Algorithms in MacroMolecular Modeling

November 11-15, 2009

The University of Texas at Austin
Austin, Texas

Organizing Committee:
Ron Elber, The University of Texas at Austin
Giovanni Ciccotti, University of Rome La Sapienza
Ulrich Hansmann, Michigan Technological University
Ben Leimkuhler, University of Edinburgh
Tamar Schlick, The New York University
Robert Skeel, Purdue University
DeWitt Sumners, Florida State University
General Information

1. The registration desk, located immediately in front of the Avaya Auditorium, will be open at 8:00 am every morning. Be sure to come by the first day to pick up a name tag and other registration materials.

2. General lectures are scheduled for 40 minutes; 30 minutes with 10 minutes discussion.

3. Short talks are scheduled for 15 minutes in length; 10 minutes with 5 minutes discussion.

4. The Avaya Auditorium is equipped with microphone and projector for either PC or Mac laptop computers.

5. Wireless access is available throughout the ACES building. You may obtain a logon ID and password from the registration desk.

6. For those presenting posters, bring your posters to the registration desk at noon on Thursday. We will have supplies available for you to assemble your poster.

7. No food or drink is allowed in the Avaya Auditorium.

8. Lunch will be provided each day for paying registrants. Lunch will be held in the lobby of the ACES building, which is next to the auditorium.

9. Coffee, tea, juice and pastries will be provided each morning in the lobby of ACES for paying registrants; coffee will also be provided at the breaks.

10. There will be a riverboat dinner cruise on Friday evening, November 13th. Buses will leave from the conference hotel promptly at 5:30 pm.

11. Extra tickets for the cruise may be purchased for $45 at the registration desk on Wednesday only.

12. A list of restaurants within walking distance of the campus and the conference hotel (AT&T Executive Education and Conference Center) will be provided at registration.

13. If you are not staying at the conference hotel and will be driving to the conference, be aware that there is a public parking garage on San Jacinto (indicated on the map at the back of the program). You may bring your parking ticket to the registration desk and we will validate it.

14. Taxi service in Austin (for getting around town and to the airport) is provided by Yellow Cab, 512-452-9999.

15. You may call Ruth Hengst at 512-743-3273 for emergencies.
Schedule
Algorithms in MacroMolecular Modeling
November 11-15, 2009
ACE 2.302, The University of Texas at Austin

**Wednesday, November 11**
*Registration desk opens at 8:00 am in front of Avaya Auditorium (ACE 2.302)*

9:00–9:20 Introduction

**Session 1: Potential Design**
9:20–10:00 Bob Jernigan, Iowa State University
*Evaluating Coarse-Grained Protein Structures*

10:00–10:40 Carlos Simmerling, State University of New York
*Using NMR Data to Evaluate and Improve Empirical Force Fields*

10:40–11:00 BREAK

11:00–11:40 Jarek Meller, University of Cincinnati
*1Djury: Fast and Accurate Method for Protein Model Quality Assessment*

**Session 2: Simulations of Systems in Equilibrium**
11:40–12:20 Ulrich H.E. Hansmann, Michigan Technological University
*Simulations of Small Globular Proteins*

12:20–14:00 LUNCH

14:00–14:40 Ben Leimkuhler, University of Edinburgh
*Novel Stochastic-Dynamical Sampling Methods*

Short Talks (10 minutes for talk; 5 minutes for discussion)

14:40 Sara Bonella, University of Rome "La Sapienza"
*Symmetrized Correlation Functions via Path Integrals in Time and Temperature*

14:55 Santanu Chatterjee, Notre Dame
*String Method with Collective Variables from Normal Modes*

15:10–15:35 BREAK

15:35–16:15 Jiali Gao, University of Minnesota
*X-Pol Potential: From Lifson Molecular Mechanics to a Quantal Force Field for Biomolecular Simulations*

Short Talks (continued)
Constructing Multi-Resolution Markov State Models (Msms) To Elucidate Biomolecular Folding Mechanism

Phosphoryl Transfer in Solution and in Enzymatic Active Sites: Insights from Ab Initio Metadynamics

Long-Range Coulomb Interactions and QM/MM Simulation in Grid Computation

Sampling Conformations in High Dimensions Using Low Dimensional Distribution Functions

AFM – A Systematic Approach for Developing High-Quality Force Fields

Maximum Flux Transition Paths and Their Relative Probabilities

Predicting Continuous Local Structure and the Effect of its Substitution for Secondary Structure in Fragment-Free Protein Structure Prediction

Thursday, November 12

9:00 – 9:40 Steve Bond, University of Illinois at Urbana-Champaign
A Goal-Oriented Adaptive Finite Element Method for the Poisson-Boltzmann Equation

Session 3: Advances in Hardware and Software

9:40 – 10:20 D.E. Shaw, D.E. Shaw Research, LLC.
Millisecond-Long Molecular Simulations of Proteins on the Anton Machine

10:20 – 11:00 Robert Skeel, Purdue University
Structure and Parallelization of N-Body Solvers

11:00 – 11:20 BREAK

11:20 – 12:00 L.V. Kale, University of Illinois at Urbana-Champaign
Challenges and Opportunities in Simulations of Biomolecular Systems at Petascale and Beyond

