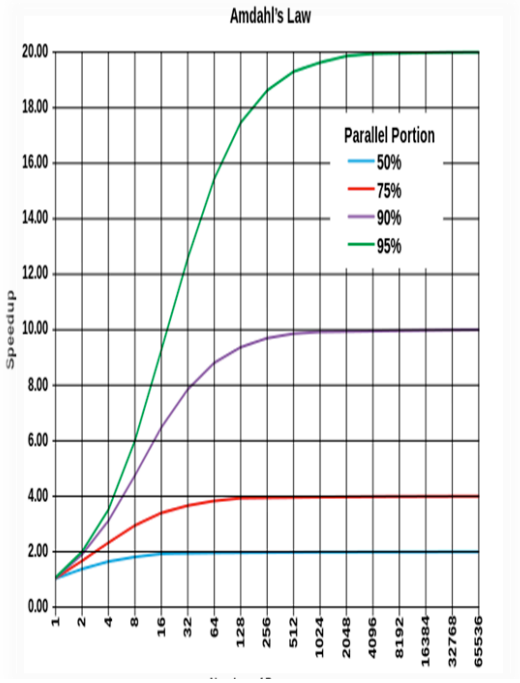
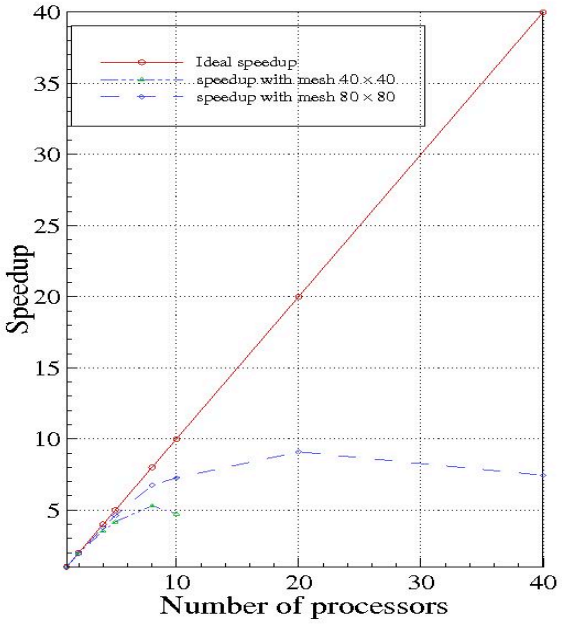
Abstract

The understanding of heat and mass transfer is important for the design and usage of metal hydrogen storage system. The system is modelled by a set of partial differential equation and then solved by finite difference method. The simulation results showed the temperature distributions and its evolution, the evolution of density of hydrogen gas in the porous material La-Ni5. Given the parameters to obtain the distribution of temperature by solving the mathematical model is the forward problem. But not all system parameters can be measured easily, sometimes the value of parameter comes from the estimation of researchers. Inverse problem is trying to solve this problem. In our setting, we have measurements of temperature and we want to get the estimation of some system parameters. When solving inverse problem by utility of inverse problem techniques, solving the forward problem is implicit in the process. The time spent on the forward problem determined the total time needed for the whole inverse problem. By using MPI and the utility of LONI we parallelize the program (parallelize the Jacobi iteration), and we get substantial speedup for the parallel code. The maximum speed up we get is around 9.





Comparison of different models of electron and nuclear couplings in biomolecules and clusters: High Performance Computing (HPC) at LSU

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and

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Adaptive models of ultrafast polarization phase-selective (UF-PPS) EM radiation structures and their signatures have been tested on probing dynamics and structure (imaging) of even highly coherent correlated electrons in molecules. New theoretical and experimental studies indicate their comparative advantages when applied to ultrafast events[1] Recently discovered[2] unusual cluster structures as well as unusual enzymatic, photonic and redox synthesis and electron transfers and turnovers question validity of previous models. Here we provide a brief review of calculations using different models, including DFA, on bio-molecules and related redox reactions. The focus is on the work done as a set of research projects assignments for Chemistry graduate and undergraduate students. We investigate and compare predictions of these models in order to find where the significant differences may exist. Of particular interest for the theoretical modeling is identification of electron spins and vibrational coupling.

Acknowledgement

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Parallel Covariance Matrix Adaptation-Evolution Strategy for Modeling of Complex Groundwater Systems

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Abstract

The inverse problem in groundwater modeling deals with a rugged (i.e. ill-conditioned and multimodal), nonseparable and noisy function that involves solving second-order nonlinear partial differential equations with forcing terms. Traditional derivative-based optimization algorithms such as Gauss-Newton method take less iteration to converge, but may fail to reach a near global solution due to their stagnation at a local minimum solution. Derivative-free optimization methods such as Covariance Matrix Adaptation-Evolution Strategy (CMA-ES) can avoid entrapment in a local optimum and enhance search efficiency especially with the use of large population size. However, this approach requires not only more iterations, but also extremely high computational cost. It seems to be unrealistic for modeling complex groundwater systems.

This study developed a parallel version for CMA-ES to accelerate the calibration process of the groundwater flow model. Owing to the population-based method, CMA-ES was easily to be parallelized by the embarrassingly parallel algorithm, which requires little or no communication of results between tasks. The parallel CMA-ES has been successfully implemented to both High Performance Computing (HPC) systems of Louisiana State University (LSU) and Louisiana Optical Network Initiative (LONI). To obtain the most efficiency of parallel implementation, the number of processors was always chosen the same as the population size in this study.

