3rd Annual High Performance Computing User Symposium

Louisiana State University, Baton Rouge

June 4 - 5, 2014

3^{rd} Annual High Performance Computing User Symposium

Louisiana State University, Baton Rouge, LA 70803
June 4-5, 2014

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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 3^{rd} 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 3^{rd} 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 and LONI. Special thanks to NVIDIA Corporation for organizing the GPU Workshop immediately following the Symposium and John Stone for agreeing to be the keynote speaker for the Symposium.

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

Symposium Program

June 4th, 2014	Louisiana Digital Media Center Lobby
6:00 pm - 8:00 pm	Registration and Poster Session
June 5th, 2014	Louisiana Digital Media Center Theatre
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8:15 am - 8:30 am	Welcome
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9:30 am - 10:00 am	*Theoretical and Computational Physics Research at Primarily Undergraduate Institution* Hye-Young Kim Department of Chemistry and Physics, Southeastern Louisiana University
10:00 am - 10:15 am	Break
Session II	Chair: Abdul Khaliq, Louisiana Tech University
10:15 am - 11:00 am	*Red Queen Evolution of Testes Mass and Sperm Competition* Jacob A. Esselstyn Department of Biological Sciences, Louisiana State University
11:00 am - 11:20 am	*Modeling silicate glasses: insights from first principles molecular dynamics simulations* Dipta Ghosh School of Electrical and Computer Science, Louisiana State University
11:20 am - 11:40 am	*Numerical Simulation of the early Universe in Loop Quantum Cosmology* Brajesh Gupt Department of Physics & Astronomy, Louisiana State University
11:40 am - 12:00 pm	*Simulation of Immunoprecipitation Bead Mass Transport* Nicholas Richardson Department of Mathematics and Engineering Technology, Northwestern State University of Louisiana
12:00 pm - 1:00 pm	Lunch (provided)

Symposium Program

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1:45 pm - 2:05 pm	*Simulation for the International Space Station CALET Experiment* Nicholas Cannady Department of Physics & Astronomy, Louisiana State University
2:05 pm - 2:25 pm	*Large Eddy Simulation Investigations of Wave Hydrodynamics at the Marsh Edge in presence of a Breakwater* Agnimitro Chakrabarti Department of Civil & Environmental Engineering, Louisiana State University
2:25 pm - 2:45 pm	*First Principle Modeling of Atomic Nuclei in the Era of Petascale Computing* Tomáš Dytrych Department of Physics & Astronomy, Louisiana State University
2:45 pm - 3:00 pm	Break
Session IV	Chair: Le Yan, Louisiana State University
3:00 pm - 3:45 pm	*Molecular Simulations of Earth Materials for Environmental and Energy Applications* Jianwei Wang Department of Geology & Geophysics, Louisiana State University
3:45 pm - 4:05 pm	*Ultrafast Transient Absorption in a Helium Gas* Mengxi Wu Department of Physics & Astronomy, Louisiana State University
4:05 pm - 4:25 pm	*Accelerating the pace of protein functional annotation with Intel Xeon Phi coprocessors* Wei Feinstein Department of Biology, Louisiana State University
4:25 pm - 4:45 pm	*Theoretical Studies of the Structural, Electronic, and Optical Properties of Carbazole-Imidazolium based GUMBOS* Chengfei Lu Department of Chemistry, Louisiana State University
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Cain Department of Chemical Engineering, Louisiana State University

2 Molecular Dynamics Simulation of Oil Alkanes and Dispersants in Atmospheric Air/Salt Water Interfaces

Zhengui Zhang
Cain Department of Chemical Engineering, Louisiana State University

3 Density of hydrous model basalt melt at mantle pressure regime

Suraj K. Bajgain
Department of Geology and Geophysics, Louisiana State University

4 Structure, Dynamics and Crystallization of Ionic Liquids under Confinement and Low Temperature

Xiaoxia He
Cain Department of Chemical Engineering, Louisiana State University

5 Solitary wave forces on Biloxi Bay Bridge decks

Guoji Xu
Department of Civil and Environmental Engineering, Louisiana State University

6 Microscopic Structure of Self-Assemblies composed of VECAR molecules

Bijay Shrestha
Department of Chemistry and Physics, Southeastern Louisiana University

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Jumao Yuan
Department of Chemistry, Louisiana State University

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Richard Platania
School of Electrical Engineering and Computer Science, Lousisiana State University

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Yun Ding
Department of Physics & Astronomy, Louisiana State University

Abstracts

Programming for Hybrid Architectures Today and in the Future

John Stone

Beckman Institute for Advanced Science and Technology,
University of Illinois at Urbana-Champaign, Urbana, IL 61801

Abstract

Hybrid or heterogeneous computing architectures combine conventional multi-core CPUs with massively parallel microprocessors such as GPUs to create a platform that is well suited to the needs of many high performance computing workloads. Hybrid architectures have demonstrated significant benefits for application performance and also energy efficiency over conventional architectures. As of November 2013, several of the top ten fastest supercomputers in the world were based on hybrid many-core and GPU architectures, and all of the top ten systems in the Green500 list were hybrid GPU-accelerated systems. The most efficient Green500 system, Tsubame-KFC, achieved a record 4.5 GFLOPS/Watt. While it is clear that hybrid systems offer tremendous potential for increased performance and energy efficiency, they also pose challenges in terms of the adaptation of legacy application software to fully exploit massively parallel microprocessors such as those in GPUs. This presentation will outline the development and subsequent evolution of hybrid computing approaches in HPC, describe challenges and solutions for adapation of legacy software to current state-of-the-art hybrid computing platforms, and forecast hybrid computing technologies and changes to HPC workloads and usage models that are expected to impact the HPC user community in the next two to five years.

Theoretical and Computational Physics Research at PUI

Hye-Young Kim

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

Abstract

Southeastern Louisiana University is a primarily undergraduate institution (PUI). I offer research projects to undergraduate students in computational and theoretical physics. I had many number of students who participated in nano-material science research using both theoretical methods and the molecular dynamics simulations. In this presentation, I would present both the recent outcomes of my research group and my teaching experience working with undergraduate student researchers.

Current research is supported by Louisiana BOR grant (LEQSF(2012-15)-RD-A-19) and by the Louisiana Optical Network Institute (LONI).

Modeling silicate glasses: insights from first principles molecular dynamics simulations.