12:00 – 12:40 Keshav Pingali, ICES, The University of Texas at Austin
Towards A Science of Parallel Programming

12:40 – 14:00 LUNCH

Session 4: Soft Matter

14:00 – 14:40 Greg Voth, University of Utah
Multiscale Simulation of Biomolecular Assemblies
14:40 – 15:20  Dmitrii Makarov, UT-Austin  
*Computer Simulations of Protein Translocation*

15:20 – 17:00  Posters (ACES Lobby) Coffee/refreshments will be served

Guilherme Menegon Arantes, Institute of Chemistry, University of Sao Paulo  
*Flexibility and Molecular Recognition in A Cdc25 Phosphatase Ensemble*

Santanu Chatterjee, Notre Dame  
*String Method with Collective Variables from Normal Modes*

Ivaylo Ivanov, University of California, San Diego  
*Monoubiquitin - PCNA Complexes: A Multiscale Modeling Approach*

Serdal Kirmizialtin, The University of Texas at Austin  
*Computational Exploration of Thermodynamics and Kinetics of Mobile Ions Around RNA Duplex*

Peter Majek, The University of Texas at Austin  
*Revisiting Milestoning with Generalized Voronoi Cells*

Naoyuki Miyashita, RIKEN Computational Science Research Program  
*Simulation Studies on the Differences in the Binding Mechanism of LILRB1/HLA-G And LILRB2/HLA-G*

Nikolay Shestopalov, UT-Austin  
*Controlled Self-Assembly of Charged Particle Monolayers*

Sandeep Somani, University of Maryland, College Park  
*Sampling Conformations in High Dimensions Using Low Dimensional Distribution Functions*

Yuji Sugita, RIKEN  
*Generalized-ensemble Simulations of Proteins in Explicit Solvent*

Yoshiteru Yonetani and Hidetoshi Kono, Japan Atomic Energy Agency  
*Sequence Dependencies of DNA Deformability and Hydration in the Minor Groove*

Jiajing Zhang, UT – Austin  
*Implicit Solvent Trypsin-ligand Binding Free Energy Calculation with Polarizable Potential*

### Friday, November 13

**Session 5: Protein Folding and Protein-Protein Interactions**

9:00 – 9:40  David Beveridge, Wesleyan University  
*Molecular Dynamics of T. aquaticus MutS: Interdomain Communication and Allosterism*

9:40 – 10:20  Peter Wolynes, University of California, San Diego  
*Recent Successes of the Landscape Theory of Protein Folding*
10:20 – 11:00 Harold Scheraga, Cornell University  
*Calculation of Folding Pathways and Native Structures of Proteins*

11:00 – 11:20 BREAK

11:20 – 12:00 Jeff Skolnick, Georgia Tech  
*New Approaches to Drug Discovery and Cancer Metabolomics*

**Session 6: Nucleic Acid Complexes**

12:00 – 12:40 Tamar Schlick, New York University  
*All-Atom Studies of DNA Polymerase Mechanisms and Coarse-Grained Simulations of Chromatin Fiber Folding*

12:40 – 14:00 LUNCH

14:00 – 14:40 John Marko, Northwestern University  
*Micromechanical Study of DNA-Protein Interactions and Chromosome Structure*

14:40 – 15:20 Christine Heitsch, Georgia Tech  
*Analysis, Prediction, and Design of Viral RNA Secondary Structures*

15:20 – 15:45 BREAK

17:30 Bus departs for riverboat dinner cruise from AT&T Executive Education and Conf. Ctr, 1900 Martin Luther King Boulevard

18:00 – 20:00 Riverboat dinner cruise; Lady Bird Lake

**Saturday, November 14**

9:00 – 9:40 Thomas Cheatham, University of Utah  
*Perils and Promise in Simulation of RNA-Ligand Interaction*

9:40 – 10:20 De Witt Sumners, Florida State University  
*The Writhe – A Macromolecular Shape Descriptor*

**Session 7: Kinetics and Mechanism**

10:20 – 11:00 Eric Vanden-Eijnden, Courant Institute  
*Theory and Modeling of Reactive Events*

11:00 – 11:20 BREAK

11:20 – 12:00 Vijay Pande, Stanford University  
*Insights from All-Atom Simulations of Protein Folding on the Millisecond Timescale and Beyond*

12:00 – 12:40 John Straub, Boston University  
*Generalized Replica Exchange Method: Optimal Combination of Generalized Ensemble Methods and Replica Exchange Method*
12:40 – 14:00 LUNCH

14:00 – 14:40 E. Darve, Stanford
*Computing Reaction Rates in the Presence of Multiple Energy Barriers*

14:40 – 15:20 Rob Coalson, University of Pittsburgh
*Calculating Ion Permeation through Protein Channels*

15:20 – 15:45 BREAK

15:45 – 16:25 Giovanni Ciccotti, University of Rome "La Sapienza"
*Back to Time-dependent Non-equilibrium Molecular Dynamics*

**Sunday, November 15**

**WORKSHOP:**
Introduction to calculations of reaction paths and rates in the software MOIL. The workshop will be offered depending on a sufficient number of registrations (to the workshop). Bring your problem. We will help you set it up during the workshop.
Abstracts

Evaluating Coarse-Grained Protein Structures
Robert Jernigan
Iowa State University

The complexities of densely packed proteins may be better understood with simple models. We have been investigating two highly cooperative representations – 4-body contact potentials for energies and elastic network models for entropies.