We implemented the parallel CMA-ES to calibrate the three-dimensional groundwater flow model in the "1,200-foot" sand, "1,500-foot" sand, and "1,700-foot" sand of the Baton Rouge area. The model was developed based on MODFLOW-2005, which had a grid of 93 rows, 137 columns and 45 layers. The model also included the east-west trending Baton Rouge fault and the Denham Springs-Scotlandville fault. The simulation period was from 1975 to 2010 using 432 one-month stress periods. We used 2,805 groundwater head records from 21 USGS observation wells to estimate hydraulic conductivity, specific storage, and fault permeability. The CMA-ES minimized the root mean square error (RMSE) of the simulated to the observed groundwater heads.

Our results showed that increasing the number of processors, which equals to the population size, significantly decreases the number of iterations. To reach the RMSE of 1.66 meters, it required 96 iterations by using the population size of 16 in comparison with 58 iterations by using the population size of 48. However, the speedup of parallel CMA-ES only scaled up with increasing the number of processors to a certain point. Increasing the number of processors to 96 still required 60 iterations to reach the RMSE of 1.66 meters. In this study, we used 48 processors to calibrate the groundwater flow model. The speedup was 48 times. The model converged after 58 iterations. The total execution time given by the QueenBee supercomputer of LONI and the SuperMike of LSU HPC was 178 hours and 43 hours, respectively. The calibration result showed that the Baton Rouge fault and the Denham Springs-Scotlandville fault are low-permeability faults that restrict horizontal groundwater flow. There is a strong groundwater flow interactions between the "1,200-foot" sand and the "1,500-foot" sand in the area between two faults.

High Performance Computing for Region-Scale Groundwater Recharge Estimation in Southeastern Louisiana and Southwestern Mississippi

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Abstract

Groundwater recharge is an important hydrologic process to replenish an aquifer and plays an important role in groundwater resources availability. Groundwater recharge study is imperative to the Southern Hills aquifer system (a sole source aquifer) underneath southeastern Louisiana and southwestern Mississippi, which provides more than 50 percent of the drinking water consumed in the area and has no substitute drinking water source(s). This study developed a Geographic Information System-based integrated framework and incorporated a high-resolution hydrologic model to quantify long-term groundwater recharge. We employed the Hydrologic Evaluation of Landfill Performance (HELP3) model as our hydrologic water budget model to estimate spatial-temporal distribution of potential recharge for a regional scale. In addition, in order to obtain a high resolution spatial recharge map, the study area was divided into 286,355 confined homogeneous subdivisions by intersecting GIS datasets of significant variables affecting groundwater recharge such as; soil type, land use/land cover, leaf area index, topographic slope, and climate zones. A program module was developed in Python programming language to execute HELP3 and to estimate recharge for individual subdivisions. However, due to a great number of subdivisions, recharge estimation became practically impossible if executing HELP3 sequentially in one processor. This study developed a parallel procedure using high performance computing to distribute required HELP3 model runs to a number of processors. As a result, groundwater recharge for all subdivisions was calculated with extremely less computational time. As recharge is the residual term in water budget method, the accuracy of estimated recharge relies upon the accuracy of other estimated budget terms such as runoff and evapotranspiration. We re-estimated curve numbers and calibrated the HELP3 using the computed runoff of individual hydrologic units in terms of Hydrologic Unit Codes (HUCs) from the USGS WaterWatch database. Also, the HELP3 computed evapotranspiration compared well to the estimated evapotranspiration dataset obtained from MODIS Global Evapotranspiration Project. The results determined a recharge index (RI) map, the percentage of precipitation that recharges aquifers. A recharge lag map was also determined to understand the travel time of infiltrated precipitation reaching to the last soil layer. Moreover, the results showed spatial-temporal variation of recharge in the Southern Hills aquifer system due to variations in land use, soil characteristics and predicted meteorological variables.

GPU Enabled Simulation of Free Boundary Flow using Smoothed Particle Hydrodynamics

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Abstract

The interaction of a fluid and elastic solid object in the fluid is modeled with the Smoothed Particle Hydrodynamics (SPH), a mesh-free Lagrangian method. The computational domain changes in space and time. The shape of the fluid boundary is unknown and is a part of the solution. The fluid and the elastic solid are discretized into groups of particles and their properties at certain positions are interpolated with kernel function based on surrounding particles. Owing to the built-in parallel features of SPH method, Graphic Processing Unit (GPU) was implemented in SPH-based modeling and was used to provide simulation data, which is an improvement on the speed and memory over a single CPU computation. NVIDIA CUDA-based GPU optimization of free surface fluid-solid interaction using SPH will be presented, in which the moving boundaries between fluid and elastic solid are handled by treating the solid and the fluid as two different types of particles. The performance of SPH implemented on GPU architecture is evaluated and compared with the result from conventional SPH. Results illustrate that the GPU-SPH approach is deal to simulate free boundary fluid-solid interaction problems with numerous particles involved and is faster and more efficient than conventional mesh-based numerical methods within a moderate error tolerance.

Parallel Simulation of Particulate Flow with Virtual Identity Particles and Spectral Modal Element Method

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Abstract

Particulate flow has wide applications in engineering and industry, and is of great interest to researchers in both academia and industry. The challenges in modeling particulate flow phenomena include tracking moving internal boundaries which are part of the solution and quantifying large amount of interactions among particles and the fluid. Existing methods such as direct numerical simulation in conjunction with arbitrary Lagrangian-Eulerian, distributed Lagrangian Multiplier, fictitious domain, and mesh-free discrete methods are effective for certain conditions. However, when the number of particles becomes significantly large and near-particle details are desired, the entire system with coupled momentum exchange between the two phases - fluid and particles becomes too stiff or even intractable to handle numerically.

