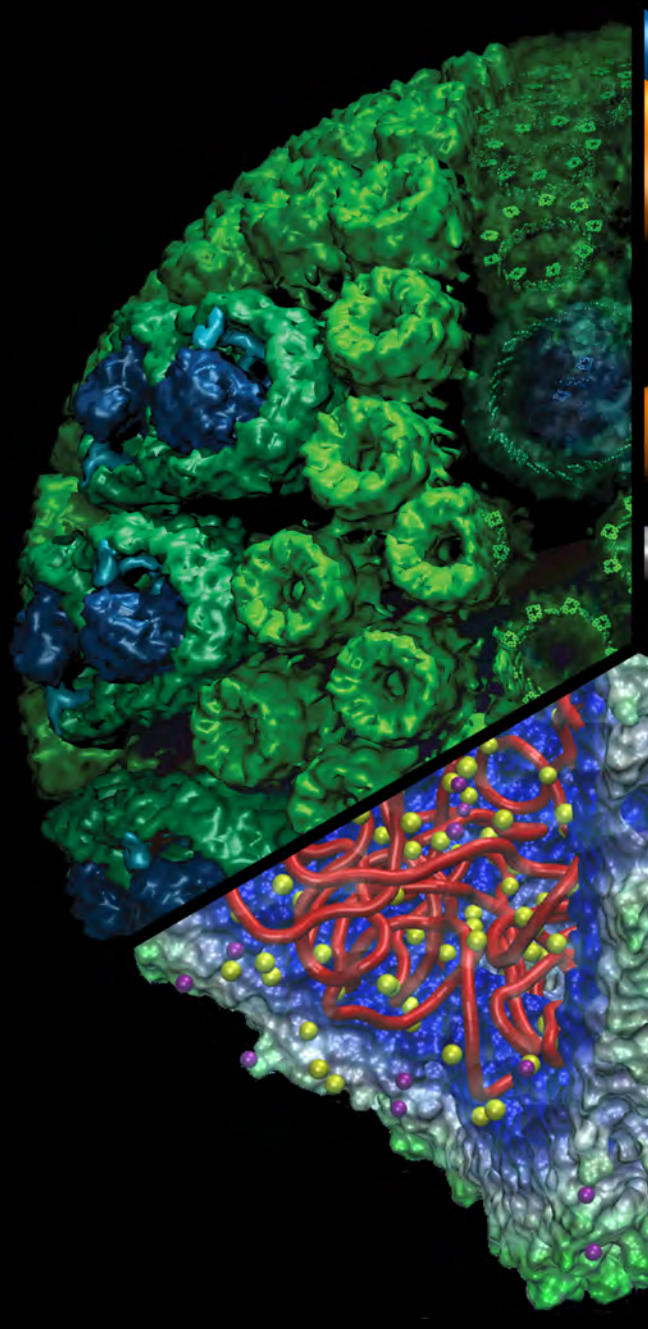
Theoretical and Computational Biophysics Group
20th Anniversary Symposium

Computational Biology of the Cell
The Next Decade

September 21-23, 2009
Beckman Institute
www.ks.uiuc.edu/symp09/

Book of Abstracts



Images (clockwise): fullerene orbitals, satellite tobacco mosaic virus, photosynthetic chromatophore vesicle

Speakers:
Charles L. Brooks, *U. Michigan*
Valerie Daggett, *U. Washington*
Angel E. García, *Rensselaer*
Angela Gronenborn, *U. Pittsburgh*
Helmut Grubmüller, *Max Plank Inst.*
Stephen Harvey, *Georgia Tech*
Gerhard Hummer, *NIH*
Michael L. Klein, *U. Pennsylvania*
Petros Koumoutsakos, *ETH Zurich*
J. Andrew McCammon, *UC San Diego*
Vijay Pande, *Stanford U.*
Richard Pastor, *NHLBI/NIH*
Benoît Roux, *U. Chicago*
Andrej Sali, *UC San Francisco*
David E. Shaw, *D. E. Shaw Research*
Jeffrey Skolnick, *Georgia Tech*
Devarajan Thirumalai, *U. Maryland*
Gregory A. Voth, *U. Utah*

Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign

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20th Anniversary Symposium

Computational Biology of the Cell

The Next Decade

September 21-23, 2009

Beckman Institute for Advanced Science and Technology

University of Illinois at Urbana-Champaign

WELCOME

The Theoretical and Computational Biophysics Group of the Beckman Institute welcomes all symposium participants and we look forward to exciting days of learning, discussion, and friendship.

Twenty years ago a few students and a professor, along with a self-built 60 processor parallel computer that fit into a backpack, arrived from Bavaria and moved into the brand new Beckman Institute. The move soon led to the formation of a wonderful team of physicists, computer scientists, chemists, biochemists, biophysicists and staff, who worked side-by-side as scientific programmers and cell biologists. Assisted by wonderful administrators, and funded generously through NIH, NSF, the Beckman Foundation, and the State of Illinois, the team embarked on the historic venture of building the Computational Microscope, an instrument of amazing resolving power that lead to many discoveries.

While the last twenty years have been great, the next twenty years promise to be even greater as the past efforts of computational biologists all around the world promise to bear more fruits than ever. Technological advances are once again opening doors wide for breakthroughs and entirely new views of the living cell.

Technologies in the form of petascale computers, the Shaw computer, and graphics processing units, promise millisecond simulations soon. Coarse-grained algorithms will permit explorations into entirely new scales of time and space. Force fields accounting for atomic polarizabilities and linking to quantum chemistry on-the-fly promise to make simulations significantly more accurate. Hybrid computational - experimental (X-ray, EM) methods will reveal large cellular machines from the ribosome to the flagellum. Partnerships between computing and biotechnology/pharmacology are hugely promising.

For us computational cell biologists this symposium is a unique opportunity, as it is entirely focused on our field. Unlike at other conferences where we are usually a minority among experimentalists or among a broader range of computational scientists, during the next three days we will just address our immediate computational cell biology peers. We can talk shop to "family" and can be frank; we can discuss our future in broad terms, while reaching above particular methodology and application.

To keep our feet on the ground, though, there will be experimentally-oriented colleagues among the speakers and many more in the audience; the University of Illinois at Urbana-Champaign has a great history of closely linking experimental, theoretical, and computational science and I know that our experimental friends in the audience will keep a fire under our feet.