Dipta B. Ghosh and Bijaya B. Karki

School of Electrical Engineering and Computer Science,
Department of Geology and Geophysics, and Center for Computation and Technology
Louisiana State University, Baton Rouge

Abstract:

Melts are of particular geophysical interest owing to their ubiquitous role in the early stages of accretion of the Earth and also in its present day dynamics. Owing to the experimental inaccessibility of the in-situ "high-temperature – high-pressure" conditions, a requisite in the study of geophysically relevant melts, silicate glasses are often considered as accessible analogs to high-pressure melts. Because of the lack of data on silicate liquids, it is not known however, how closely the behavior of silicate glasses corresponds to that of liquids at high pressure. To understand and gain some insight on the issue, we investigate the equation of state, structural and elastic properties of $MgSiO_3$ glass at 300 K as a function of pressure from first-principles molecular-dynamics (FPMD) simulations. We explore two different compression paths: cold compression, in which the zero pressure quenched glass is compressed at 300 K, and hot compression, in which the liquid is quenched in-situ at high pressure to 300 K. We also study decompression and associated irreversible densification. Our simulations show that the glass at the zero pressure is composed of primarily Si-O tetrahedra, partially linked with each other via the bridging oxygens (present in 35%; the remaining being the non-bridging oxygens). With increasing pressure, the mean Si-O coordination number gradually increases to 6, with 5-fold and subsequently 6-fold replacing tetrahedra as the most abundant coordination environment. The Mg-O coordination comprising of a mixture of four-, five- and six-fold species at zero pressure picks up more high-coordination (seven- to nine-fold) species on compression and its mean value increases from 4.5 to 8 over the entire pressure range studied. Consistently, the anion-cation coordination numbers increase on compression with appearance of oxygen tri-clusters (three silicon coordinated O atoms) and mean O-Si coordination eventually reaching 2. Hot compression produces greater densities and higher coordination numbers at all pressures as compared with cold compression, reflecting kinetic hindrances to structural changes. On decompression from 6 GPa, the glass regains its initial uncompressed structure with almost no residual density. Decompression from 27 GPa produces significant irreversible compaction, and the peak-pressure of decompression significantly influences the degree of density retention with as high as 15% residual density on decompression from 170 GPa. Irreversibility arises from the survival of high coordination species to zero pressure on decompression. With increasing pressure, the calculated compressional and shear wave velocities (about 5 and 3 km/s at the ambient conditions) of $MgSiO_3$ glass increase initially rapidly and then more gradually at high pressures. Our results suggest that hot-compressed glasses perhaps provide closer analog to high-pressure silicate melts than the glass on cold compression.

Numerical simulation of the early universe in loop quantum cosmology

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

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[2]*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803*

Loop quantum cosmology (LQC) is a theory of quantum cosmology based on loop quantum gravity (LQG) which gives a quantum geometric description of the spacetime. Due to the underlying quantum geometric effects, LQC resolves all the physical singularities in a homogeneous and isotropic universe by replacing big bang by a big bounce bridging two disparate phases of universe, namely the expanding and contracting phases which were otherwise disjoint in the classical theory. In this talk, we present numerical techniques recently developed at LSU to study the evolution of a bouncing quantum universe in its early stages in the paradigm of LQC. We describe the numerical scheme as well as its implementation with high performance computers and GPUs using the computational resources at CCT, LSU to simulate the evolution of anisotropic universe. We describe the advantages of the numerical scheme and some of the results. We will also discuss the future impact of the numerical scheme in terms of its potential to compute corrections to the observational effects of quantum geometry.

Simulation of Immunoprecipitation Bead Mass Transport

Jinko Kanno[1], Adarash Radadia[2], and Nicholas Richardson[3]

[1] *Department of Mathematics and Statistics, Louisiana Tech University, Ruston, LA 71272*
[2] *Institute for Micromanufacturing, Louisiana Tech University, Ruston, LA 71272*
[3] *Department of Mathematics and Engineering Technology, Northwestern State University of Louisiana, Shreveport, LA 71101*

Abstract

Antibodies immobilized on micron-sized beads have been heavily used for capture and purification of specific bacteria, viruses, or proteins from complex clinical samples for biomedical diagnostics. This process is referred to as immunoprecipitation. In this process, beads of well-characterized size are mixed in known amounts (or concentration) with the clinical sample potentially containing pathogenic bacteria or viruses. For simplicity we will only consider bacteria for our studies. Ability to predict the bacteria isolation efficiency based on estimated bacteria concentration, known bead size and concentration, and mixing time, will reduce the amount of time and cost of material spent by biotech researchers in optimizing their immunoprecipitation assays. Decreasing the bead size results in increased surface area and thus the amount of antibodies, however this reduces the total fluid volume swept by the beads and the bacteria-bead interaction probability. We hypothesize that there is an optimum bead size that provides an optimum balance between the two. The overall goal of this project is to create a simple simulation calculator that predicts the bead-bacteria interaction probability based on known bacterial concentration, bead size and concentration, and mixing time.

We have created a simulation to model the movement of beads and bacteria in a solution to determine the capture efficienct E. By adjusting the parameters for bead and bacteria size, concentration, capture probability, and capture range, the simulation will determine the capture efficiency.

The simulation currently represents the beads and bacteria as spherical objects. We simulate their movement by projecting a random placement of beads and bacteria in a simulation area onto a plane. The simulation time, t_{mix} is set by the capture range where a larger range will result in a longer mixing time. Using the simulation area to project onto a plane, each bacteria is checked to determine if a bead is within its capture range. Each bead has a specified probability to capture the bacteria. Since the simulation is dependent on probability, we run multiple simulations in parallel on LONI. Since each simulation is independent, the only communication needed is to combine the results in the end.

Insights Into the Structure and Function of Glycosylated Proteins

Dhruva K. Chakravorty
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University of New Orleans
New Orleans, LA 70148

Abstract.
Using computational methods we explore the structure and function of glycogen binding proteins Glucose Oxidase (GoX) and the *Streptococcus pneumomiae* surface adhesion protein PfbA. (GOX) is a redox enzyme that uses flavin adenine dinucleotide (FAD) as a cofactor to reduce β-D-glucose into δ-gluconolactone via a ping-pong steady-state kinetic mechanism. While it remains a candidate for developing alternative fuel cells, instability of the dimeric interface remains a concern. Electrochemistry experiments have determined that enzymatic efficiency depends upon the orientation of FAD to the electrode. Our hypothesis is that the orientation of FAD effects the conformational space sampled by the protein. *S. pneuomoniae* PfbA is a Ca2+ and Mn2+ binding beta-sheet protein that binds sugar molecules as part of its virulence mechanism. We present early results on the role of sugar molecules on these enzymes. In close agreement with literature, molecular dynamics simulations find that these proteins undergo large conformational changes that have been implicated in the modulating the glycosylation reaction. Our long-term goal is to develop computational chemistry methods in order to simulate the protein-protein and protein-electrode interactions to understand the impact of crowding environments on the protein.