Focusing on the momentum exchange in an integral averaged sense and avoiding resolving moving boundaries in the system, we simulate the equivalent effect of particulate flow with virtual particles in the domain using Virtual Identity Particles model (VIP). In VIP, we impose tailored force fields and distribute them with spatial kernel functions which are generated based on the actual shape and positions of particles. The modified Navier-Stokes equations for the fluid field are solved before particles move to their new positions. This relieves the expensive work to fully solve Navier-Stokes equations with numerous non-slip boundary conditions imposed on particles' surfaces - moving internal boundaries for the fluid. Spectral Modal Element method was used to provide numerical solutions.

The parallelization was accomplished through domain decomposition via *mpmetis* developed by George Karypis et al. and implemented in C++ with the aid of standard MPI library functions. The communication overhead for particles-phase computation is much less than the combined time for the fluid field solver in acquiring high order finite element solution of fluid velocity, triple integral evaluations, and temporal integration for particles. High scalability and accuracy make VIP a valuable alternative for modeling particulate flows involving numerous moving internal particles in the system on one fixed mesh while avoiding fully resolving boundary layers around particles.

Applications of a finite volume immersed boundary method for complex geometries in river environments.

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Immersed boundary methods have emerged in recent years as a good alternative to conventional body-fitted methods especially in problems involving complex geometries. For moving boundaries, the need to establish a new body-conformal grid at each time can significantly simplify and decrease the solution procedure and also eliminates issues related to grid non-orthogonally and skewness compared to domain remeshing for body-fitted grids. For this study, we used an immersed boundary method based on a finite volume solver, OpenFOAM. It is implemented using a discrete forcing approach with direct imposition of the boundary conditions.

Our objective is to examine the mean flow and turbulent quantities for bed geometries that are typical of two dimensional dunes. We performed Large Eddy Simulation of flow using dune shapes of Nelson et al. (1993). The instantaneous flow field was investigated with special emphasis on the occurrence of coherent structures. To assess the applicability of the immersed boundary method, we compared results from a body-fitted grid of a similar numerical setup at different locations on the dune cross-section.

For validation, profiles of velocities and turbulent intensities calculated by the numerical model are compared with experimental measurements and we found that the immersed boundary method gives results which are in good agreement with the experimental data.

Parallel Computation of a Finite Volume Coastal Ocean Model

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Abstract

In this study, we investigated the performance of a portable parallelized Finite Volume Coastal Ocean Model (FVCOM). The programming paradigm of FVCOM parallelization is based on domain decomposition with message-passing interface (MPI), a standard API for distributed-memory.

In order to examine the performance of parallelized FVCOM with different computer architectures, we conducted efficiency analysis of this parallelized model on two supercomputers, Tezpur and SuperMike-II. The model efficiency under various number of processor assignment is measured by total simulation time and speedup. In addition, a scientific simulation of a rotating-table experiment, which will be used to discuss the evolution of freshwater plumes, was performed. By comparing with laboratory experiment results, we concluded that accuracy of simulation result is highly correlated to the mesh resolution, especially along the lateral boundary. We need to implement the non-slip boundary condition with very fine mesh resolution (~ 0.01cm) within the lateral boundary layer to resolve the viscous flow, whereas in the interior region, where fluid flow is slow, coarse mesh resolution (~ 0.2 cm) is applicable.

Clutter Reduction in Visualization of Atomic Trajectories with Position Merging

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Abstract

Visualization of position-time series data from molecular dynamics simulations as particle (atomic) trajectories helps us gain insight into the structural and dynamical behavior of the material system under consideration. However, these trajectories generally overlap with each other significantly, and the associated clutter/occlusion problem becomes serious even for moderate-sized data sets. Here, we propose an adaptive hierarchical scheme for merging multiple positions along the trajectories in order to significantly reduce the number of points or line segments to be rendered. Our approach finds positions, which lie within a finite space window (cutoff distance) from a reference position, and merges them into single point. The space window is then moved in time order with merging performed at each successive location. The process continues until all original positions are considered thereby producing a reduced number of merged positions. A next level merging then processes new positions that are derived in the previous level with the same or a different cutoff. This hierarchical merging continues until the number of merged positions does not decrease further or desired visibility is achieved. At each level, the merged positions can be rendered with additional information such as time elapsed, 3D location, merge count, etc. color-coded along the trajectories. The geometry of individual trajectories on merging becomes increasingly visible so that the nature and extent of atomic movements can be better assessed. Improved visualization of trajectories also allows us to display the underlying atomic structure and how it evolves with time.

First principles calculations of grain boundaries in Mg_2SiO_4 at high pressure

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Abstract:

Grain boundary structures are known to have significant influence on the materials propertie (such as: strength, diffusion, electrical conductivity). In this study we explore the effects of pressure o the structural properties of Forsterite (Mg_2SiO_4) grain boundaries (GB) by first principles densit functional calculations. We have modeled Mg terminated stepped {010} surfaces (keeping tetrahedra Si units intact) with step walls made up of {001} and {100} surfaces. A number of tilt angles startin from 18° – 65°, and for each angle a set of two configurations: coherent and incoherent wer considered. All the configurations were fully relaxed (cell shape and size) at three pressure point starting from 0 – 17 GPa. Simulation results at ambient conditions show that on relaxation, the initiall separated (by an order of inter-atomic distance) grains come closer (coherent) or coalesce (incoherent into each other forming islands that are connected by channel like structures. Structural changes occu predominantly around the GB region. Away from the GB region, average bond lengths an coordination numbers remain practically same as with their calculated crystalline values (1.638 Å fo Si-O tetrahedra and 2.086 and 2.114 Å for two different type of Mg-O octahedra). Some 3-, 4- and 5 coordinated Mg atoms are also (in addition to Mg – O octahedra) present around the GB region wit average bond lengths varying from 1.975 – 2.122 Å. For either of the step walls ({100} and {001} incoherent configurations are more favorable. Calculated GB energies in the range of ~ (1.9 – 3.0) J/m compare very well with the study of De Leeuw et al (2000). Based on the angles considered here, mis-orientation angle of ~30° gives the most stable configuration for the {001} step wall while for th {100} step wall it is 65°. The shape, size and number of the islands change with compression. The fac that many of the interfacial Mg atoms remain under-coordinated even at the highest compressio studied here suggest continuing interconnectivity of these islands. For all the simulated incoheren configurations GB energy and the GB excess volume display a linear increasing trend for the entir pressure range considered here.