We have derived four-body contact potential energies as a way to consider protein interactions in more cooperative model. We demonstrate that around 500 chains are sufficient to provide a good estimate of these four-body contact potentials by obtaining convergent threading results. They rely upon reduced amino acid alphabets for 3 of the four members of each quartet. We also have chosen two sets of protein native structures differing in resolution, one with all chains’ resolution better than 1.5 Å and the other with 94% of the structures having a resolution worse than 1.5 Å to investigate whether potentials from well-refined protein datasets perform better in threading. Potentials from well-refined proteins did not generate better threading results than those from more diverse structures. Our four-body contact potentials can discriminate well between native structures and partially unfolded or deliberately misfolded structures, when combined with short range energies.

Elastic network models provide strong evidence that proteins control their functional motions through their slow, domain motions. These models represent the structures as highly cohesive rubbery materials. Such models exhibit strong control over their motions, including control of the motions of functional surface loops by domain motions and even the motion of reactive atoms at enzyme active sites in coordination with domain motions. The elastic network models are entropic models, and their success in describing protein functional motions suggests their utility for estimating folded protein entropies. We learn that protein entropies depend more on the shape characteristics of the entire structure and less on the details within the structure.

Using NMR Data to Evaluate and Improve Empirical Force Fields
Carlos Simmerling
State University of New York

The quality of results from molecular simulations depends strongly on the accuracy of the underlying force field that describes the physical interactions in the system. These functions include various approximations, and validation is essential for the identification of weaknesses in current models and development of more accurate models of biomolecules. In this presentation we will discuss the ff99SB protein force field and performance as compared to data from solution NMR measurements. Specific areas of worse agreement are used to guide the slight modification of the force field parameters to provide more accurate simulations. The effect of water model on the results will also be discussed.
1Djury: Fast and Accurate Method for Protein Model Quality Assessment

Jarek Meller
University of Cincinnati

Model quality assessment (MQA) is an integral part of protein structure prediction methods that typically generate multiple candidate models. The challenge lies in ranking and selecting the best models using a variety of physical, knowledge-based and geometric (clustering-based) scoring functions. In particular, 3D-Jury and related structural consensus methods assume that well predicted (sub-)structures are more likely to be similar in a population of candidate models, compared to incorrectly folded ones. While in general very accurate in the context of diversified sets of models, this approach is computationally expensive since it relies on MaxSub, or related heuristics, to identify similar substructures in pairs of models. To overcome this problem, we consider a simple alternative, in which structural similarity is assessed in terms of 1D profiles consisting of relative solvent accessibilities and secondary structures of equivalent amino acid residues in the respective models. The resulting 1Dsim measure is shown to correlate strongly with MaxSub structural similarity scores, and provides a basis for an efficient clustering-based MQA method, which is dubbed 1D-Jury. 1D-Jury does not require the computationally expensive 3D superposition of pairs of models, and its computational complexity for the problem of ranking a set of models is linear in the number of models, as opposed to quadratic complexity for 3D-Jury and related methods. At the same time, the accuracy of the new approach in terms of the ability to select the best models as top candidates is shown to be on par with that of 3D-Jury. Implications for the design of improved scoring functions for model quality assessment and protein structure prediction are discussed.

Simulations of Small Globular Proteins

Ulrich H.E. Hansmann
Michigan Technological University

Proteins are nanomachines that perform a large number of diverse functions in cells. Despite decades of research we still do not understand in complete detail the mechanism by which a protein folds into its biologically active form. Computational tools that allow one to evaluate the sequence-structure relationship and the folding process would therefore lead to a deeper insight into the molecular machinery of cells. Unfortunately, computer simulations are extremely difficult for detailed protein models. This is because the energy landscape of all-atom protein models is characterized by a multitude of local minima separated by high energy barriers. While there has been remarkable progress there is still a need for improved algorithms to overcome this multiple-minima problem. I will discuss some of these approaches, and their potential and limitations in protein science.

References

Novel Stochastic-Dynamical Sampling Methods

Ben Leimkuhler
University of Edinburgh

We consider three methods to enhance canonical sampling of biomolecular landscapes. These methods build on previous schemes (Nose-Hoover/Nose-Poincare, Langevin Dynamics, Hybrid Monte-Carlo) but achieve good results with only one or two scalar noise processes. (1) The Nose-Hoover-Langevin scheme provides an ergodic alternative to Nose Hoover Chains [1]; (2) by embedding a dynamical scheme like Nose-Hoover into a hybrid Monte-Carlo-like framework, the ergodicity problem is overcome and even stepsize-dependent truncation errors may be corrected [2]; and (3) an intriguing new class of dynamical-stochastic schemes can be designed by looking beyond the traditional Bulgac-Kusnezov framework for techniques based on innovative coupling to artificial baths, in particular a partial force-based thermostat can be constructed using these ideas [3]. I will describe each of these approaches and provide numerical experiments to illustrate their performance.