Simulation for the International Space Station CALET Experiment

Bethany Broekhoven, Nick Cannady, Doug Granger, T. Gregory Guzik, Amir Javaid, Seth Junot, and Michael Stewart

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

Abstract

The CALorimetric Electron Telescope (CALET) instrument is being developed by an international collaboration of researchers in Japan, Italy, and the United States and is designed to explore the High Energy Universe. The instrument is a large, deep calorimeter designed primarily to measure the spectrum of cosmic ray electrons up to 20 TeV but also gammas and nuclei (Z=1 to Z=40) from several MeV up to 1000 TeV within a field of view of 45 degrees. The primary science goals of CALET are to address outstanding questions such as (1) the nature of the sources of high energy particles and photons, (2) the details of particle transport in the Galaxy, and (3) signatures of dark matter, in either the high energy electron or gamma ray spectrum. LSU is the lead institution for the U.S. portion of the CALET collaboration.

One of the many objectives of the U.S. collaboration is to develop a software model of the CALET main telescope whose output is identical to the CALET flight data. The model is based on an existing simulation code which is configured to include an accurate physical description of the CALET main telescope hardware and an accurate electrical description of the telescope's operation. Output from the model will be used to validate the data processing and analysis software as well as to evaluate backgrounds and other physical or systematic effects that will be encountered during in-orbit operations.

CALET instrument modeling and simulations are carried out using a combination of M.C. simulation code packages EPICS (Electron-Photon Induced Cascade Simulator) and Cosmos as well as the software code for the CALET instrument model. Together, EPICS and Cosmos successfully simulate cosmic ray events in the detector environment, including deposition of energy and development of particle showers. A large set of simulation runs are required, filling the energy, solid angle and particle type “phase space”, for a proper evaluation of the instrument design. To do this, a large amount of processing power is required. For instance, one simulation of a particle shower for Iron at 500GeV/n takes on average fifteen minutes and for a proper evaluation, we will need over 100,000 of these events. By utilizing the HPC resources available, we will be able to effectively and efficiently generate the data needed to fully characterize the CALET instrument.

Further, in order to cover the required “phase space” we will need many runs of the simulation code and generate hundreds of individual output files, creating a management issue. In order to address this issue we have developed an online Simulation Log database as well as a Management Checklist in order to track and control how HPC resources are used. The database allows users to log information about the simulation data as well as job parameters. Once required fields are entered into the Log, a job name and unique ID are returned to the user that are then used in the naming convention of a simulation input and output files. Characteristics of the job, such as run time, errors, size of output data files, are also logged. The Simulation Log database provides a sortable listing of all jobs to assist in locating particular results or assessing the status of our overall HPC computations.

This presentation will discuss the CALET science mission and instrument, the specific modeling tasks to be undertaken by LSU and our methodology for managing the computation results.

Large Eddy Simulation Investigations of Wave Hydrodynamics at the Marsh Edge in presence of a Breakwater

Agnimitro Chakrabarti[1], and Qin J. Chen[1,2,3]

[1]*Department of Civil & Environmental Engineering, Louisiana State University*
[2] *Center for Computational Technology, Louisiana State University*
[3] *Coastal Studies Institute, Louisiana State University*

Abstract

Louisiana has lost 1833 sq miles of wetlands between 1932-2010 (Couvillion et al, 2011) with recent trends (Dahl and Stedman, 2013) from 2004-2009 showing almost doubling of the erosion rate compared to the previous data from 1988-2004, largely due to the increased occurrence of catastrophic hurricanes and associated storm surge and wave induced damage at the marsh fringes. In fact erosion of the marsh edge by high frequency, moderate to high energy wind waves is a major cause of wetland loss in coastal Louisiana accounting for almost 26% of the total land loss. To combat the devastating wetland loss, rock dikes, nearshore breakwaters, artificial oyster reefs, among other structures have been built in south Louisiana. However due to soft soils and fine sediments in Louisiana's estuaries and bays, innovative engineering design of shoreline protection systems that are different from those applied to sandy coasts is needed. The authors' research group is using Computational Fluid Dynamics (CFD) tools to understand the hydrodynamics causing erosion around the marsh edge under a variety of wave conditions and submergence levels, both under no-structure (natural) conditions and with-structure (constructed) conditions. The study aims to lay out design guidelines by optimizing the height, degree of submergence, structure footprint and distance from the shoreline for rubble mound breakwaters based on erosive shear stress potential of the transmitted waves, wave reflection and transmission efficiency, as well as the vertical and horizontal circulation patterns at different critical design water levels. We use the open-source CFD package OpenFoam, developed by OpenCFD Ltd at the ESI Group for simulating the complex three-dimensional (3D) flow field around the marsh edge as well as the breakwaters using dynamic Large Eddy Simulation (LES) closure schemes.

The accuracy of the model is verified against laboratory measurements of wave breaking on a beach, the resultant wave height variation and undertow, and wave transmission and reflection by a semi-circular breakwater. Good agreement between the numerical result and laboratory data has been found. It is found that a submerged breakwater placed within two wavelengths in front of a marsh edge can create complex circulation patters in the vertical plane. Such a circulation is absent without the structure and likely has important sediment transport potential.

References:
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2. Dahl, T. and Stedman, S. (2013). Status and trends of wetlands in the coastal watersheds of conterminous united states 2004-2009. Technical report, U.S. Department of the Interior, Fish and Wildlife Service and National Oceanic and Atmospheric Administration, National Marine Fisheries Service.