Toward tangible genomic user interfaces for enhancing mobile element research and education engaging multi-genome sequencing data

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Abstract

The combination of advanced genomic technologies and computational tools enables researchers to conduct large-scale experiments that answer biological questions in unprecedented ways. However, present user interfaces for computational genomics have rarely ventured beyond traditional graphical interaction techniques, thus missing opportunities from a fertile period in human-computer interaction (HCI) design. One such prospect involves tangible interfaces, which use systems of physical artifacts as representations and controls for digital information. Both individually and collectively, our teams have begun developing user interfaces employing tangible interfaces for engaging with genomic information. Here, we summarize these earlier individual examples, and describe our efforts toward tangible engagement with whole and multi-genome datasets. These efforts focus on mobile element analyses of primate genomes by distributed human teams, as mediated by multitouch tables, mixed commercial and research tangibles, and interactive high-performance computing backends.

Effective Thermal Control Techniques for Liquid-Cooled 3D Multi-Core Processors

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Abstract

Microchannel liquid cooling shows great potential in cooling 3D processors. However, the cooling of 3D processors is limited due to design-time and run-time challenges. Moreover, in new technologies, the processor power density is continually increasing and this will bring more serious challenges to liquid cooling.

In this paper, we propose two thermal control techniques: 1) Core Vertically Placed (CVP) technique. According to the architecture of a processor core, two schemes are given for placing a core vertically onto multilayers. The 3D processor with the CVP technique can be better cooled since its separate hotspot blocks have a larger total contact area with the cooler surroundings. 2) Thermoelectric cooling (TEC) technique. We propose to incorporate the TEC technique into the liquid-cooled 3D processor to enhance the cooling of hotspots. Our experiments show the CVP technique reduces the maximum temperature up to 29.58 ℃, and 16.64 ℃ on average compared with the baseline design. Moreover, the TEC technique effectively cools down a hotspot from 96.86 ℃ to 78.60 ℃.

Inferring the Expression Variability of Human Transposable Element-Derived Exons by Linear Model Analysis of Deep RNA Sequencing Data

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Abstract

The exonization of transposable elements (TEs) has proven to be a significant mechanism for the creation of novel exons. Existing knowledge of the retention patterns of TE exons in mRNAs were mainly established by the analysis of Expressed Sequence Tag (EST) data and microarray data.

This study seeks to validate and extend previous studies on the expression of TE exons by an integrative statistical analysis of high throughput RNA sequencing data. We collected 26 RNA-seq datasets spanning multiple tissues and cancer types. The exon-level digital expressions (indicating retention rates in mRNAs) were quantified by a double normalized measure, called the rescaled RPKM (Reads Per Kilobase of exon model per Million mapped reads). We analyzed the distribution profiles and the variability (across samples and between tissue/disease groups) of TE exon expressions, and compared them with those of other constitutive or cassette exons. We inferred the effects of four genomic factors, including the location, length, cognate TE family and TE nucleotide proportion (RTE, see Methods section) of a TE exon, on the exons' expression level and expression variability. We also investigated the biological implications of an assembly of highly-expressed TE exons.

Our analysis confirmed prior studies from the following three aspects. First, with relatively high expression variability, most TE exons in mRNAs, especially those without exact counterparts in the UCSC RefSeq (Reference Sequence) gene tables, demonstrate low but still detectable expression levels in most tissue samples. Second, the TE exons in coding DNA sequences (CDSs) are less highly expressed than those in 3' (5') untranslated regions (UTRs). Third, the exons derived from chronologically ancient repeat elements, such as MIRs, tend to be highly expressed in comparison with those derived from younger TEs. Furthermore, our study resulted in several novel findings. They include: (1) for TE exons, a high TE nucleotide proportion can lead to lower retention rates in mRNAs; (2) the previously observed negative relationship between the lengths of exons and the inclusion levels in transcripts is also true for exonized TEs; (3) The expression level and expression variability of TE exons are inversely impacted by the considered genomic features (i.e. a continuous variable such as the exon length or a category indicator such as 3'UTR); (4) not only the exons derived from Alu elements but also the exons from the TEs of other families were preferentially established in ZNF genes.

Alu Distribution and Mutation Types of Cancer Genes

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Abstract

Alu elements are the most abundant retrotransposable elements comprising ~11% of the human genome. Many studies have highlighted the role that *Alu* elements have in genetic instability and how their contribution to the assortment of mutagenic events can lead to cancer. As of yet, little has been done to quantitatively assess the association between *Alu* distribution and genes that are causally implicated in oncogenesis.

We have investigated the effect of various *Alu* densities on the mutation type based classifications of cancer genes. In order to establish the direct relationship between *Alu*s and the cancer genes of interest, genome wide *Alu*-related densities were measured using genes rather than the sliding windows of fixed length as the units. Several novel genomic features, such as the density of the adjacent *Alu* pairs and the number of *Alu*-Exon-*Alu* triplets, were developed in order to extend the investigation via the multivariate statistical analysis toward more advanced biological insight. In addition, we characterized the genome-wide intron *Alu* distribution with a mixture model that distinguished genes containing *Alu* elements from those with no *Alus*, and evaluated the gene-level effect of the 5'-TTAAAA motif associated with *Alu* insertion sites using a two-step regression analysis method.