I hope we seize the opportunity and, in our discussions, dare to weave our past accomplishments into a vision of future opportunities and challenges, as well as ask hard questions about where we should be moving as a field.

We very much look forward to exciting lectures, lively disputes, and to having a good time together.

Klaus Schulten and the Theoretical and Computational Biophysics Group

Schedule At A Glance

Monday, September 21, 2009

11:30-	REGISTRATION
11:45-1:00	LUNCH BREAK*
1:00-1:15	**Tamer Başar and Klaus Schulten**, "Welcome"

Session I: Meeting the Grand Challenges

	Session Chair: Martin Gruebele
1:15-1:45	**Michael L. Klein** "Computer Simulation: Challenges for the Next Decade and Beyond"
1:45-2:15	**J. Andrew McCammon** "Prospects for Enhanced Sampling in Molecular Dynamics"
2:15-2:45	**Petros Koumoutsakos** "Computational Biology = ? + Biology"
2:45-3:05	DISCUSSION
3:05-3:30	BREAK (Room 1005)

Session II: Towards Subcellular and Cellular Assemblies and Processes

	Session Chair: Ido Golding
3:30-4:00	**Helmut Grubmüller** "Simulation of Life at the Meso-scale"
4:00-4:30	**Gerhard Hummer** "Protein-Protein Binding: from Encounter Complexes to Multi-Protein Assemblies"
4:30-5:00	**Gregory Voth** "Systematic Multiscale Modeling of Biomolecular Systems
5:00-5:20	DISCUSSION
5:20-5:45	BREAK (Room 1005)
5:45-6:15	**Steve Harvey** "The Puzzle of Viral Packaging: What We Know, and What Still Puzzles Us"
6:15-6:45	**Charles Brooks** "Building Virus Capsids: from Design Principles Assembly Mechanisms"
6:45-7:05	DISCUSSION
7:05-7:30	RECEPTION
7:30-	DINNER* Klaus Schulten after dinner talk, "Can Modelers be Nice to Each Other?"

* Catered lunches (Room 1005) and dinners (Atrium) are by invitation only.
Lectures are held in the Beckman Auditorium, Room 1025.

Tuesday, September 22, 2009

Session III: Milliseconds and Beyond

	Session Chairs: Thom Dunning and Wen-mei Hwu
8:30-9:00	**David E. Shaw** "Unsupported Speculation on Future Opportunities and Challenges for Millisecond-Scale Molecular Dynamics Simulations"
9:00-9:30	**Laxmikant Kale** "Challenges and Opportunities in Simulations of Biomolecular Systems Beyond Petascale"
9:30-10:00	**Angel E. Garcia** "Microsecond Simulations of the Detailed folding/unfolding Thermodynamics of Proteins"
10:00-10:20	DISCUSSION
10:20-10:45	BREAK (Room 1005)
10:45-11:15	**Vijay Pande** "A Paradigm Shift for Simulation: Viewing Simulations from a Statistical Perspective"
11:15-11:45	**Benoit Roux** "Treatment of Slow and Complex Conformational Transitions"
11:45-12:15	**Zaida Luthey-Schulten** "Challenges in Simulating RNA Systems"
12:15-12:35	DISCUSSION
12:35-1:45	LUNCH BREAK*

Session IV: The Big Picture

	Session Chair: Steve Sligar
1:45-2:15	**Jeffrey Skolnick** "New Approaches to Drug Discovery and Cancer Metabolomics"
2:15-2:45	**Valerie Dagget** "Dynameomics"
2:45-3:15	**Thorsten Ritz** "Can We Use Physics to find Laws of Biology? Towards Quantifying Biological Function in the Context of Evolutionary Constraints"
3:15-3:35	DISCUSSION
3:35-4:00	BREAK (Room 1005)

Session V: Hand in Hand With Experiment

	Session Chair: Taekjip Ha
4:00-4:30	**Angela Gronenborn** "Structural Studies of HIV-1 capsid: Synergy Between cryo-EM, NMR and X-ray"
4:30-5:00	**Andrej Sali** "Computational Integration of Diverse Structural and Kinetic Data for Visualizing Macromolecular Assemblies and Processes"
5:00-5:30	**Dave Thirumalai** "Universality and Specificity in Protein Folding"
5:30-6:00	**Olga Dudko** "Single Molecules Under Force: Kinetics of Rupture in 1D and Beyond"
6:00-6:20	DISCUSSION
6:20-6:50	RECEPTION
6:50-	DINNER*

Wednesday, September 23, 2009

Session VI: Special Systems

Session Chair: Greg Timp

9:00-9:30	**Richard W. Pastor** "Why Pure Lipid Systems Remain Challenging"
9:30-10:00	**Emad Tajkhorshid** "Simulating The Art of Active Transport Across the Cellular Membrane"
10:00-10:30	**Alek Aksimentiev** "Molecular Modeling in Nanobiotechnology"
10:30-10:50	DISCUSSION
10:50-11:20	BREAK (Room 1005)
11:20-11:50	**Klaus Schulten** "Molecular Assembly and Teamwork - Bridge Between Inanimate and Animate Matter"
12:00-1:00	LUNCH BREAK*

Symposium Program

Monday, September 21, 2009

11:45am-1:00pm

REGISTRATION AND LUNCH

1:00-1:15pm

Klaus Schulten, "Welcome"

Session I: Meeting the Grand Challenges

Session Chair: Martin Gruebele

1:15-1:45pm

Computer Simulation: Challenges for the Next Decade and Beyond
Speaker: Michael L. Klein, University of Pennsylvania

I entered Bristol University in 1958 as an undergraduate and received my BSc three years later. This was of course after the pioneering papers in the 1950's that heralded computer simulation methodologies: I refer to the work of Metropolis, Teller et al via Monte Carlo (1953) and molecular dynamics by Berni Alder et al (1957). Or was molecular dynamics really due to Enrico Fermi (1953)? Anyway, I was fortunate enough to get to learn to use a computing machine during my research as a graduate student in the UK. In 1963 I attended a conference in Copenhagen at which George Vineyard showed a movie of particles being fired at a crystal. He was interested in modeling radiation damage. This simulation predated the seminal work of Aneesur Rahman on liquid Argon, which appeared in 1964 when I was already a post-doc in physics at Rutgers. At that time I was using computers to evaluate Feynman diagrams for phonon-phonon scattering in solid Argon. A chance encounter a couple of years later with Bob Zwanzig pointed me to the possibility of using molecular dynamics to test the convergence of my calculations, which seemed to be at best asymptotically converging. I was struggling with a problem, which even the great physicist Rudolf Peierls had not been able to help me deal with. So, in 1968 I started collaboration with Bill Hoover, at Lawrence Livermore National Lab, which allowed access to the necessary computational resources and we used Monte Carlo to test my semi-analytic perturbation theory calculations.