First Principle Modeling of Atomic Nuclei in the Era of Petascale Computing

Tomáš Dytrych, Kristina D. Launey, and Jerry P. Draayer

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

Abstract

Over the past decade, major progress in the development of realistic internucleon interactions along with the emergence of petascale computing resources have advanced considerably predictive capabilities of ab initio modeling of nuclear structure and reaction processes. However, a widespread application of first principle studies to heavier nuclei, crucial for advancing our knowledge about the element formation and stellar evolution, still remains beyond computational reach. The progress is hindered by the nearly combinatorial growth of many-nucleon basis, that comes with the addition of oscillator shells and the number of nucleons. We developed a novel ab initio framework that utilizes state-of-art techniques and formalism of the group theory to solve Schrödinger equation for a system of strongly interacting nucleons. We implemented this theoretical framework as a hybrid MPI/OpenMP computer code that scales well up to 365,000 cores and possibly beyond. We will present results that clearly unveil a remarkable feature common to the low-energy structure of nuclei that has heretofore gone unrecognized in other ab initio studies – the emergence of simple orderly patterns that favor strongly deformed configurations and low intrinsic spin values [1]. We will show how one can use this feature to quell computational explosion associated with rapidly increasing size of model space while ensuring that important properties of atomic nuclei, e.g., enhanced BE2 strengths and nucleon cluster substructures [2], are appropriately accommodated in ab initio studies.

References

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[2] A. C. Dreyfuss, K. D. Launey, T. Dytrych, J. P. Draayer, and C. Bahri, Phys. Lett. B 727 (2013) 511.

Molecular Simulations of Earth Materials for Environmental and Energy Applications

Jianwei Wang

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Abstract: Knowledge of earth materials is essential to their environmental and energy applications. Because of the difficulties in direct observation of earth materials under various conditions, molecular modeling becomes indispensable in understanding their structure and properties. These simulations provide greatly increased understanding and atomistically detailed otherwise unobtainable information of the structure, dynamics, spectroscopy, and energetics. I will use a few examples to illustrate how these atomic-scale simulations can provide a bridge between theories and observations of earth materials using high performance computing facilities. In low temperature geochemistry, water exchange reaction at water-mineral surfacs is fundamentally importan to the understanding of the interfcial chemistry of minerals in the environment. Molecular dynamics and rare event sampling methods are used to compute the reaction rate and to understand how the exchange rate scales from aqueous ion, nanoparticles, to mineral surfaces. For hydrogen storage materials, hydrogen clathrate hydrate is environmentally friendly because upon combustion it simply releases water. Direct calculations of the vibrational spectra of hydrogen clusters in hydrogen hydrate cages from first-principles improve the understanding of the experimental Raman spectra of the hydrogen molecules and provide a guild on the synthesis of hydrogen gas hydrate. For uranium dioxide, or a mineral called uraninite, one of the unique properties is its non-stoichiometry. First-principles molecular dynamics simulations of hyperstoichiometric uranium dioxide suggest that the well-known structural model for the oxygen defect cluster in UO_{2+x} needs a revision. The simulations show the dynamic nature of the defect cluster, which consists of three interchanging configurations, in contrast to the averaged structure established from early neutron diffraction data.

Ultrafast Transient Absorption in a Helium Gas

Mengxi Wu[1], Shaohao Chen[2], Seth Camp[1], Kenneth Schafer[1], Mette Gaarde[1]

[1] *Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803*
[2] *High Performance Computing, Louisiana State University, Baton Rouge, LA 70803*

Abstract

We present an example of the theoretical ultrafast transient absorption studies in our group, in which we consider the absorption of an attosecond pulse by a laser-dressed inert gas. We use a weak attosecond pulse to excite the gas to some transient excited states, which are then probed by an intense femtosecond pulse, and the absorptions of the attosecond pulse is detected. We vary the delay between the two pulses and use this delay-dependent absorption spectrum as a tool to learn the ultrafast electron dynamics in the atom. Most of our theoretical calculations involve the coupled solutions of the time-dependent Schrodinger equation and the Maxwell's wave equation, which require high-performance computing resources. The computational resources are provided mostly by the Louisiana Optical Network Initiative and the High Performance Computing at Louisiana State University. We will show an example in which the attosecond pulse is temporally reshaped while propagating through the gas medium.

Accelerating the pace of protein functional annotation with Intel Xeon Phi coprocessors

Wei Feinstein[1,3], Juana Moreno[2,3], Mark Jarrell[2,3] and Michal Brylinski[1,3]

[1]Department of Biology, Louisiana State University, Baton Rouge, LA 70803
[2] Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803
[3] Center for Computation and Technology, Louisiana State University, Baton Rouge, LA 70803

Abstract

Intel Xeon Phi is a new addition to the family of powerful parallel accelerators. The range of its potential applications in computationally driven research is broad; however, at present, the repository of scientific codes is still relatively limited. In this study, we describe the development and benchmarking of a parallel version of *e*FindSite, a structural bioinformatics algorithm for the prediction of ligand-binding sites in protein models. Implemented for the Intel Xeon Phi platform, the parallelization of the structure alignment portion of *e*FindSite using pragma-based OpenMP brings about the desired performance improvements, which scale well with the number of computing cores. Compared to a serial version, the parallel code runs 11.8 and 10.1 times faster on the CPU and the coprocessor, respectively; when both resources are utilized simultaneously, the speedup is 17.6. For example, ligand binding predictions for 501 benchmarking proteins are completed in 2.1 hours on a single Stampede node equipped with the Intel Xeon Phi card compared to 3.1 hours without the accelerator and 36.8 hours required by a serial version. In addition to the satisfactory parallel performance, porting existing scientific codes to the Intel Xeon Phi architecture is relatively straightforward with short development times due to the support of common parallel programming models by the coprocessor.

THEORETICAL STUDIES OF THE STRUCTRURAL, ELECTRONIC, AND OPTICAL PROPERTIES OF CARBAZOLE-IMIDAZOLIUM BASED GUMBOS

Chengfei Lu, Nuoreen Siraj, Paul Magut, , Lucy W. Kiruri, Kenneth Lopata, Isiah Warner

Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803, United States

Abstract

We report on a joint theoretical and experimental studies of the electronic structure of a series of carbazole-imidazolium $[CI]^+$ based GUMBOS with $[OTf]^-$, $[NTf_2]^-$, and $[BETI]^-$ as anion. The theoretical studies were carried out using the density functional theory (DFT) with valence split 6-31+G(d,p) basis set. The ground state geometries optimization and electrostatic potential surfaces (ESP) of $[CI]^+$ and anions were calculated to estimate the hydrogen bonding interaction between the cation and the anions. The groud state geometries of GUMBOS were also optimized, showing a reduction of in the dihedral angel between carbazole ring and imidazoulium ring as well as in the band gap going from $[OTf]^-$ to $[BETI]^-$. The electron densities of LUMO were moving from carbazole ring to imidazolium ring as anion going from $[OTf]^-$ to $[BETI]^-$, which led to a S0 to S1 transition increase with this trend. The calculated reorganization energy for hole and electron indicates that three compounds are in favor of hole transport than electron transport.