The study resulted in several novel findings worthy of further investigation. They include: (1) Recessive cancer genes (tumor suppressor genes) are enriched with *Alu* elements ($p < 0.01$) compared to dominant cancer genes (oncogenes) and the entire set of genes in the human genome; (2) *Alu*-related genomic features can be used to cluster cancer genes into biological meaningful groups; (3) The retention of exon *Alus* has been restricted in the human genome development, and an upper limit to the chromosome-level exon *Alu* densities is suggested by the distribution profile; (4) For the genes with at least one intron *Alu* repeat in individual chromosomes, the intron *Alu* densities can be well fitted by a Gamma distribution; (5) The effect of the 5'-TTAAAA motif on *Alu* densities varies across different chromosomes.

miRNA-Mediated Relationships between Cis-SNP Genotypes and Transcript Intensities in Lymphocyte Cell Lines

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Abstract

In metazoans, miRNAs regulate gene expression primarily through binding to target sites in the 3′ UTRs (untranslated regions) of messenger RNAs (mRNAs). Cis-acting variants within, or close to, a gene are crucial in explaining the variability of gene expression measures. Single nucleotide polymorphisms (SNPs) in the 3′ UTRs of genes can affect the base-pairing between miRNAs and mRNAs, and hence disrupt existing target sites (in the reference sequence) or create novel target sites, suggesting a possible mechanism for cis regulation of gene expression. Moreover, because the alleles of different SNPs within a DNA sequence of limited length tend to be in strong linkage disequilibrium (LD), we hypothesize the variants of miRNA target sites caused by SNPs potentially function as bridges linking the documented cis-SNP markers to the expression of the associated genes. A large-scale analysis was herein performed to test this hypothesis. By systematically integrating multiple latest information sources, we found 21 significant gene-level SNP-involved miRNA-mediated post-transcriptional regulation modules (SNP-MPRMs) in the form of SNP-miRNA-mRNA triplets in lymphocyte cell lines for the CEU and YRI populations. Among the cognate genes, six including ALG8, DGKE, GNA12, KLF11, LRPAP1, and MMAB are related to multiple genetic diseases such as depressive disorder and Type-II diabetes. Furthermore, we found that ~35% of the documented transcript intensity-related cis-SNPs (~950) in a recent publication are identical to, or in significant linkage disequilibrium (LD) ($p<0.01$) with, one or multiple SNPs located in miRNA target sites. Based on these associations (or identities), 69 significant exon-level SNP-MPRMs and 12 disease genes were further determined for two populations. These results provide concrete *in silico* evidence for the proposed hypothesis. The discovered modules warrant additional follow-up in independent laboratory studies.

*e*RefSite: Local Structure Refinement of Ligand Binding Sites in Protein Models

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Abstract

Computational modeling has become an integral component of modern structure-based drug development and design. Amongst numerous algorithms developed to date, molecular docking, i.e. the modeling of ligand binding to receptor proteins, has profound applications in lead discovery and drug repositioning. The latter can be accomplished by inverse virtual screening of a drug candidate against all possible binding sites across the human proteome. Consequently, an exhaustively large repository of protein candidates is requisite. To address this issue, protein models constructed by computational approaches can be included to significantly expand the structural coverage of drug targets in the human proteome from approximately 15% to 70%. However, the quality of computer-generated models is notably lower than those solved experimentally, which represents a significant challenge for molecular docking approaches. A local binding site refinement can be applied to improve the structural quality of protein models making them better targets for drug repositioning. Towards this goal, we developed *e*RefSite, a new refinement procedure to rebuild the side chains of drug binding residues using template-based modeling extensively supported by machine learning. The scoring function implemented in *e*RefSite comprises knowledge-based, side-chain rotamer, and conformational energy terms. Initial benchmarks carried out for a large dataset of 2,292 modeled binding sites demonstrate that *e*RefSite effectively refines binding pockets in 58.2% of the cases. On average, using only top-ranked predictions, the initial structural quality of 4.74Å heavy atom RMSD (root-mean-square-deviation from crystal) improves to 4.69Å. Moreover, the integrated non-linear scoring function significantly outperforms individual terms by 7.5-17.2%. If the best constructed models are considered, the average structural quality of refined binding sites further improves to 4.61Å suggesting that additional enhancements should include better ranking protocols.

Developing Large-scale Scientific Applications in Life Sciences Using High-Performance Computing (HPC) and Cloud Computing

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Large-scale computation is increasingly becoming pivotal in many life science research topics. The advent of High-performance distributed computing (HPDC) approaches and the emergence of cloud computing are providing viable solutions for roadblocks that are associated with scalability, scale-across support, distributed data processing and management, multi-level parallelism, and others critically required for efficient large-scale scientific computation. We present our recent research outcomes and efforts in that direction with four different topics in computational biology and structural bioinformatics.