[2] A metropolis-adjusted Nose-Hoover thermostat, Leimkuhler, B. and Reich, S., Multiscale Modelling and Numerical Analysis, DOI: 10.1051/m2an/2009023

X-Pol Potential: From Lifson Molecular Mechanics to a Quantal Force Field for Biomolecular Simulations

Jiali Gao
University of Minnesota

At the heart of dynamics simulations is the potential energy function that describes intermolecular interactions in the system, and often it is the accuracy of the potential energy surface that determines the reliability of simulation results. The current generation of force fields was essentially established in the 1960s. While the accuracy has been improved tremendously by systematic parameterization, little has changed in the formalism and in the representation of the system. The explicit polarization (X-Pol) potential is a quantal force field based on electronic structure theory, designed for molecular dynamics simulation and modeling of biopolymers. In this approach, molecular polarization and charge transfer effects are explicitly treated by an electronic structure method, and the wave function of the entire system is variationally optimized. We illustrate the possibility of parametrizing the X-Pol potential to achieve the desired accuracy as that in MM force fields, and demonstrate the feasibility of carrying out molecular dynamics (MD) simulation of solvated proteins. We use a system consisting of 14281 atoms and about 30,000 basis functions, including the protein bovine pancreatic trypsin inhibitor (BPTI) in water with periodic boundary conditions, to show the efficiency of an electronic structure-based force field in atomistic simulations. The X-POL force field permits the inclusion of time-dependent quantum mechanical polarization and charge transfer effects in much larger systems than was previously possible. We illustrate a unified approach to modeling biological and materials systems from atoms to macromolecular systems using electronic structure theory.
A Goal-Oriented Adaptive Finite Element Method for the Poisson-Boltzmann Equation
Steve Bond
University of Illinois at Urbana-Champaign

The Poisson-Boltzmann equation (PBE) is a nonlinear elliptic partial differential equation (PDE), which can be used to describe the electrostatic potential for a biomolecule immersed in a solvent. The PBE is known as a "implicit solvent" model, since there are no explicit solvent atoms, with the solvent (and protein) modeled as a dielectric continuum. Once one obtains the electrostatic potential, important quantities, such as solvation free energy, can be computed using an appropriate functional of the solution. In this talk, we show how one can efficiently compute quantities like solvation free energy using an adaptive finite element method. In our scheme, the mesh refinement is driven by goal-oriented error estimation based on the free energy functional. Hierarchical basis methods are used to precondition the resulting algebraic systems arising in the multilevel finite element discretization.

Milliseconds-Long Molecular Dynamics Simulations of Proteins on the Anton Machine
David E. Shaw
D. E. Shaw Research and Center for Computational Biology and Bioinformatics, Columbia University

The ability to perform long, accurate, atomic-level molecular dynamics (MD) simulations could in principle provide insights into the structural, dynamic, and functional characteristics of proteins at an atomic level of detail. Many biologically important phenomena, however, occur over timescales that have thus far fallen far outside the reach of MD technology. We have constructed a specialized, massively parallel machine, called Anton, that is capable of performing all-atom simulations of proteins in an explicitly represented solvent environment at a speed roughly two orders of magnitude beyond that of the previous state of the art. Using novel algorithms developed within our lab, the machine has now simulated the behavior of a number of proteins for periods as long as a millisecond -- approximately 100 times the length of the longest previous MD simulation -- revealing aspects of protein dynamics that were previously inaccessible to both computational and experimental study.

Structure and Parallelization of N-Body Solvers
Robert Skeel
Purdue University

There are two fundamentally different types of fast N-body solvers. Hierarchical clustering methods, such as tree codes and the fast multipole method, partition interactions based on pairs of clusters at a various length scales and do each part either exactly or using a separable approximation of the interaction kernel. Kernel-splitting methods, such as FFT-based method and the multilevel summation method (MSM), separate the kernel into a short-range part that is calculated exactly and a smooth part that is interpolated from a grid. The structure and properties of these various methods are compared, and opportunities offered by modern computer hardware are outlined, including general purpose graphics processing units (GPGPUs) and distributed memory machines. It is shown how these can be exploited for methods such as MSM, and numerical results and timings are presented. This is joint work with David J. Hardy, University of Illinois.
Challenges and Opportunities in Simulations of Biomolecular Systems at Petascale and Beyond

Laxmikant (Sanjay) Kale
University of Illinois at Urbana-Champaign

We are entering an era which presents us with unprecedented opportunities to perform scientific research through simulation of biomolecular systems. These opportunities will come in the form of new hardware and in the adoption of new methods for improved accuracy. On the hardware dimension, we already have petascale machines, and within a couple of years multi-petaFLOPS systems will be available for most researchers. However, utilizing these effectively for classical MD still remains a challenge. As exemplar, I will address our efforts in scaling NAMD to the Blue Waters System. This will be NSF’s premier “Track 1” machine, to be available to end users in mid-2011. Accelerators, such as GPGPU, Cell, and Larrabee, provide another opportunity to increase performance of specific subcomputations. These will be augmented by more specialized accelerators, either with reconfigurable logic, or with chips designed specifically for an application. The exascale era, which is being predicted in 2018-2020 timeframe, is likely to combine accelerators with further scaling of the petascale machines. At the same time, newer modeling techniques will lead to more accurate simulations. These involve modeling of quantum effects on one end and coarse models on the other end, along with techniques for combining multiple resolutions and multiple physical models in a single simulation. Mapping of these sophisticated algorithms onto the heterogeneous and complex hardware is a tall challenge for the software. Although much research is needed to that end, I believe that the object-based decomposition, as represented by Charm++, has a potential to be a foundation of such research, because of its ability to concurrently compose multi-physics modules, and to handle accelerators in a portable manner. I will explain the reasons for this, and outline an agenda of future work in software frameworks and strategies.