Molecular dynamics simulations of hydrophobins at hydrophobic/hydrophilic interfaces: the feasibility of hydrophobins as oil dispersant

Yuwu Chen[1], Thilanga P. Liyana-Arachchi,[2] Paul S. Russo[3] and Francisco R. Hung[1]

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Abstract

We present the feasibility of a unique bio-surfactant: hydrophobin as oil dispersant. These small surface-active proteins can self-assemble at a variety of hydrophobic/hydrophilic interfaces, efficiently encapsulating oil (to form "blob") and air (to form "bubble"). By performing classic molecular dynamics (MD) simulation and potential of mean force (PMF) calculations with both all-atom and coarse-grained representations of a class I hydrophobin EAS, interfacial properties of hydrophobin at gas/water and oil/water interfaces were probed. According to the PMF calculation results, EAS molecule was likely to stay at the hydrophobic/hydrophilic interface, and the adsorption behavior of EAS at the interface was strong and irreversible. Moreover, according to classic MD simulations, EAS would strongly bind at the gas/water and oil/water interfaces, indicating the self-assembling process occurs at the molecular level.

Molecular Dynamics Simulation of Oil Alkanes and Dispersants in Atmospheric Air/Salt Water Interfaces

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Molecular dynamics simulations were conducted to investigate the properties of several intermediate- and semi-volatile *n*-alkanes from oil, as well as model dispersants, at the air/salt water interface. These studies are relevant to the possible transport of oil and dispersants from the sea surface into the atmosphere via mechanisms such as bubble bursting and whitecaps (breaking waves). Our simulations show that the *n*-alkanes and the model dispersants have a strong preference to remain at the air/salt water interface, as indicated by the presence of deep free energy minima at these interfaces; therefore, *n*-alkanes are very likely to adsorb at the surface of bubbles or droplets and be ejected to the atmosphere by sea surface processes such as whitecaps and bubble bursting. The free energy minimum at the interface becomes deeper as the chain length of the *n*-alkanes increases, and as the concentration of dispersant at the interface increases. These simulation results are consistent with experiments using a laboratory aerosolization reactor, where it was found that more oil hydrocarbons are ejected when Corexit 9500A is present in the system. These trends strongly suggest that aerosolization through bubble bursting and breaking waves at the sea surface is an important transport mechanism for the ejection of spilled oil hydrocarbons into the atmosphere.

Density of hydrous model basalt melt at mantle pressure regime

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Seismic observations indicate the presence of low velocity zone (LVZ) at 410 km depth and ultra-low velocity zone (ULVZ) at 2890 km depth below the surface of the Earth. These observations suggest the existence of partial melts within the solid mantle. Silicate melts might have played more important role in the Earth's early history when the Earth was fully molten. Thus, the knowledge of physical properties (i.e., density and Diffusivity) of silicate melts at high pressure and temperature are necessary to understand the melt segregation and transportation. Silicate melts are known/expected to be hydrous. Water can make large impact on density and mobility of melt. Despite of many implications, experiments at mantle pressure and temperature conditions are difficult to conduct. On the other hand, first principle molecular dynamics (FPMD) simulation is a robust computational technique that can be complement to the experiment. In this study, FPMD simulation of hydrous model basalt melt is performed to study the density and diffusivity of the melt. Results of this study indicate that hydrous model basalt melt (with 3 wt. % of water) can be neutrally buoyant in the mantle that can contribute a probable explanation of a low-velocity layer found above the 410 km discontinuity. Conductivity of hydrous model basalt based on proton diffusivity is estimated to be 25 Sm^{-1} at 410 km depth (14 GPa, 1800 K). Assuming that a 20 km thick slab containing 5 % neutrally buoyant hydrous melt, estimated conductivity is capable to produce the conductance anomaly that can be detected with the use of electromagnetic sounding.

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Structure, Dynamics and Crystallization of Ionic Liquids under Confinement and Low temperature

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Molecular dynamics simulations were used to study the structure, dynamics and crystallization of the ionic liquids(IL). The IL 1-butyl-3-methylimidazolium bis(trifuluoromethanesulfonyl)imide [$BMIM^+$][NTf_2^-] were confined inside the ordered mesoporous carbon CMK-3 and CMK-5. CMK-3 and CMK-5 consists of nanorods that are made of amorphous carbon. This material exhibits interconnected nanopores, which are promising candidates for applications in electrochemical double-layer capacitor EDLCs. The properties of IL confined in CMK-3 at different temperatures were obtained and compared with the experiment results. We also compare the properties of IL confined in CMK-5 with different surface charge densities. Our results indicate that variables such as pore size, pore morphology, temperature and surface charge density have a profound influence on the structural and dynamical properties of the confined IL. Ions inside the pore form different layers, with the number of layers and the relative positions of the density peaks of the ions varying with pore size, pore morphology and surface charge density. The radial distribution functions suggest that the structure of the confined IL in the neutral CMK-3 and CMK-5 is similar to that of bulk IL; however, the IL confined in different charged CMK-5 shows different peaks compared to the bulk. The mean squared displacement of the confined ions near the surface of CMK-3 and CMK-5 show slower dynamics than the ions far from the surface. In particular, as the surface charge density rises, the dynamical properties of the counter ions in the layers near the surface decrease. Another observation is that the ions near the surface of CMK-3 and CMK-5 exhibit longer decorrelate time than the bulk ions. Crystallization is another important physical property of IL, which can be used in the synthesis of optically-active and magnetic nanomaterials. String method in collective varaibles (SMCV) is used to study how the IL 1,3-dimethylimidazolium chloride [$DMIM^+$][Cl^-] aggregate and organize themselves into the crystals. Order parameters(OPs) are defined to distinguish different transition states between the crystal and liquid. Our simulation proves that the SMCV method associated with OPs can be used to estimate the minimum free energy path, the molecular-level structure along it, as well as activation barriers and mechanism of crystallization of ILs.