- Development of a new implementation of Replica Exchange Statistical Temperature Molecular Dynamcis (RESTMD) with Hadoop MapReduce
- Enhancing eThread, a meta-threading pipeline for protein structure modeling with Amazon EC2 cloud
- Long-time all atom molecular dynamics simulation revealing the riboswitch branch migration mechanism
- Next-generation sequencing (DNA) data analytics using HPCs and Clouds

First-Principles Identification of Nitrogen-Doped Fullerene as Potential Cathode Catalyst for Hydrogen Fuel Cells

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Abstract

In this work, we examine the possibility of nitrogen-doped C_{60} fullerene (N-C_{60}) as a cathode catalyst for hydrogen fuel cells. We utilize first-principles spin-polarized density functional theory (DFT) calculations to simulate the electrocatalytic reactions on N-C_{60}. The first-principles results show that the O_2 molecule can be adsorbed and partially reduced on the N-C complex sites (Pauling sites) of N-C_{60} without any activation barrier. Through a direct pathway (DPW), the partially reduced O_2 can further react with H^+ and additional electrons and complete the water formation reaction (WFR) without any activation energy barrier. In the indirect pathway (IDPW), reduced O_2 reacts with H^+ and additional electrons to form water molecule through a transition state (TS) with a small activation barrier (0.22~0.37 eV). From an intermediate state to a TS, H^+ can obtain a kinetic energy of about 0.95~3.68 eV due to the Coulomb electric interaction, and easily overcome the activation energy barrier during WFR process. The full catalytic reaction cycles can be completed energetically and N-C_{60} fullerene recovers to its original structure for next catalytic reaction cycle. N-C_{60} fullerene is a potential cathode catalyst for hydrogen fuel cells.

GPU-accelerated ligand docking

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Abstract

Computational modeling of drug binding to proteins has become an integral component of modern drug discovery pipelines. A typical application is structure-based virtual screening, which involves molecular docking of hundreds of thousands of drug candidates to the functional sites in pharmacologically relevant macromolecular targets. This approach can dramatically reduce the overall costs of discovering lead compounds by limiting the size of a screening library to these compounds that most likely exhibit the desired biological activity. Consequently, significant efforts are currently directed towards the development of faster and more accurate molecular docking algorithms. To improve the state-of-the-art, we develop a multi-scale approach to ligand docking and binding affinity prediction, with primary application in genome-scale drug discovery and design. This approach breaks down into two consecutive stages: 1) low-resolution docking of small organic compounds, e.g. drug candidates, to receptor proteins, and 2) high-resolution refinement of the generated binding poses. The docking procedure employs a novel combined force field that integrates physics-based energy terms with statistical potentials and evolutionary restraints. Monte Carlo Replica Exchange is used to efficiently sample the conformational space. The modeled binding poses of drug candidates are then subject to all-atom refinement using a physics-based molecular mechanics approach. During this step, the binding affinity of a drug candidate to the receptor protein is estimated from molecular interactions at the atomic level. Our implementation will exploit two levels of parallelism: coarse- and fine-grained. The former considers a simultaneous processing of series of replicas using multiplexed-REMC; the latter parallelizes the calculation of N-body interactions within each individual replica. Furthermore, docking computations are fairly regular with intensive floating-point arithmetic and relatively small data sizes. These characteristics inspired us to target the cost-effective Graphics Processing Unit (GPU) architecture, which features wide vector processing units, but relatively small on-chip scratchpad memory. Our preliminary benchmarks indicate that significant speed-ups over CPU implementation can be achieved.

A density functional study of the reactions of 2-chlorophenol, 1, 2-Dichlorobenzene, Chlorobenzene with CuO - Cu_8O_8 clusters

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Abstract

The surface-mediated reactions of 2-chlorophenol, 1, 2-dichlorobenzene, phenol, and chlorobenzene were modeled using CuO - Cu_8O_8 clusters and ab initio calculations. The phenols, chlorinated phenols, and chlorinated benzenes are precursors that have been implicated in the formation of polychlorinated dibenzo-p-dioxins and polychlorinated dibenzofurans (PCDD/Fs). Adsorption of 2-chlorophenol and 1, 2-dichlorobenzene resulted in the formation of identical surface-bound species followed by a concomitant reduction of a copper atom. Using three density functionals (B3LYP, M06, and PBE1PBE) calculations we found the stable structures and calculated the reaction energies of the title reactions. In all cases, the reaction energies of the small clusters ($<Cu_5O_5$) were more exothermic than large clusters ($>Cu_5O_5$). The reaction of 2-chlorophenol to yield 2-chlorophenoxyl was found to be slightly endorthemic compared to that of 1, 2-dichlorobenze to yield 2-chlorophenoxyl. The favorable sites for addition of water molecule was found using Bader charge analysis. We found that the Cu atom with the largest Bader charge provided the most reactive site for the organic compounds. We also determined the extent of copper reduction during reaction with an organic precursor. There is a significant charge reduction of copper on small clusters (CuO - Cu_5O_5). For larger clusters ($>Cu_5O_5$), copper reduction was negligible.

Synthetic libraries of drug-target complexes for structure-based drug design

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Abstract

Over the past few decades structural bioinformatics has become an increasingly important component of modern drug discovery. Structural knowledge helps scale down the size of compound libraries in virtual screening experiments and supports the chemical optimization of lead compounds in order to improve their potency, selectivity and pharmacokinetic parameters. This can immensely benefit drug discovery process by reducing the cost and increasing the quality of the final product. Although protein three-dimensional structures are best determined by experimental methods such as X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy, the number of experimentally resolved structures is low compared to the number of available protein sequences. Despite significant advances in these techniques, their limitations and expensive procedures make it unlikely to have experimentally resolved structures of all known protein sequences in the near future. For example, as of May 2013, the number of gene products in the Reference Sequence Database is $>3.1\times10^7$; in contrast, the number of experimentally determined structures deposited in the Protein Data Bank is only 91,190. Considering a much slower pace of experimental structure determination compared to genome sequencing, this disparity continues to grow. Protein structure prediction attempts to bridge the gap between the available sequence and structure data and therefore is playing an important role in structure-based drug development. Nevertheless, traditional structure modeling from raw sequence data typically leads to protein models in the unbound conformational state. On the other hand, other publicly available resources, such as BindingDB, provide large repositories of protein-ligand interactions collected from inexpensive, high-throughput binding assays. Experimental data routinely generated by these assays is uni-dimensional and could be used in conjugation with protein structure modeling to generate three-dimensional models of drug-protein complexes. Importantly, due to a high evolutionary conservation of functional sites in proteins, the structures of the majority of drug targets can be effectively modeled in their bound conformations. Our objective is to leverage 1-dimensional information on protein-ligand interactions from BindingDB to support large-scale homology-based structure modeling of pharmacologically relevant molecular assemblies. Towards this goal, we have modeled 2,245 individual drug targets, which will be used as a basis to construct the molecular structures of 235,957 drug-target complexes. Our preliminary analysis suggests that using existing structural information from Protein Data Bank, the majority of BindingDB assemblies can be confidently predicted at near-atomic level. This will greatly expand the repertoire of molecular interactions between proteins and small molecules to further support contemporary structure-based drug discovery and design.