Towards a Science of Parallel Programming

Keshav Pingali
The University of Texas at Austin

Like most fields of science, computational biology uses a wide range of algorithms from n-body methods and sparse linear solvers to event-driven simulation and SAT solvers. What are the right abstractions for reasoning about parallelism and locality in these kinds of algorithms? In this talk, I will argue that the abstractions we currently use such as dependence graphs are fundamentally broken and are not useful outside the realm of dense matrix computations. I will then describe a novel data-centric abstraction called "amorphous data-parallelism" that provides a simple and unified picture of parallelism in these kinds of applications, and an implementation of these ideas in the ParaMeter system.
Multi-scale Simulation of Biomolecular Assemblies

Gregory A. Voth
University of Utah

A multiscale theoretical and computational methodology will be presented for studying biomolecular systems across multiple length and time scales. The approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the approach is the multiscale coarse-graining method for rigorously deriving coarse-grained models from the underlying molecular-scale interactions. Applications of the multiscale approach will be given for membranes and proteins, although the overall methodology is applicable to many other complex condensed matter systems. Recent applications to membrane remodeling phenomena by proteins and to large protein complexes will also be described. The computational challenges and opportunities for this area of molecular modeling will be especially emphasized.

Computer Simulations of Protein Translocation

Dmitrii Makarov
The University of Texas at Austin

I will report on some of our group’s theoretical and computational efforts to understand the molecular mechanisms of protein translocation and unfolding inside pores. In a nutshell, the problem we are trying to solve is to compute the time it takes a protein, driven by an external force, to traverse a pore whose size is smaller than that of the protein itself. While I will discuss some biological implications of our work, the emphasis of the talk will be on the computational challenges associated with calculating the rates of large conformational rearrangements of biopolymers in confined spaces.

Molecular Dynamics of *T. aquaticus* MutS: Interdomain Communication and Allosterism

David L. Beveridge, Susan N. Pieniazek, and Manju M. Hingorani
Wesleyan University

Communication events within multifaceted protein architectures play critical roles in many complex biological processes, including DNA mismatch repair (MMR). MutS and its homologs, highly conserved proteins in both prokaryotes and eukaryotes, are responsible for the initiation of MMR. MutS binds to DNA at sites of base pair mismatches or insertions/deletions and summons the participation of downstream repair proteins. ATPase activity at the nucleotide binding sites ~70 Å distant from the DNA binding site coordinates the downstream events in MMR. All-atom molecular dynamics (MD) simulations including explicit consideration of solvent at the level of ~100 ns trajectories have been performed and analyzed to elucidate the nature of the recognition of DNA lesions and the interdomain allosteric communication between the DNA binding site and the twin ATP/ADP sites in prokaryotic *T. aquaticus* MutS and homologs. Two models for the propagation of the allosteric signal are investigated a) via contacts between amino residues in a physical pathway connecting the functional and allosteric sites, and b) via correlations among collective atomic fluctuations. This issue is explored further using non-equilibrium MD simulations.
Recent Successes of the Landscape Theory of Protein Folding

Peter G. Wolynes
University of California, San Diego

Protein folding can be understood as a biased search on a funneled but rugged energy landscape. This picture can be made quantitative using the statistical mechanics of glasses and first order transitions in mesoscopic systems. The funneled nature of the protein energy landscape is a consequence of natural selection. I will discuss how this rather simple picture quantitatively predicts folding mechanism from native structure and sequence. Recent advances using the energy landscape ideas to design algorithms to predict protein structure from sequence will also be reviewed.

Calculation of Folding Pathways and Native Structures of Proteins

Harold A. Scheraga
Cornell University

An all-atom and coarse-grained approach to the protein folding problem will be discussed. Previous and current results, and anticipated directions will be presented.

New Approaches to Drug Discovery and Cancer Metabolomics

Jeffrey Skolnick
Georgia Institute of Technology

The growing number of predicted protein structures requires robust methods that can utilize low-quality receptor structures for protein function identification and ligand screening. Here, FINDSITE, a new method for ligand-binding site prediction and functional annotation based on binding site similarity across groups of weakly homologous template structures identified from threading is described. For crystal structures, considering a cutoff distance of 4 Å as the hit criterion, the success rate is 70.9% for identifying the best of top five predicted ligand-binding sites. The ability to accurately assign a molecular function to the protein model and to predict the binding site is sustained when approximate protein models (<35% sequence identity to the closest template structure) are used, showing a 67.3% success rate. FINDSITE tolerates inaccuracies in protein models up to a root-mean-square-deviation, RMSD, from the crystal structure of 8-10 Å, because many of these models have a local RMSD from the native binding site < 2 Å. Furthermore, the chemical properties of template-bound ligands can be used to select ligands from large compound libraries. This approach is completed by Q-DOCK, a low-resolution structure-based flexible ligand docking/ranking approach. In docking against distorted receptor models with a RMSD from native of ~3 Å, Q-Dock recovers on average 15-20% more specific contacts and 25-35% more binding residues than all-atom methods. Finally, we describe a recent approach to cancer metabolomics, COMET, that shows considerable ability to predict metabolites with significant antiproliferative activities in cancer cell lines.
All-atom Studies of DNA Polymerase Mechanisms and Coarse-Grained Simulations of Chromatin Fiber Folding