As a result, I became converted to the power of computation as an indispensable research tool. But where to find a suitable computer, which typically only existed in the US National Labs? It turned out that another chance encounter - this time with Jean-Pierre Hansen - solved this problem. At the time (1969), Jean-Pierre was a post-doc at Cornell and I was working at the NRC in Ottawa Canada but we agreed to collaborate on using molecular dynamics to study dynamical properties of rare gas solids once he returned to Paris. Jean-Pierre began an independent research career associated with the group of Loup Verlet, who had recently bought a UNIVAC machine; offering a level of computational resources typically not available to casual researchers.

So, from the early 1970's my research focused increasingly on the use of computer simulation to study solids primarily but also liquids. Inspired by the simulation of water by John Barker and Bob Watts (1969) and Aneesur Rahman and Frank Stillinger (1971) I also began to focus on molecules - first Monte Carlo studies of small linear molecules (N2 and CO2) and eventually 'real' molecules. In the mid 1970's others pushed the frontiers of molecular dynamics simulations into the domain of chemical biology: Michael Levitt and Arieh Warshel along with Martin Karplus and his many disciples led the charge. Throughout this evolutionary period of the field, progress often depended on the development of novel algorithms and methodologies, which were even more important than the increasing capability of the computing machines. The mid-1980's saw enormous progress on algorithms and gave birth to the Car-Parrinello methodology that linked electronic structure and dynamics. The ensuing 25 years has seen many advances and developments in bold new directions by many outstanding researchers, many of whom are at this meeting.

I will review some of the history as a prelude to attempting to set out a number of challenges for computation in the domain of chemical biology in the decades ahead.

1:45-2:15pm

Prospects for Enhanced Sampling in Molecular Dynamics
Speaker: J. Andrew McCammon, Howard Hughes Medical Institute

The many-dimensional configuration spaces and rough potential energy surfaces of proteins and other biopolymers present severe challenges for configurational sampling. This talk will describe methods for speeding the sampling of configurations and the calculation of structural and thermodynamic properties. The potential of such methods for characterizing biomolecular mechanisms, for interpreting experimental data, and for structure-based drug discovery will be briefly considered. Information related to this work can be found at the website http://mccammon.ucsd.edu/ .

2:15-2:45pm

Computational Biology = ? + Biology
Speaker: Petros Koumoutsakos, Swiss Federal Institute of

Technology (ETH)

In this talk I hope to present examples that stimulate a discussion on the following questions: What kinds of Computational tools are needed for making advances in Biology? Can an we exploit computational advances made in other sciences? Do we need new computational tools and if so what should they be like?

2:45-3:05pm

DISCUSSION

3:05-3:30pm

BREAK (Beckman Garden or Room 1005)

Session II: Towards Subcellular and Cellular Assemblies and Proceses

Session Chair: Ido Golding

3:30-4:00pm

Simulation of Life at the Meso-scale
Speaker: Helmut Grubmüller, Max-Planck-Institute for Biophysical Chemistry

"It is difficult to make predictions, especially about the future" is a famous quote, which is certainly appropriate for the meeting. It is equally inspiring, though, to stretch one's imagination, and to share dreams. Would we have expected a decade ago to be able to simulate a whole virus, as we can now? A whole organelle, as we will be able to do soon? A whole cell? In a way – yes, simply on the grounds of Moore's Law, which continued to hold for the past five decades. Parallel computers, introduced into the field by Klaus, further pushed the limits and enabled Moore's Law to remain valid for another one or two decades. Probably GPUs will provide the next leap. So the hardware track seems to be reasonably predictable; what about the software, the physics and modeling part? Strangely, in my view not too much has happened on this side since 1975. True, the algorithms have become much better, the force fields, too, and a number of conceptual advances have been made, pertaining to non-equilibrium physics, or enhanced sampling methods such as replica exchange and so on. It is only recently, however, that the underlying model – essentially interacting atoms – has been extended towards coarse graining. (I'm skipping QM/MM here, which is of course equally important.) Despite the fact that multiscale modeling has been proposed already many years ago, only recently we have seen significant advances – it seems to be really hard! And so it is. The core of any good theory or model is a clever selection of relevant versus irrelevant degrees of freedom, and a sufficiently accurate – but not over-accurate – treatment of the effect of the latter onto the dynamics of the former. To be able to treat, e.g., a whole cell, what needs to be done now is to automize this process, to devise clever heuristics which dynamically decide which level of coarse graining is appropriate within which region of the simulation system, and to systematically derive each level from the underlying, more detailed one, on which it is based. This is a strict bottom-up program, and I am convinced it's the only one which has the chance to succeed. To me, one of the most fascinating achievements of science is when Gedankenexperiments come into reality, such as EPR. The – provocative – Gedankenexperiment which has yet to be realized is to describe a frog by solving the Schrodinger equation. Within 30 years, we have almost arrived at viruses, and are now approaching systems which are generally called alive. What could be more exciting?

4:00-4:30pm

Protein-Protein Binding: from Encounter Complexes to Multi-Protein Assemblies
Speaker: Gerhard Hummer, National Institute of Health

The formation of protein complexes is a central element of the function of biological systems at the molecular level. With advances in molecular and structural biology, and the advent of proteomics, it is now increasingly recognized that much of biology is influenced, if not dominated, by weak and transient binding. Important biological functions are carried out by multi-protein assemblies that form transiently and are held together by relatively weak pairwise interactions, with dissociation constants in the micro- to millimolar regime. In my talk, I will describe models developed specifically to study weak protein binding. In these models, we use different coarse-graining strategies, including both structure-based and transferable energy functions. In simulations of the binding of a natively-unstructured transcription factor pKID/CREB to its co-activator KIX/CBP, we find that binding precedes folding [1]. Our observation of an unstructured transition state of the coupled folding/binding reaction, with structural stabilization actually slowing down the binding process, helps explain how being unstructured can confer an advantage in protein target recognition. To study the structure and motions of large multi-protein assemblies, we have developed a transferable energy function [2]. With this model, we were able to study protein binding and dissociation at equilibrium, including the formation of both the specific and non-specific complex structures (i.e., transient encounter complexes), as validated by paramagnetic relaxation enhancement NMR experiments [3]. From simulations of the Vps27 complex of the ESCRT membrane-protein trafficking system [2,4], we conclude that this membrane-bound multi-protein assembly is dynamic and open, allowing it to bind to a diverse set of ubiquitinated target proteins. We also find that the binding of its different domains is highly cooperative, which is essential for the proper function at the low protein concentrations inside the cell.