Keywords: molecular dynamic simulation; ionic liquids; confinement; crystallization

Solitary wave forces on Biloxi Bay Bridge decks

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Abstract

Hurricane Katrina in 2005 destroyed a number of coastal bridges, including the Biloxi Bay Bridge. In this study, a wave model based on a solitary wave theory is developed to investigate the time-history of wave forces on the Biloxi Bay Bridge considering three different still water levels. A commercial CFD program of Fluent is employed to conduct this investigation. The results show that the wave forces on the bridge deck vary with the submersion coefficient under the same water depth and wave height. The wave forces also exhibit different characteristics under different still water depths, although with the same wave height.

Microscopic Structure of Self-Assemblies composed of VECAR molecules

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Abstract

A series of MD simulations has been performed using GROMACS and LONI resources to study the micellization of VECAR molecules in water. VECAR is a newly synthesized amphiphilic antioxidant molecule [1]. The force field generated from the Automatic Topology Builder demonstrates that both ends (vitamin E and Carnosine) of the molecule are hydrophilic and the carbon chain linking these two in the middle is hydrophobic. This structure differs from the common structure of amphiphilic molecules which has a hydrophilic head and a long hydrophobic tail attached at the opposite ends of the molecule. As a result, VECAR molecules self-assemble into atypical nano-structures. Recent results of data analyses on the microscopic structure of the self-assemblies will be reported. *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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Workflow Software for Keck & CAMD Tomography Systems

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Abstract

Neutron & X-ray interferometry is now possible with micro-fabricated gratings. With M.W. Keck funding, we will build a laboratory X-ray tomography/interferometry system; construction of similar interferometers is underway at the LSU CAMD synchrotron and the UC Davis McClellan Nuclear Research Center.

The data rate requires new workflow software and collaborative efforts. Highlighted here are joint efforts with Center for Computation & Technology (CCT) on High-Performance Computing (HPC) on Mathematica or MATLAB, New York University on VisTrails and City University of New York on SNARK09. These collaborations have the potential for great advances. HPC achieved parallel computing and contemporary processing which can happen at speeds of nanoseconds. VisTrails could become the standard for materials science tomography workflow. SNARK09 could provide the development framework for advanced interferometry data processing.

In our research, we consider three image sets: absorption, dark-field and phase-contrast. Particularly, for phase-contrast, single-shot and phase-stepping are the most commonly used methods in analysis. Single-shot is a technique that finds vertical and horizontal phase components using the Fourier transform. Phase-stepping is a technique that eliminates the mechanical scanning of the grating while still retaining the maximum spatial resolution. It scans the source of the x-ray tube with an electromagnetic field. This causes the projection of the object to move in the opposite direction, and also causes a relative movement between the projection and the moir fringes. The images are digitally shifted to realign the projections. The end result is that the projection of the object is stationary, while the moir fringes move over it.

SNARK09 is a software package for reconstruction of 2D image from 1D projection. It includes some features, such as projection computation, digital difference analyzer (DDA), and over 30 reconstruction algorithms.

VisTrails is a new system combining features of workflow management and visualization systems, including several packages, such as VTK (Visualization Toolkit), matplotlib and ImageMagick. VisTrails also supports user-created packages including our Mathematica and Matlab scripts.

KiwiViewer is a free, open source visualization app for exploring scientific and medical datasets that runs on Android and iOS mobile devices with multi-touch interaction. KiwiViewer supports a variety of file formats, including obj, stl, ply, and vtk. Datasets may be loaded into KiwiViewer from an SD card, email attachment, DropBox, or URL download.

We use *bullet* data for absorption study, *neutron battery* data from a neutron interferometer for dark-field study, *flame retardant* data for single-shot study and *Foraminifera* data for phase-stepping study.

RESTMD: Large Scale Sampling with Distributed HPC Systems

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Abstract

Conformational sampling of large biological molecules, such as proteins, RNAs, and DNAs, is crucial for an understanding of their function and roles in gene expression and regulation mechanisms in a living cell, which is still challenging if all-atom simulations are needed primarily due to computational costs. Here, we present our recent development of a novel sampling method, Replica Exchange Statistical Temperature Molecular Dynamics (RESTMD) that effectively avoids the drawbacks of the widely popular Replica Exchange Molecular Dynamics (REMD).

In this work, we compare different outcomes of the two RE schemes, Replica Exchange Molecular Dynamics (REMD) and Replica Exchange Statistical Temperature Molecular Dynamics (RESTMD). The replica exchange portion of both implementations is handled by the Hadoop MapReduce framework, allowing for simple parallelization of the simulations and serialization of the exchanges between them. The STMD and MD simulations are carried out by using the CHARMM (Chemistry at Harvard Molecular Mechanics) package which was modified by us for running the STMD portion. We demonstrate that RESTMD, taking advantage of the STMD algorithm as well as replica exchange, provides a more efficient sampling simulation by requiring a lesser number of replicas to achieve the same amount of sampling results compared to REMD. RESTMD takes advantage of the RE scheme by exchanging more frequently and allows exchanges between any replicas, consequently exploring more conformational space in a shorter time window and being able to deal with sizable molecular systems. Collectively, RESTMD enables an individual researcher to pursue more challenging problems associated with biological processes, such as interactions between nc-RNAs and proteins or between DNAs and proteins occurring in various epigenetic mechanisms.

HEP and Grid Computing on HPC Clusters

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Abstract

This presentation describes how LONI and Louisiana Tech's HPC cluster Cerberus has been utilized and the tools that have been employed while collaborating with High Energy Physics (HEP) experiments and grid organizations. HEP deals with a uniquely large amount of data to be used in large scale Monte Carlo production and large scale data analysis. The solution to these tasks is to utilize tools such as the Hadoop Distributed File System (HDFS) for scalable and reliable data storage while relying on grid computing setups like the Open Science Grid (OSG) Toolkits designed for distributed High Throughput computing. To help facilitate the work, other tools such as the CernVM File System (CVMFS) allow users to checkout bulky software to be used in analysis over NFS. The HPC cluster Cerberus already employs these tools to process data generated at CERN over the grid via a local OSG installation. This project is a successor to the highly successful Monte Carlo Production program for the Dzero Experiment that was done on the LONI network previously. A primary goal for the grid computing setup at Louisiana Tech is to have ATLAS Experiment Production jobs submitted to Cerberus via a CERN PanDA Queue.