Tamar Schlick
New York University

With significant software and hardware advances, molecular dynamics (MD) simulations have become important for studying the motions of complex biological systems. For various DNA polymerases in the X family, classical as well as classical/quantum-mechanical simulations have uncovered conformational pathways to relate enzyme architecture to fidelity behavior. Going beyond MD, however, is necessary to capturing large-scale conformational changes and chemical pathways. Such methods include transition path sampling and coarse grained modeling approaches. For DNA polymerase beta, transition path sampling and hybrid classical/quantum approaches help relate free energy pathways to biological function. Studies of pol lambda and pol X elucidate the distinct pathways of these polymerases from each other and from pol beta. Applications to chromatin folding require a drastic reduction of the number of degrees of freedom by a coarse-grained approach. Using such a model of oligonucleosome chains in combination with tailored sampling protocols, we elucidate the energetics of oligonucleosome folding/unfolding and the role of each histone tail, linker histones, linker DNA length, and divalent ions in regulating chromatin structure. The resulting compact topologies reconcile features of the zigzag model with straight linker DNAs with the solenoid model with bent linker DNAs for optimal fiber organization.

Recent references


Micromechanical Study of DNA-Protein Interactions and Chromosome Structure

John F. Marko
Northwestern University

I will discuss the use of micromechanical experiments – essentially measurements of elasticity - as methods to study how DNA is organized by being folded by proteins, ultimately into whole chromosomes. I will discuss studies at three scales of complexity. First, I will present results of single-DNA micromanipulation studies of proteins which compact the chromosome in the bacterium E. coli. I will then discuss how we have used similar techniques to study the dynamics of assembly of nucleosomes into chromatin fiber onto a single DNA molecule. Finally I will discuss experiments which probe the internal organization of entire mitotic chromosomes isolated from dividing cells.

Analysis, Prediction, and Design of Viral RNA Secondary Structures

Christine Heitsch
Georgia Tech

Understanding how biological sequences encode structural and functional information is a fundamental scientific challenge. For RNA viral genomes, the information encoded in the sequence extends well-beyond their protein coding role to the role of intra-sequence base pairing in viral packaging, replication, and gene expression. Working with the Pariacoto virus as a model sequence, we investigate the compatibility of predicted base pairings with the dodecahedral cage known from crystallographic studies. To build a putative secondary structure, we first analyze different possible configurations using a combinatorial model of RNA folding. We give results on the trade-offs among types of loop structures, the asymptotic degree of branching in typical configurations, and the characteristics of stems in "well-determined" substructures. These mathematical results yield insights into the interaction of local and global constraints in RNA secondary structures, and suggest new directions in understanding the folding of RNA viral genomes.

Perils and Promise in Simulation of RNA-ligand Interaction

Thomas Cheatham, III
University of Utah

The structure of RNA is profoundly influenced by its surroundings of solvent, ligands, and ions. Moreover, RNA is highly dynamic with motions across many time scales, motions that have the potential to sample multiple distinct conformational substates. Can the current generation of empirical force fields and molecular dynamics methods model this complexity? Nucleic acid helices are well modelled, however there are still questions regarding the balance of interactions (stacking, hydrogen bonding, ...) for non-canonical structure. For example, simulation suggests that well-defined loop, bulge and other interesting structures are not well maintained in longer MD runs. In addition to validation and assessment results on large tetraloop datasets and well-resolved RNA NMR structures, we'll discuss recent work on drug interactions with the Hepatitis C IRES and new structures from NMR refinement with modern simulation protocols.
The Writhe—A Macromolecular Shape Descriptor  
De Witt Sumners  
Florida State University

The directional writhe of a spatial closed curve is the sum of the signed crossings in the projection of the curve in the given direction. The writhe of a simple closed curve in 3 space is the average over all directions of directional writhe. We extend [1] this definition to apply to edge-oriented (each edge has an arrow on it) finite spatial graphs. This definition of writhe covers spatial polygonal arcs and non-connected graphs, and does not require the ad hoc closing of arcs to eliminate the problems posed by endpoints. This talk will discuss the properties of writhe of graphs, and the proof of writhe additivity for connected sums, with applications to DNA and RNA.

Theory and Modeling of Reactive Events  
Eric Vanden-Eijnden  
Courant Institute

In the first part of the talk, I will explain why we may need to go beyond the standard framework of transition state theory (TST) to describe activated processes and reactive events, and I will present another framework, termed transition path theory (TPT), that permits to do that. Unlike TST, which gives mainly an expression for the rate of the reactive event, TPT describes more fully the statistical properties of the reactive trajectories (i.e. those trajectory by which the reactive event occurs), in particular in terms of their probability density function and their probability current.