References:

1. Turjanski AG, Best RB, Gutkind JS, Hummer G. Binding-induced folding of a natively unstructured transcription factor. PLoS Comp. Biol. 4,

e1000060, 2008.

2. Kim YC, Hummer G. Coarse-grained models for simulations of multiprotein complexes: application to ubiquitin binding. J. Mol. Biol. 375:1416-33, 2008.

3. Kim YC, Chun T, Clore GM, Hummer G. Replica exchange simulations of transient encounter complexes in protein-protein association. Proc. Natl. Acad. Sci. 105, 12855, 2008.

4. Prag G, Watson H, Kim YC, Beach BM, Ghirlando R, Hummer G, Bonifacino JS, Hurley JH. The Vps27/Hse1 Complex Is a GAT Domain-Based Scaffold for Ubiquitin-Dependent Sorting. Dev. Cell 12: 973-86, 2007.

5. Ren X, Kloer DP, Kim YC, Ghirlando R, Saidi LF, Hummer G, Hurley JH, Structure 17, 406, 2009.

4:30-5:00pm

Systematic Multiscale Modeling of Biomolecular Systems
Speaker: 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 large protein complexes will also be described. The computational challenges and opportunities for this area of molecular modeling will be especially emphasized.

5:00-5:20pm

DISCUSSION

5:20-5:45pm

BREAK (Beckman Garden or Room 1005)

5:45-6:15pm

The Puzzle of Viral Packaging: What We Know, and What Still Puzzles Us
Speaker: Steve Harvey, Georgia Institute of Technology

The formation of small icosahedral viruses requires the assembly of a protein capsid around a core of nucleic acids. This can happen in either of two ways. The capsids of DNA bacteriophage assemble spontaneously, in the absence of DNA. The genome is then driven into the capsid by an ATP-consuming motor. In contrast, capsid formation in RNA viruses does not consume ATP, but the proteins do not assemble into a capsid unless the RNA is present. This talk will present the results of recent computational studies on both of these problems. The models illuminate aspects of viral assembly that are not revealed by experiment, and they make testable predictions aimed at promoting future experiments.

6:15-6:45pm

Building Virus Capsids: from Design Principles Assembly Mechanisms
Speaker: Charles L. Brooks, University of Michigan

In this talk I will discuss recent work on elucidating physical constraints that define the principles from which viral capsid architecture and dynamics emerge. Questions to be addressed include the ubiquitous "shape" of viral capsid proteins and how this limits their structure and dynamics. Additionally, I will provide an overview of applications of coarse-grained models to the kinetics and thermodynamics of viral capsid assembly and the morphology of assembled capsules that occur.

6:45-7:05pm

DISCUSSION

7:05-7:30pm

RECEPTION

7:30pm-

DINNER

(catered dinner in Atrium by invitation only)

Klaus Schulten after dinner talk, "Can Modelers be Nice to Each Other?"

Tuesday, September 22, 2009

Session III: Milliseconds and Beyond

Session Chairs: Thom Dunning and Wen-mei Hwu

8:30-9:00am

Unsupported Speculation on Future Opportunities and Challenges for Millisecond-Scale Molecular Dynamics Simulations
Speaker: David E. Shaw, D. E. Shaw Research

A special-purpose machine, together with novel algorithms developed in conjunction with that hardware, has recently enabled the first atomic-level molecular dynamics simulation of a protein over a period of more than a millisecond – approximately 100 times the length of the longest previously published simulation. This tool is already allowing the observation of certain slow, large-scale conformational changes on a qualitatively distinct, temporally well-separated timescale. At this point, however, relatively little is known about the range of applicability of such simulations and technologies or about the new set of binding constraints that will inevitably be uncovered by this significant extension of the timescales accessible to MD simulation. After reviewing the current state of the art and the set of challenges that are already visible, I plan to indulge in reckless, largely ungrounded prognostication about such matters in the hope that a decade from now, nobody in the audience will remember what I've predicted in this talk.

9:00-9:30am

Challenges and Opportunities in Simulations of Biomolecular Systems Beyond Petascale
Speaker: Laxmikant Kale, University of Illinois at Urbana-Champaign

We already have petascale machines, and within a couple of years, systems with multi-petaFLOPS peak performance 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. I will speculate on possible hardware technologies needed, and software techniques desired, to harness the exascale computers for the purposes of biomolecular modeling.

9:30-10:00am

Microsecond Simulations of the Detailed folding/unfolding Thermodynamics of Proteins
Speaker: Angel E. Garcia, Rensselaer Polytechnic Institute

The development of new force fields combined with enhanced sampling methods enable us to calculate detailed stability diagrams of proteins and small RNA molecules as a function of temperature, pressure, and urea concentration. These calculations reveal a complex dependence of protein stability on hydration. The balance between folded and unfolded states can be changed adding co-solvents or changing the system volume. Combined studies of the folding of the TRP-cage protein under various conditions reveal the mechanisms for urea denaturation in which van der Waals interactions (not hydrogen bonding) drives the unfolding.

This work is supported by the National Science Foundation, MCB-0543769.

10:00-10:20am

DISCUSSION

10:20-10:45am

BREAK (Beckman Garden or Room 1005)

10:45-11:15am

A Paradigm Shift for Simulation: Viewing Simulations from a Statistical Perspective
Speaker: Vijay Pande, Stanford University

Traditionally, researchers have used a handful of simulation trajectories, usually as long as possible, to address questions of interest. More recently, a new paradigm has emerged to use many, potentially shorter simulations in a statistical scheme to address issues of long experimental timescales, heterogeneous dynamics, and as a means to gain an understanding of the underlying system. I will discuss my predictions for how these methods could change simulation methodology in the next decade, showing how such methods can draw together additional key aspects in simulation, especially novel multiscale simulations and means to directly connect experiment to theory.