Numerical Simulations of Cuttings Transport Process in Horizontal Wells Using Discrete Element Method

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Abstract

Flow of particulate materials in the carrier fluid plays a significant role in petroleum engineering applications. In structural complex geometries such as extended-reach, deviated and horizontal wells, transport phenomena can be a critical issue. Effective hole cleaning is essential to reduce the cost of deep-water rig operations. Otherwise, insufficient cuttings transport may lead to some crucial problems such as pipe sticking, increasing in torque and drag, decreasing in drilling rate, material damage, and bad cementing quality. Transportation of drilled cuttings can be affected by several parameters resulted from fluid properties, physical characteristics of particles and operational parameters. All these key elements are required to be considered simultaneously for an effective hole cleaning.

In this study, a coupling between Computational Fluid Dynamics (CFD) and Discrete Element Model (DEM) will be performed in order to predict the accurate particle velocities. Discrete Phase Model (DPM) is also used to estimate particle trajectory. Even though DPM is not computationally time consuming and performed for cuttings transport, DEM is considered to be more robust because of its particle-particle interaction. DEM will simulate the particle trajectory taking account fluid-particle and particle-particle interactions. In addition, CFD will be used for the fluid flow calculation. Different types of turbulent models will be used to carry out the best physical phenomena. CFD solves the Navier-Stokes Equation in order to analyze the fluid flow in the computational domain. The model being developed by the CFD-DEM coupling will represent the more accurate model to understand the drilled cuttings transport.

Loop Quantum Cosmology with High Performance Computers

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Loop quantum cosmology (LQC) is a quantum theory of cosmology, that attempts to describe the early evolution of the universe, in particular, close to the big bang, where classical general relativity fails. Notably, early numerical simulations of sharply peaked states, which correspond to a universe that becomes classical a late times, show a singularity resolution, where the big bang of the classical theory is replaced by a "big bounce".

The evolution of states in LQC is governed by difference equations with a fixed 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 a very large computational domain. These simulations, hence, would be computationally very expensive. In this work we implement an efficient hybrid numerical scheme based on the fact that the LQC difference equations can be approximated by partial differential equations (PDE's) in the large spatial volume regime. This scheme implements two grids: One covering the low volume regime, where the LQC difference equations are solved, and one covering the large volume regime where the PDE's are solved. By a simple change of coordinate in the large volume grid, we obtain a surprising reduction in the computation cost. This scheme enables us to explore regions of the parameter space that were previously unachievable.

We describe the numerical properties and present the results of the simulations for various states. All the cases studied show quantum bounces in the high curvature regime, while agreeing with classical general relativity in the low curvature regime.

Delft3D modeling of hurricane-induced surge and waves in coastal Louisiana

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Abstract

The Louisiana coast is extremely susceptible to the impacts of frequent tropical storms and hurricanes because of its unique geometry and position within the Gulf of Mexico. When tropical cyclones approach the coast or make landfall, they often generate very large storm surges and high wind waves. As these events are significant drivers of coastal land change, the ability to accurately predict and model these phenomena is important.

We focus our numerical modeling on Hurricane Isaac, a category 1 storm that made landfall in Louisiana on August 28, 2012, and induced a storm surge greater than 4 m in upper Breton Sound. Simulations of hurricane-induced surge and waves were executed with the Delft3D model. First, an improved asymmetric hurricane wind model integrated with background winds was employed to generate surface wind fields. The waves and surge at the open boundaries were provided by a gulf-scale Delft3D simulation, and two sets of meshes covering southeastern Louisiana were generated for nesting computations. Two fully-coupled Delft3D modules, Delft3D-Flow and Delft3D-Wave, were used to hindcast the water levels and waves, respectively. Vegetation effects were explicitly considered by a sub-module in Delft3D. The spatial distributions of the maximum surge heights, maximum significant wave heights, as well as their temporal variations were examined, and model results agree well with field observations. The effects of hurricane forward speed, wind intensity and vegetation properties such as height and stem density on storm surge were also probed by a series of numerical experiments.

All Delft3D simulations were carried out on SuperMike-II, a large Linux cluster at Louisiana State University. Considering a four-day-simulation job, it takes about 18 hours when using 48 processors (3 nodes). The size of total input and output job files is about 20G. Till now, we have used about 0.5M SUs on SuperMike-II for Delft3d-related jobs. In addition, we carried out a series of scaling tests of ADCIRC with different meshes on SuperMike-II. An empirical formula was achieved to estimate wall times. The study has been supported in part by the NSF and NOAA.

Delft3D modeling of storm surge, hurricane waves and sediment transport in coastal Louisiana

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Abstract

Louisiana is highly susceptible to the impacts of frequent tropical storms and hurricanes. Hurricanes generate high surge and large waves. And the resultant strong physical forcing could potentially suspend and redistribute sediments in a large area. Considerable concerns have been raised over the issues such as:

- What is the role of hurricanes in coast sediment dynamics?
- Does a hurricane cause erosion or deposition on wetlands?
- How would hurricanes distribute sediment along the coast?

Answers to these questions are of great scientific and economic significance for the protection and restoration of the vanishing Louisiana coast.

This study utilizes Delft3D to predict storm surge, waves and sediment dynamics on the Louisiana coast. Hurricane Gustav is chosen as an example to illustrate the sediment deposition and erosion pattern relative to cyclone conditions.

Numerical simulation shows that, after Hurricane Gustav, deposited sediments were widely distributed along the Louisiana coast, which can be attributed to the flood water that carried suspended sediments and distributed them onshore. Part of the result is validated qualitatively by observation in Tweel and Turner(2012). Significant erosion was found offshore between Terrebonne Bay and Barataria Bay due to the large waves and strong currents generated by the hurricane at landfall.