Ab-initio Calculations of Accurate Electronic Properties of ZnS

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We present results from *ab-initio,* self consistent, local density approximation (LDA) calculations of electronic and related properties of zinc blende zinc sulphide (zb-ZnS). We employed the Ceperley and Alder LDA potential and the linear combination of atomic orbital (LCAO) formalism in our non relativistic computations. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams' method as enhanced by Ekuma and Franklin (BZW-EF). The BZW-EF method includes a methodical search for the optimal basis set that yields the minima of the occupied energies. This search entails increases of the size of the basis set and the related modifications of angular symmetry and of radial orbitals. Our calculated, direct gap of 3.72 eV, at the Γ point, is in excellent agreement with experiment. We have also calculated the total (DOS) and partial (pDOS) densities of states and electron and hole effective masses for ZnS. Research funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE-NA0001861), LaSPACE, and LONI-SUBR.

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Validation and Application of LES Modeling of Unidirectional and Wave Flow through Submerged Vegetation

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Abstract:

The State of Louisiana has witnessed the loss of 1883 sq. miles of wetland between 1932-2012 due to a number of factors among which wave erosion and lack of sediment supply[1] are very important. Coastal vegetation offers cost efficient, environmentally sustainable wave damping and sediment trapping solutions and has thus received a lot of attention in recent years[2]. Waves lose their energy due to turbulent interactions as they move over and through vegetation arrays, but our understanding of the inherent hydrodynamics is limited. In this work we will present results from our ongoing research on numerical simulations of water waves and unidirectional flows through submerged vegetation, idealized as a rectangular array of rigid cylinders using the fully three-dimensional Navier-Stokes Equation involving Large Eddy Simulation (LES) turbulence closure scheme. LES provides more accurate flow fields than Reynolds Averaged Navier-Stokes (RANS) models by resolving the larger eddies which govern most of the flow dynamics while the effects of the smaller (sub-grid scale) eddies are modelled using the eddy-viscosity approach. The free surface is handled by a Volume of Fluid (VOF) model. The simulations are being carried out using the open source CFD software OpenFOAM[3], on massively parallel clusters provided by LSU High Performance Computing (LSU-HPC) and the Louisiana Optical Network Initiative (LONI). In this presentation we will show the validation of the model with laboratory experiments for unidirectional flow and investigate the vertical variation of mean and turbulence quantities as well as visualizations of the three dimensional coherent vortex structures generated from individual stems within the canopy scale due to the periodic variation of the surrounding hydrodynamic field. In addition, calculation of bulk drag coefficients using the energy conservation approach will also be made and comparisons presented with available experimental results. The results of this work are expected to improve our understanding of wave hydrodynamics through vegetation arrays as well as highlight the applicability of cutting-edge computational research to answer fundamental science and engineering research questions. Computational resources for the research have been provided by the Center for Computation and Technology at Louisiana State University.

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GPU IMPLEMENTATION OF A VARIATIONAL MONTE CARLO STUDY

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Understanding the mechanism which leads to various exotic phases in strongly correlated systems is important from the perspectives of both theoretical physics and practical applications. Unfortunately, analytical techniques for studying strongly correlated systems are limited. Over the last two decades or so, various numerical methods had been proposed to tackle such problems. Different Quantum Monte Carlo methods have been successfully applied to study various strongly correlated systems. While those methods are usually unbiased, for some of the most physically interesting regimes, they suffer from the minus sign problem. Variational Monte Carlo (VMC) is a useful numerical method for obtaining ground state wave function by minimizing the ground state energy of strongly correlated systems. This method can provide fairly accurate results in some interesting phases, such as the spin liquid phase and the superconducting phase without the minus sign problem. The main obstacle for VMC is the large statistical fluctuations from the Monte Carlo sampling. Therefore, large number of samples are needed to reduce the noise of the data. The GPU computing allows to overcome the obstacle by accelerating the VMC simulations by generating a large number of independent samples in parallel. We have implemented the VMC algorithm for the single band Hubbard model for the tilted square lattice in GPU. Our present GPU implementation has produced about 100 times speedup compared to the CPU code in a single core. We expect the present code will provide us the capability to study larger system sizes with higher accuracy which is hitherto difficult.

Quantum Cosmology with High Performance Computers

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The evolution of a semi-classical state in isotropic LQC is governed by difference equations with uniform discretization in the spatial direction. We study the numerical simulations of widely spread states corresponding to quantum universes which, due to the large spread, require large computational domain. These simulations, hence, would be computationally very expensive. In this work we present an efficient hybrid numerical scheme based on the fact that LQC difference equations can be approximated by partial differential equations (PDE's) in the large spatial volume domain. We introduce a hybrid spatial grid where we solve the LQC difference equations in small volume regime and the PDE's in the large volume regime. By a simple change of co-ordinate, we obtain a surprising reduction in the cost of computation. This scheme enables us to explore the regions of the parameter space which was previously unachievable. We describe the numerical properties and present the results of the simulations for various states, and compare them with the results of effective dynamics.