11:15-11:45am

Treatment of Slow and Complex Conformational Transitions
Speaker: Benoit Roux, University of Chicago

One of the most outstanding challenges in calculations of free energies, which is the treatment of very large conformational changes in a protein. The recently developed string method of Maragliano et al. (JCP, 2006) is a good starting point. This method aims to discover the minimum free energy path (MFEP) and the free energy along the path in the subspace corresponding to a large but finite set of coordinates, z, referred to as "collective variables". In the string method, the transition path is represented as a "chain of state" by an ordered sequence of M discrete "images" {z(1), z(2), ..., z(M)} in the space of collective variables z (the path is built onto the free energy surface as a function of the collective variables). We have proposed a different algorithm to optimize the path in the string method that we call the "swarms-of-trajectories" (JPC, 2008). The optimized paths can then be utilized to construct reduced stochastic models to extract long-time behavior as well as equilibrium properties for the system. An important requirement for constructing reliable reduced models is to include a set of representative states by focusing on the dynamically meaningful regions of phase space involved in the transition. The optimized path from the string method is a good starting point to split the complete configurational space of the system into small discrete regions. I will describe the theory and recent applications of those methods.

11:45am-12:15pm

Challenges in Simulating RNA Systems
Speaker: Zaida Luthey-Schulten, University of Illinois at Urbana-Champaign

RNA:protein complexes form the largest assemblies in the cell and control its information processing systems that are universal across all three domains of life. The size and inherent flexibility of the highly charged RNA systems present challenges in long timescale simulations of such processes like translation. Comparative evolutionary analysis of the translational machinery provides important insight into the mechanism of recognition between its components. We examine the dynamical network of interactions involved in the migration of tRNA among the complexes that set and maintain the genetic code [1-3] and discuss problems that need to be addressed for in vivo simulations of translation.

References:

1. A. Sethi, J. Eargle, A. Black, and Z. Luthey-Schulten, "Dynamical Networks in Protein:RNA Complexes", Proc. Natl. Acad. Sci. USA, 106, 6620-5 (2009).

2. J. Eargle, A. Black, A. Sethi, L. Trabuco, and Z. Luthey-Schulten, "Dynamics of Recognition between tRNA and elongation factor TU", J. Mol. Biol. 377, 1382-405 (2008).

3. E. Roberts, A. Sethi, J. Montoya, C. Woese, and Z. Luthey-Schulten, "Molecular Signatures of Ribosomal Evolution", Proc. Natl. Acad. Sci. USA 105, 13953-8 (2008)

12:15-12:35pm

DISCUSSION

12:35-1:45pm

LUNCH BREAK

(catered lunch in Room 1005 by invitation only)

Session IV: The Big Picture

Session Chair: Steve Sligar

1:45-2:15pm

New Approaches to Drug Discovery and Cancer Metabolomics
Speaker: 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.

2:15-2:45pm

Dynameomics
Speaker: Valerie Dagget, University of Washington

The dynamical behavior of proteins is important to understand their function and folding. We have performed molecular dynamics simulations and analyses of the native state and unfolding pathways of about 1000 proteins, representing the majority of folds that are present in known and soluble proteins. This data set contains both the largest collection of protein simulations and protein structures in the world. These data, stored and organized using an innovative database approach, are used to obtain information about the dynamics and (un)folding of the overall protein fold space, relevant subsets thereof, and individual proteins. Using state-of-the-art analysis methods, questions relevant to evolution, protein folding and disease are investigated. The collected data can further be used for drug design and protein engineering. Our native state simulation data and analyses for the 100 most populated metafolds, together with related resources, will be made publicly accessible through www.dynameomics.org.

2:45-3:15pm

Can We Use Physics to find Laws of Biology? Towards Quantifying Biological Function in the Context of Evolutionary Constraints
Speaker: Thorsten Ritz, University of California at Irvine

The past decade has seen a close and fruitful relationship between structural biology and computational biology. However, despite the greatly increased ability to relate structures to functions at the protein level, we still have not seen universal biological principles emerging from such studies. In fact, most biological principles currently discussed are high-level concepts, such as the handicap principle or the interface theory of perception, that seem rather disconnected from molecular computational biology. One reason for this may be that quantifying biological function has been treated in a comparatively ad-hoc fashion. The next decade of computational biology will likely see an increased sophistication in quantifying biological function, in close interaction with experimental biologists interested in understanding design principles of biological systems. Drawing on research examples from behavioral biology, genetics, and development, I will attempt to outline which roles physics, computation, evolutionary and experimental biology might play in this interaction. I will conclude by presenting a set of next-decade questions for the computational biology community that, if answered, may pave the way towards the uncovering of universal biological principles, or laws.

3:15-3:35pm

DISCUSSION

3:35-4:00pm

BREAK (Beckman Garden or Room 1005)

Session V: Hand in Hand With Experiment

Session Chair: Taekjip Ha

4:00-4:30pm

Structural Studies of HIV-1 capsid: Synergy Between cryo-EM, NMR and X-ray
Speaker: Angela Gronenborn, University of Pittsburgh

Mature HIV-1 particles contain a conical-shaped capsid that encloses the viral RNA genome and performs essential functions in the virus life cycle. Previous structural analysis of two- and three-dimensional arrays provided a molecular model of the capsid protein (CA) hexamer and revealed three interfaces in the lattice. We will present a cryoEM study of a tubular assembly of CA and a high-resolution NMR structure of the CA C-terminal domain (CTD) dimer. In the solution dimer structure, the monomers exhibit different relative orientations compared to previous X-ray structures. The solution structure fits extremely well into the EM density map, suggesting that the dimer interface is retained in the assembled CA. We also identified a novel CTD-CTD interface at the local three-fold axis in the cryoEM map and confirmed its functional importance by mutagenesis. In the tubular assembly, CA intermolecular interfaces vary slightly, accommodating the asymmetry present in tubes. This provides the necessary plasticity to allow for controlled, asymmetric virus capsid assembly. This work was supported by the National Institutes of Health (GM082251 and AI076121).