In the second part of the talk, I will describe how TPT can be use to design and/or improve numerical methods for computing the pathways and rate of reactive events. I will focus in particular on the string method and milestoning. These techniques will be illustrated via several examples.

Insights from All-Atom Simulations of Protein Folding on the Millisecond Timescale and Beyond  
Vijay Pande  
Stanford University

For those interested in grand-challenge class HPC calculations, all one really wants is a single processor with petaflop scale speed. Unfortunately, we may likely never get such a system. Instead, we can get today petaflop (sustained) class performance from clusters of exotic "stream" processors, such as the Cell processor or modern GPU's. While distributed computing of these stream processors is by no means a panacea for petaflop scale computing, one may be surprised to what degree algorithms that were traditionally tightly coupled can be ported to this platform. I will talk about our experience in this area, in particular with applications to simulations of biomolecular kinetics and thermodynamics performed on the Folding@home computing platform (which currently sustains over 5 petaflops of aggregate performance); I will also discuss how these methods could impact and influence HPC computing for other groups and other disciplines in the future.
To explore these issues in the context of a particular application area, I will discuss applications of these methods to the challenges of simulating proteins in a cellular context. While there has been much progress in understanding how proteins fold in vitro, i.e. in infinite dilution. The much more biologically relevant question is how do proteins fold in the cell, especially in the context of cellular crowding, chaperonins, and other biological machinery of the cell. We have simulated folding extensively in vitro and are now simulating in the context of chaperonins, the ribosome, and cellular crowding. We find significant differences in these environments vs the in vitro case, suggesting how some of the most fundamental aspects of protein biophysics (i.e. the role of hydrophobicity and hydrogen bonding in protein stability) must be reconsidered in the cellular context. I will also highlight some new results on protein aggregation, a key aspect of proteins in the cellular environment.

**Generalized Replica Exchange Method: Optimal combination of generalized ensemble methods and replica exchange method**

*John Straub*
Boston University

In recent years, the Replica Exchange Method (REM) and Parallel Tempering have become the standards for workhorse equilibrium sampling of systems exhibiting complex energy landscapes. However, the standard temperature REM (tREM) often struggles to attain its maximum advantage when the system size becomes large or the system manifests an “energy gap” near a first-order transition region. We present a general sampling scheme to mitigate the limitations of the tREM by systematically combining various generalized ensemble methods, such as the Statistical Temperature sampling and Tsallis-Weight Sampling, with the replica exchange scheme via the effective temperature formulation.

**Computing Reaction Rates in the Presence of Multiple Energy Barriers**

*Éric Darve*
Stanford University

Many methods to calculate reaction rates depend on defining a reaction coordinate or a good approximation of it. However, in practice, finding such a coordinate is difficult, and one often has to rely on physical intuition of the chemical process. We will present and discuss a new approach to calculate reaction rates based on a partitioning of space and minimum (free) energy pathways, which does not require defining a reaction coordinate. We borrow from the concepts of macrostates (Swope & Pitera, J. Phys. Chem. B 108, 2004), Voronoi cells, Weighted Ensemble (Huber & Kim, Biophys. J. 70, 1996), and non-Markovian Fokker-Planck equations (Darve, Solomon, and Kia, P.N.A.S. 27, 2009).
Calculating Ion Permeation through Protein Channels
Rob Coalson
University of Pittsburgh

We will describe a Brownian Dynamics algorithm for computing the flux of simple ions (e.g., Na+ and Cl-) through channel proteins in their open pore configuration when subjected to transmembrane concentration or electric potential gradients. After basic methodological issues are reviewed, we will present applications to ligand gated ion channel proteins, including the acetylcholine receptor (nAchR) and the glycine receptor (GlyR). If time permits, suggested chemical modifications of these channels which may have biotechnological utility will be proposed.

Back to Time-dependent Non-equilibrium Molecular Dynamics
Giovanni Ciccotti
University of Rome "La Sapienza"

[Abstract to be provided]
SHORT TALK ABSTRACTS

Symmetrized Correlation Functions via Path Integrals in Time and Temperature
Sara Bonella, University of Rome "La Sapienza"
A new approach for computing quantum time correlations functions is presented. The approach starts from a path integral representation of symmetrized time correlation function and employs a linearized approximation of the dynamics to derive a hybrid Monte Carlo - Molecular Dynamics algorithm that calculates this quantity iteratively. The procedure converges to the exact quantum result with increasing number of iterations. The performance of the algorithm for model systems will be described.

String Method with Collective Variables from Normal Modes
Santanu Chatterjee, Notre Dame
The on-the-fly String Method may be used to find the minimum free energy paths (MFEP) between meta-stable states of a molecule. This requires the choice of a set of non-trivial reaction coordinates, or collective variables, along which the transition takes place. We propose the use of low frequency normal modes as the reaction coordinates. This choice is based on the observation that normal mode analysis can provide the direction of the low frequency motion of interest. We also show that the choice of the normal modes confers simplifications in the string method itself. This choice of variables leads to efficient numerical discretization.