Replica Exchange Dynamic Molecular simulations of Cyclic and Linear Amphiphilic Homopolymer

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Abstract

Polymer-based micelles had been raised particular interests in application as drug delivery material because their spontaneously forming core-shell structure with hydrophobic core encapsulating solvent-compatible particles as long as hydrophilic corona imparting water-solubility upon the aggregation. In our research work, Molecular Dynamic (MD) simulations based on a novel Amphiphilic Homopolymer c-PHS-Amph first reported by Scott Grayson's lab were performed to investigate polymer's unique topologies as well as its resulting prominent solvent-dependent character, which would progressively shed a in-depth interpretation to the molecular driving force leading amphiphilic behavior. Since Macromolecule requiring relative large scale computational work, we have cooperated with Steve Rick's group to employ Replica Exchange Dynamic Simulation (REDs) to improve sampling space and determine the global polymer conformation. Through applying REDs technique, exchange among replicas split in large potential barriers occurred efficiently and successfully deliver linear and cyclic polymer's characteristic structure corresponding with different solvents' environment. Proximal radial distribution of solvent around hydrophobic arms and hydrophilic arms was performed to validate the thermodynamic signatures as well as used to reproduce the density profile of interacting solvents.

Monte Carlo Simulations of Surface Induced Nucleation

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. Surface induced nucleation is a special case of nucleation where the vapor phase condenses on a solid surface. This type of nucleation is directly applicable to areas of interest such as nano-particle synthesis, airplane de-icing systems, etc.

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 experimental data as well as theory. 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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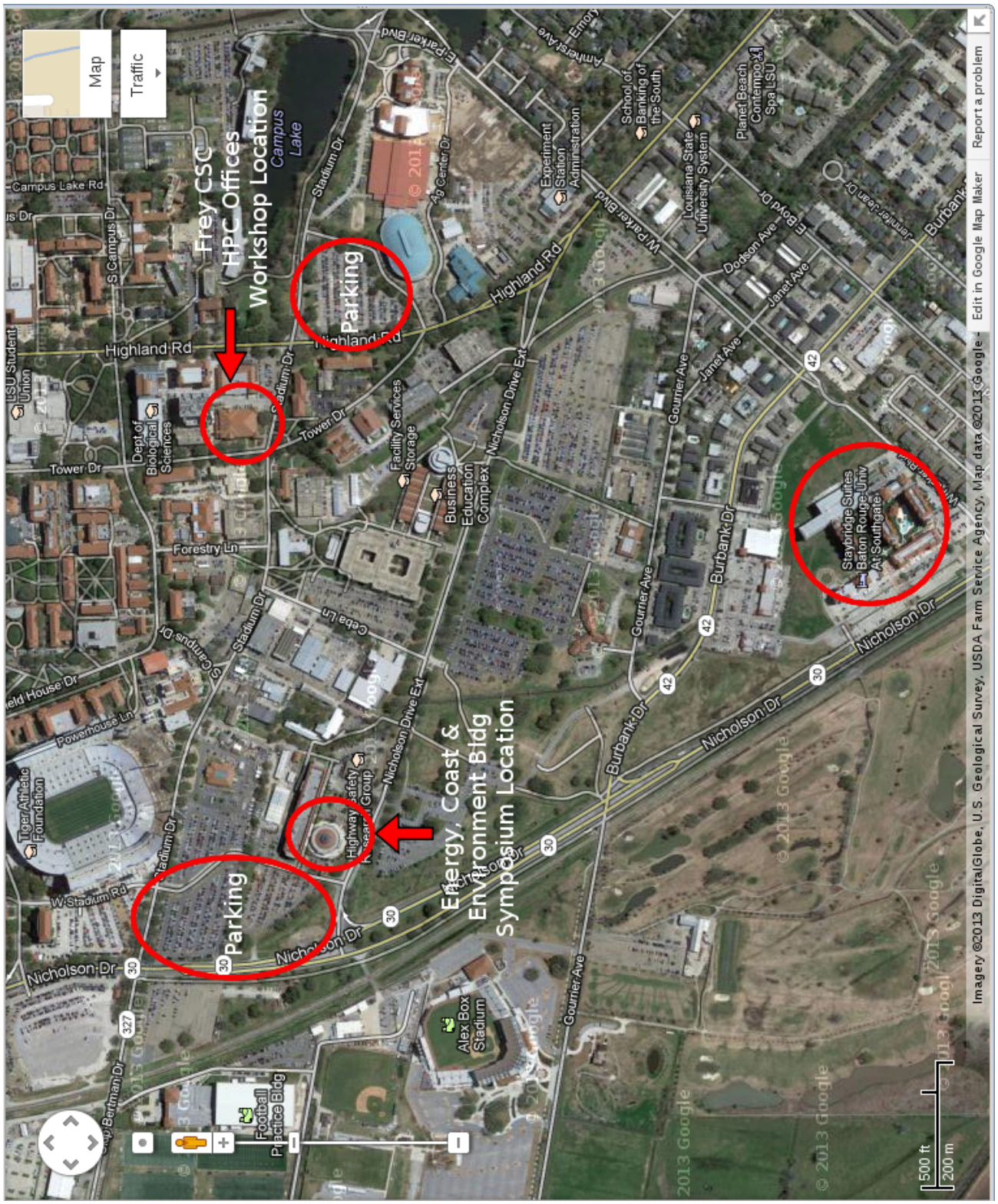
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