4:30-5:00pm

Computational Integration of Diverse Structural and Kinetic Data for Visualizing Macromolecular Assemblies and Processes
Speaker: Andrej Sali, California Institute for Quantitative Biosciences

Our broad goal is to contribute to a comprehensive structural characterization of large macromolecular assemblies. Detailed structural characterization of assemblies is generally impossible by any single existing experimental or computational method. We suggest that this barrier can be overcome by hybrid approaches that integrate data from diverse biochemical and biophysical experiments (e.g., x-ray crystallography, NMR spectroscopy, electron microscopy, immuno-electron microscopy, footprinting, chemical cross-linking, FRET spectroscopy, small angle X-ray scattering, immunoprecipitation, and genetic interactions). Even a coarse characterization of the configuration of macromolecular components in a complex (i.e., the molecular architecture) helps to elucidate the principles that underlie

cellular processes, in addition to providing a necessary starting point for a higher resolution description.

We formulate the hybrid approach to structure determination as an optimization problem, the solution of which requires three main components: the representation of the assembly, the scoring function, and the optimization method. The ensemble of solutions to the optimization problem embodies the most accurate structural characterization given the available information. The key challenges remain translating experimental data into restraints on the structure of the assembly, combining these spatial restraints into a single scoring function, optimizing the scoring function, and analyzing the resulting ensemble of solutions.

To address these challenges, we are developing the Integrated Modeling Platform (IMP) (http://salilab.org/imp). IMP is designed to allow mixing and matching of existing modeling components as well as easy adding of new functionality. It supports a wide variety of assembly representations and input data. We will also provide infrastructure that encourages and supports contributions from other laboratories.

IMP will be illustrated by its application to the determination of the molecular architecture of the Nuclear Pore Complex and the 26S proteasome.

References:

F. Alber, F. Förster, D. Korkin, M. Topf, A. Sali. Integrating Diverse Data for Structure Determination of Macromolecular Assemblies. Annual Review of Biochemistry 77, 443-477, 2008.

F. Alber, S. Dokudovskaya, L. Veenhoff, W. Zhang, J. Kipper, D. Devos, A. Suprapto, O. Karni, R. Williams, B.T. Chait, M.P Rout, A. Sali. Determining the architectures of macromolecular assemblies. Nature 450, 683-694, 2007.

F. Alber, S. Dokudovskaya, L. Veenhoff, W. Zhang, J. Kipper, D. Devos, A. Suprapto, O. Karni, R. Williams, B.T. Chait, A. Sali, M.P. Rout. The Molecular Architecture of the Nuclear Pore Complex. Nature 450, 695-701, 2007.

C.V. Robinson, A. Sali, W. Baumeister. Molecular sociology of the cell. Nature 450, 973-982, 2007.

5:00-5:30pm

Universality and Specificity in Protein Folding
Speaker: Dave Thirumalai, University of Maryland

I will use theoretical arguments to show that protein length (N) plays a crucial role in the determination of thermodynamics kinetics of protein folding. A dimensionless parameter that measures the extent of cooperativity scales as $\Omega_c \sim N^{\zeta}$ where the universal exponent $\zeta = 1 + \gamma$ where γ (≈ 1.2) is the susceptibility exponent characterizing the denatured states. We will also show that the folding time for several proteins $\tau_F \sim \exp(N^{0.5})$. I will also introduce the Molecular Transfer Model (MTM) that allows us to compute denaturant-dependent properties of folding. Applications of the MTM, which are the first simulations that have been performed under conditions that directly mimic experiments, to protein L and Cold Shock protein will be discussed. Challenges in using MTM in the context of all atom simulations will be presented.

5:30-6:00pm

Single Molecules Under Force: Kinetics of Rupture in 1D and Beyond
Speaker: Olga Dudko, University of California San Diego

Single-molecule biophysical tools permit measurements of the mechanical response of individual biomolecules to external load, revealing details that are typically lost when studied by ensemble methods. Kramers theory of diffusive barrier crossing in one dimension has been used to derive analytical solutions for the observables in such experiments, in particular, for the force dependent lifetimes. Coarse-grained simulations of molecular rupture performed over a broad range of stretching forces, beyond the range accessible experimentally, reveal a remarkable turnover in the lifetimes, which is unexpected in a one-dimensional picture, and thus calls for a higher-dimensional description. While multi-dimensional approaches to single-molecule mechanics add challenge into the interpretation of data, they at the same time reveal the richness of biomolecular interactions, providing us with tools to help comprehend the inner workings of the living cell across the scales of its organization.

6:00-6:20pm

DISCUSSION

6:20-6:50pm

RECEPTION

6:50pm-

DINNER

(catered dinner in Atrium by invitation only)

Wednesday, September 23, 2009

Session VI: Special Systems

Session Chair: Greg Timp

9:00-9:30am

Why Pure Lipid Systems Remain Challenging
Speaker: Richard W. Pastor, National Institute of Health

The talk with focus on unresolved problems in simulations of pure lipid (protein-free!) assemblies involving bilayers, monolayers, micelles, and bicelles. Topics will include surface tensions and mechanical properties in bilayers and monolayers; electrostatics, ion double layers and signaling lipids; lateral diffusion; self-assembly and effects of PEGylation; line tension

and phase separation. The (statistical) safety in large numbers of identical particles allows for both good and interesting science and, eventually, the inclusion of proteins.

9:30-10:00am

Simulating The Art of Active Transport Across the Cellular Membrane
Speaker: Emad Tajkhorshid, University of Illinois at Urbana-Champaign

Transport of materials across the cellular membrane is one of the most fundamental and highly regulated phenomena in the biology of a living cell. Molecular dynamics has been very successful in describing various aspects of the transport phenomenon in membrane channels, owing to the fact that they merely provide a passive diffusion pathway for their substrate. Active membrane transporters, on the other hand, continue to present tremendous challenges to simulation studies, not only due to their several orders of magnitude slower mode of operation and scarcity of structural data, but also due to the complexity and high dimensionality of the processes involved in their function. These complex proteins constitute sophisticated, molecular pumps that efficiently couple various sources of energy in the cell to the transport of a wide range of molecules across the membrane, often against their electrochemical gradient. Depending on the source of energy used, very different architectures and, thus, mechanisms exist for membrane transporters. Substrate binding and translocation in membrane transporters are closely coupled to numerous, mostly unknown protein conformational changes of various magnitudes that are induced by and/or coordinated with the energy-providing mechanisms. Though still extremely challenging, taking advantage of various modeling and simulation methods, and advances in computer hardware and software allowing us to push the limits of simulations, we are now in an unprecedented position to begin to expand the scope of simulation studies into the realm of membrane transporters and to study the physical basis of their function.