Constructing Multi-Resolution Markov State Models (MSMs) to Elucidate Biomolecular Folding Mechanism
Xuhui Huang, Stanford University
Simulating biologically relevant timescales at atomic resolution is a challenging task since typical atomistic simulations are at least two orders of magnitude shorter. Markov State Models (MSMs) provide one means of overcoming this gap without sacrificing atomic resolution by extracting long time dynamics from short simulations. MSMs coarse grain space by dividing conformational space into long-lived, or metastable, states. This is equivalent to coarse graining time by integrating out fast motions within metastable states. By varying the degree of coarse graining one can vary the resolution of an MSM; therefore, MSMs are inherently multi-resolution. In the talk, I will introduce a new algorithm Super-level-set Hierarchical Clustering (SHC), to our knowledge, the first algorithm focused on constructing MSMs at multiple resolutions. The key insight of this algorithm is to generate a set of super levels covering different density regions of phase space, then cluster each super level separately, and finally recombine this information into a single MSM. SHC is able to produce MSMs at different resolutions using different super density level sets. To demonstrate the power of this algorithm we apply it to a small RNA hairpin, generating MSMs at different resolutions. We validate these MSMs by showing that they are able to reproduce the original simulation data. Furthermore, long time folding dynamics are extracted from these models. The results show that there are no metastable on-pathway intermediate states. Instead, the folded state serves as a hub directly connected to multiple unfolded/misfolded states which are separated from each other by large free energy barriers.
**Phosphoryl Transfer in Solution and in Enzymatic Active Sites: Insights from ab initio Metadynamics**

Ivaylo Ivanov, University of California, San Diego

I will describe recent advances from the application of the metadynamics method to both enzymatic and non-enzymatic phosphoryl transfer. The nature of the transition state in phosphoryl transfer has been a contentious issue and one that is difficult to resolve experimentally. We have carried out large-scale ab initio molecular dynamics simulations of this class of reactions both in a biological context (catalytic RNA, group I intron catalysis) and on model compounds (methyl phosphates) in solution. The results are of fundamental significance and contribute to our understanding of the mechanisms by which enzymes such as phosphodiesterases, nucleases and ribozymes achieve their biological function.

**Long-Range Coulomb Interactions and QM/MM Simulation in Grid Computation**

Chun-Min, Q-Chem

We establish the calculation of Coulomb interactions by Fourier transforms with appropriate grid density in quantum periodic systems by separating them into long-range and short-range parts. This calculation has similar algorithm to the algorithm used in the molecular mechanics system (such as Charmm). In this way, QM and MM calculation can share the same information and their connection is faster than the traditional way.

**Sampling Conformations in High Dimensions Using Low Dimensional Distribution Functions**

Sandeep Somani, University of Maryland, College Park

This talk will describe a new approximation to a molecule’s N-dimensional conformational probability density function (pdf) in terms of marginal pdfs of highest order l, where l is much less than N. The approximation is constructed as a product of conditional pdfs derived by recursive application of the generalized Kirkwood superposition approximation. Also, a conformational sampling algorithm developed based on this approximation will be outlined. Details of the algorithm and results will be presented in an accompanying poster.

**AFM – a Systematic Approach for Developing High-Quality Force Fields**

Feng Wang, Boston University

The adaptive force matching (AFM) method developed recently is capable of producing high quality force fields for condensed phase simulations. This procedure fits simple force field terms in the condensed phase through a QM/MM approach. During the procedure, the MM part of the QM/MM is iteratively improved so as to approach ab initio quality. The method is capable of quickly sampling the configuration space described by the QM reference method and properly taking care of many-body effects. In this talk, we will briefly introduce the AFM procedure and report recent work in the quest for the best non-polarizable force field for water.

**Maximum Flux Transition Paths and Their Relative Probabilities**

Ruijun Zhao, Purdue

Given two metastable states A and B of a biomolecular system, the problem is to find a transition path from A to B by which the mechanism of reaction can be analyzed. It is often easier and sometimes necessary to calculate such a path in collective variable space rather than in configuration space. The maximum flux transition path (MFTP) is defined as a path in collective variable space that crosses each isocommittor at a point which (locally) has the highest crossing
rate of distinct reactive trajectories. (Here the committor is defined to be the probability that a trajectory at that point will reach B before A in collective variable space.) MFTP can handle the intermediate metastable states well compared with the minimum free energy path (MFEP), which often results cusps near those intermediate metastable states. Such an algorithm and its performance is discussed. There may be several isolated MFTPs. We propose an algorithm to calculate relative probabilities of these paths.

**Predicting Continuous Local Structure And The Effect of its Substitution for Secondary Structure in Fragment-Free Protein Structure Prediction**

*Yaoqi Zhou*, Indiana University

Local structures predicted from protein sequences are employed extensively in every aspect of modeling and prediction of protein structure and function. For more than 50 years, they have been predicted at a low-resolution coarse-grained level (e.g. three-state secondary structure). Here, we combine a two-state classifier with real-value predictor to predict local structure in continuous representation by backbone torsion angles. The accuracy of the angles predicted by this approach is close to that derived from NMR chemical shifts. Their substitution for predicted secondary structure as restraints for ab initio structure prediction doubles the success rate. This result demonstrates the potential of predicted local structure for fragment-free tertiary-structure prediction. It further implies potentially significant benefits from employing predicted real-valued torsion angles as a replacement of or supplement to the secondary-structure prediction tools employed almost exclusively in many computational methods ranging from sequence alignment to function prediction.
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