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. 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 experimental structures of all known protein sequences in the near future. For example, as of May 2014, the number of gene products in the Reference Sequence Database is $>3.8\times 10^7$; in contrast, the number of experimentally determined structures deposited in the Protein Data Bank (PDB) is only 100,147. Considering a much slower pace of experimental structure determination compared to genome sequencing, this disparity continues to grow. The main goal of this project is to build atomic models for sequences lacking experimentally solved structure, which can be directly used in structure-based drug development. Differ from traditional structure modeling from raw sequence data that typically leads to protein models in the unbound conformational state, our approach will bridge the gap between the available sequence and structure data by constructing protein models bound to drug compounds. Specifically, the objective is to leverage 1D information on protein-ligand interactions from the Binding to support large-scale homology-based structure modeling of pharmacologically relevant molecular assemblies. First, using template-based modeling, we constructed 2,245 highly confident models of representative drug targets from BindingDB. Subsequently, the modeled structures were structurally aligned against a set of evolutionarily related ligand-bound proteins with known structures from PDB. We identified ligands bound to these proteins that produce statistically significant structure alignment at a TM-score threshold of 0.4, which corresponds to a *p*-value of $5.0\text{x}10^{-5}$. These ligands were then compared to drug compounds associated with each drug target from BindingDB using a chemical matching algorithm. 293,619,966 pairwise comparisons picked out 2,698,553 matching pairs of BindingDB drugs and PDB ligands with a statistically significant chemical similarity at a Tanimoto coefficient of 0.4. Using a combination of protein structure alignments and ligand chemical alignments, drug compounds from BindingDB were positioned with respect to the modeled structures of their macromolecular targets. In addition, we also extracted the geometry of binding pockets from the template PDB complexes to refine the modeled binding sites in protein models shifting their structures from the unbound to bound conformational state. These extensive calculations resulted in 4,791,643 initial 3D models for known drug-target interactions from BindingDB, which comprise 118,594 unique drug-protein combinations involving 65,374 different drug compounds. The initial models will be further subject to all-atom refinement using molecular mechanics. Statistical analysis suggests that using existing structural information from PDB, the majority of binary interactions from BindingDB can be confidently modeled at near-atomic level. Our study will roughly quadruple structural information on drug-protein complexes significantly expanding the repertoire of molecular interactions between proteins and small organic molecules to further support contemporary structure-based drug discovery and design.

Bayesian designs of phase II oncology trials to select maximum effective dose assuming monotonic dose-response relationship

Beibei Guo

We consider the design of phase II oncology trials that evaluate the efficacy of a small number of doses of an anti-cancer agent with the goal of identifying the maximum effective dose, defined as the lowest dose that achieves a pre-specified target response rate and beyond which no improvement in the response will be achieved. We assume that the probability of response may increase or increase and then plateau in the tested dose range. We propose two Bayesian designs with continuous monitoring of futility and efficacy. The first design is based on Bayesian hypothesis test. In order to determine whether each dose level achieves a pre-specified target response rate and whether the response rates between doses are equal, multiple hypotheses are constructed using non-local 'alternative' prior distributions. The specification of non-local 'alternative' priors allows accumulation of strong evidence in favor of 'null' hypotheses when the 'null' hypotheses are true, thus facilitating futility early stopping and identification of the maximum effective dose. The second design is based on Bayesian model averaging, which also uses non-local priors where response rates are strictly ordered. We conduct simulation studies to evaluate the operating characteristics of the proposed designs.

Structure and Function of Helix-Turn-Helix Proteins

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Abstract

Helix-turn-helix (HTH) fold proteins are ubiquitously distributed in nature. In this study we use computational methods to investigate the function of this conserved motif in proteins that bind to other proteins or nucleotides. In the human pathogen *Staphylococcus aureus,* the QacR drug sensing protein represses expression of the QacA and QacB. Toward this, the DNA binding interface in QacR is described by a HTH fold. The interface undergoes a conformational change in response to drug binding at a distant site that reduces it DNA binding affinity. The methyltransferase (MeTr) enzyme in *Moorela thermoacetica* forms a complex with corrinoid iron-sulfur protein (CFeSP) in order to catalyze a methyl transfer reaction that is part of the Wood-Ljungdahl carbon fixation pathway. We find that the CFeSP-binding interface in MetT too shares a HTH fold. Much like the case of QacR•DNA complexes, the MetR•CFesP complex is formed and later disassociates in response to ligan binding and disassociation. Our molecular dynamics simulations have helped us identify common determinants in the function of these seemingly disparate proteins. We find that the apo forms of these proteins sample various conformational states that promote or destabilize interactions with their interacting partners. We hypothesize that these conformations are gated in response to ligand binding and the presence of their interacting partner proteins and nucleotides.

Investigating protein-protein interactions in the S100A8/S100A9 calprotectin protein complex

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ABSTRACT: Protein-protein interactions play an important role in governing metabolic and signaling pathways. Identifying the molecular determinants of these interactions will aid drug-design strategies that aim to stabilize or destabilize such interactions for therapeutic purposes. Calprotectin is an immunological response metalloprotein belonging to the S100 family of proteins are involved in cell growth and differentiation, inflammatory response, metal ion homeostasis, transcription, protein phosphorylation and secretion. Calprotectin is a heterodimer comprising of S100A8 and S100A9 homodimer proteins, and serves to capture Fe, Mn, Ca, Cu and Zn metal ions at sites of bacterial infection. The objective of this research is to utilize computational chemistry methods in order to understand the driving processes behind S100A8 and S100A9 complexation to form the heterodimer. Towards this, molecular dynamics (MD) simulations of the apo forms of the calprotectin heterodimer, S100A8 and S100A9 proteins were performed on a potential energy surface described by the ff99sb force field (AMBER) over multiple nanoseconds. Our simulations of the apo S100A8/S100A9 heterodimer find the dimeric interface maintained in the absence of the metal ion. In contrast, the S100A8 and S100A9 dimers exhibit large conformational changes akin to a breathing motion. These results are in agreement with experiments suggesting that the heterodimeric assembly is stabler. All proteins are marked by an absence of pre-organization for metal ion binding. We further identify residues involved in conserved networks of correlated motions, providing a testable hypothesis for protein conformational changes that may drive the formation of the heterodimer.

GPU-accelerated ligand docking for drug discovery

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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 a large-scale modeling of pharmacologically relevant associations between small molecules and their macromolecular targets. This approach can dramatically reduce the overall costs of discovering lead compounds by limiting the size of a screening library. At the core of virtual screening are ligand docking algorithms, which search for the global minimum of the drug-target protein conformational space.

The desire to improve state-of-the-art motivated us to develop an ultra-fast ligand docking approach that uses Monte Carlo as the sampling method and features computations on graphics processing units (GPU). Combined with an effective scoring function, this new algorithm will provide accurate predictions at a high performance/cost ratio, which is a critical factor for large-scale virtual screening applications.

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