10:00-10:30am

Molecular Modeling in Nanobiotechnology
Speaker: Alek Aksimentiev, University of Illinois at Urbana-Champaign

With ever advancing miniaturization of human technology, it becomes possible to manufacture devices with features comparable in size to the building blocks of life: DNA and proteins. Today, such devices can already detect and manipulate biological macromolecules. In the future, they will allow man-made electric circuits to interact directly with the robust machinery of a living cell. Understanding and controlling the interactions between biological and synthetic materials is critical for the development of this field. The complexity of such interactions requires computations to complement conceptual insights of nanoscale physics and molecular biology. In this talk I will highlight the opportunities for molecular modeling in nanobiotechnology and describe the unique challenges that modeling "bio-nano" systems presents.

10:30-10:50am

DISCUSSION

10:50-11:20am

BREAK (Beckman Garden or Room 1005)

11:20-11:50am

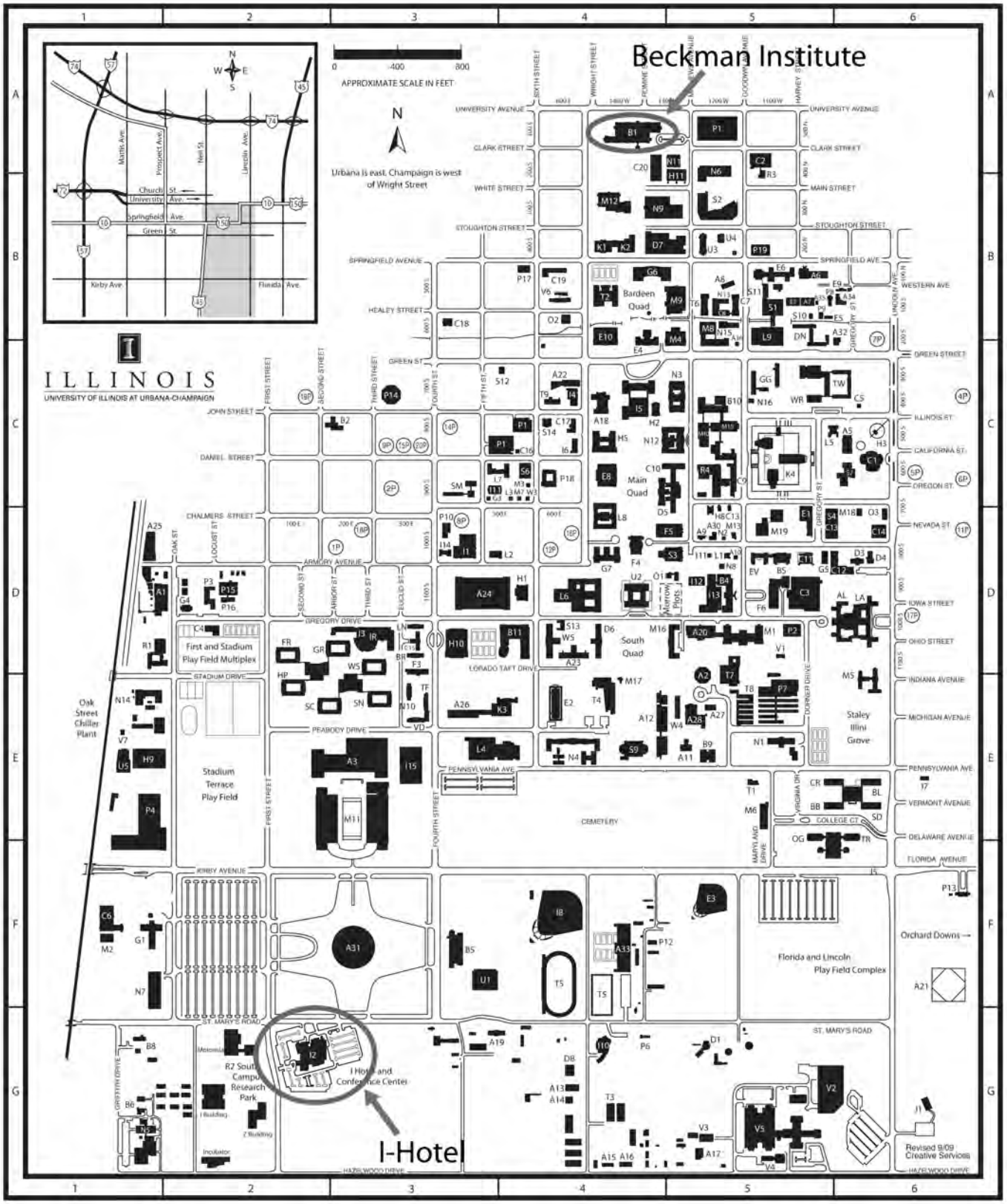
Molecular Assembly and Teamwork - Bridge Between Inanimate and Animate Matter
Speaker: Klaus Schulten, University of Illinois at Urbana-Champaign

The two-decade development of VMD and NAMD in our group sought to describe biomolecular systems on time scales and size scales relevant for answering Schroedinger's famous question "What is Life". We thought that assembly and teamwork of biomolecules is the bridge between inanimate and animate matter. It seems that in the next decade our investment will pay off since we can simulate the functional, millisecond dynamics of key biomolecular assemblies of the cell involving, hundreds of proteins. Focusing our computational microscope on cellular structures and machines, we expect to discover new principles of biological organization that could not be resolved before. Indeed, the first inroads paved in the new field of structural systems biology have lead already to exciting insights into how proteins mold cellular membranes in teams, how multi-domain proteins develop a wide range of elasticity to bear cellular forces and sustain cellular structures, and even how hundreds of membrane proteins shape a cellular organelle and then cooperate in its function. Cell biology, in the past, learned key lessons in enzymology and physiology from single protein behavior; cell biology will now learn key lessons on its large-scale structure and function from assembly behavior. We are sure that computational modeling will again play a key role in the new Science because of its unmatched resolving power.

12:00-1:00pm

LUNCH

(catered lunch in Room 1005 by invitation only)


Beckman Institute
I-Hotel
ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
APPROXIMATE SCALE IN FEET
Urbana is east, Champaign is west of Wright Street
First and Stadium Play Field Multiplex
Stadium Terrace Play Field
Oak Street Chiller Plant
Bardeen Quad
Main Quad
South Quad
Staley Illini Grove
Florida and Lincoln Play Field Complex
Orchard Downs
CEMETERY
Revised 9/09 Creative Services

CAMPUS MAP

The designation in parentheses (D1) indicates the map coordinates. An asterisk (*) indicates that a building is not included on this map.

 # Building Name (Coordinates)

A

A1 Abbott Power Plant (D1)
A2 ACES Library & Info Center (E5)
A3 Activities and Recreation Center (ARC), *formerly IMPE* (E2)
A4 Admin Info Tech Serv Bldg (H2)*
A5 Admissions and Records (C6)
A6 Advanced Computation Bldg (B5)
A7 Aerodynamics Research Lab (B5)
A8 Aeronautical Lab A (B5)
A9 African-American Cultural Prog (D5)
A10 Afro-Amer Studies & Rsch Prog (D5)
A11 Agricultural Bioprocess Lab (E5)
A12 Ag Engineering Sci Bldg (E4)
A13 Agriculture Services Bldg (G4)
A14 Ag Services Warehouse (G4)
A15 Agronomy/Plant Path Farm (G4)
A16 Agronomy Seed House (G4)
A17 Agronomy Soybean Rsch Farm (G5)
A18 Altgeld Hall (C4)
A19 Animal Science Barns (G3)
A20 Animal Sciences Lab (D5)
A21 Arboretum—Hartley Gardens (F6)
ARC—see A3
A22 Arcade Bldg (C4)
A23 Architecture Bldg (D4)
A24 Armory (D3)
A25 Armory Avenue Warehouse (D1)
A26 Art & Design Bldg (E3)
A27 Art E Annex, Studio 1 (E5)
A25 Art E Annex, Studio 2 (E5)
A29 Art Studios (H1)*
A30 Asian American Studies Bldg (D5)
A31 Assembly Hall (F3)
A32 Astronomy Bldg (B5)
A33 Atkins Tennis Ctr (F4)
A34 Atmospheric Sciences Bldg (B6)
A35 Atmospheric Sciences Annex 1 (B5)
A36 Atmospheric Sciences Annex 2 (B5)

B

B1 Beckman Institute (A4)
B2 Beckwith Hall (C2)
B4 Bevier Hall (D5)
B5 Bielfeldt Athletic Admin Bldg (F3)
B6 Biological Control Lab (G1)
B7 Biomedical Mag Res Facility (H5)*
Buell Hall—see T4
B8 Building Rsch Council (G1)
B9 Burnsides Rsch Lab (E5)
B10 Burrill Hall (C5)
B11 Business Instructional Facility (D4)

C

C1 Campbell Alumni Center (C6)
C2 Campbell Hall for Public Telecommunications (A5)
C3 Campus Recreation Ctr East (D5)
C4 Campus Rec Outdoor Ctr (D2)
Career Center—see A22
C5 Center for Advanced Study (C6)
C6 Central Receiving Bldg (F1)
C7 Ceramics Bldg (B5)
C8 Ceramics Kiln House (C5)
C9 Chemical & Life Sci Lab (C5)
C10 Chemistry Annex (C5)
C11 Child Development Lab (D5)
C12 Child Develpmnt Lab Expanded (D5)
C13 Children's Rsch Ctr (I2)*
C14 Christopher Hall (D6)
C15 Clark Hall Housing Admin (D3)
C16 CNI/Prairienet (C4)
C17 Coble Hall (C4)
C18 Colonel Wolfe School (B3)
Commerce West Bldg—see W5
C19 Computing Applications Bldg (B4)
C20 Coordinated Science Lab (A4)
C21 Credit Union Bldg (H2)*

D

D1 Dairy Exper Rnd Barns (G5)
D2 Dairy Science Rsch Farm (H6)*
D3 Dance Admin Bldg (D6)
D4 Dance Studio (D6)
D5 Davenport Hall (C5)
D6 David Kinley Hall (D4)
D7 Digital Computer Lab (B4)
D8 Duplicating/Quick Copy Bldg (G4)

E

E. Asian Lang & Cultures—see F5
E1 East Campus Commercialization Center (C5)
E2 Education Bldg (E4)
E3 Eichelberger Field (F5)
Electrical & Computer Engr Lab —see E10
E4 Engineering Hall (B4)
E5 Engineering Sr Design Studio (B6)
E6 Engineering Sciences Bldg (B5)
E7 Engineering Student Project Lab (B5)
E8 English Bldg (C4)
Enviro & Ag Sci Bldg—see N1
E9 Environmental Health & Safety (B6)
E10 Everitt Lab (B4)

F

Financial Aid—see A22
F1 Fire Service Inst Bldg (I1)*
F3 Flagg Hall (E3)
F4 Foellinger Auditorium (D4)
F5 Foreign Languages Bldg (D4)
F6 Freer Hall (D5)

G

G1 Garage/Car Pool (F1)
G3 General Curriculum Bldg (C3)
G4 Geological Survey Lab (D1)
G5 Govt & Public Affairs, Inst of (D5)
G6 Grainger Engr Library Info Ctr (B4)
G7 Gregory Hall (D4)

H

H1 Harding Band Bldg (D4)
H2 Harker Hall (C4)
Hartley Gardens—see A21
H3 Hallene Gateway (C6)
H5 Henry Admin Bldg (C4)
H8 Honors Program (D5)
H9 Housing Food Stores (E1)
H10 Huff Hall (D3)
H11 Hydrosystems Lab (A5)

I

I1 Ice Arena (D3)
I2 I Hotel and Conference Center (G2-3)
I3 Ikenberry Commons (D3)
I4 Illini Hall (C4)
I5 Illini Union (C4)
I6 Illini Union Bookstore (C4)
I7 Illinois Program for Research in the Humanities (E6)
I8 Illinois Field (F4)
IL Library Computer Sys Ofc—see L7
I9 Imported Swine Rsch Ctr (H2)*
I10 Indoor Golf Facility (G4)
International Student Affairs—see T9
I11 Intensive English Institute (D5)
I12 International Studies Bldg (C3)
Intramural and Physical Recreation (IMPE)—see A3
I13 Institute for Genomic Biology (D5)
I14 Irwin Academic Services Ctr (D3)
I15 Irwin Indoor Football Pract Fclty (E3)

J-K

J1 Japan House (G6)
K1 Kenney Gym (B4)
K2 Kenney Gym Annex (B4)
K3 Krannert Art Museum & Kinkead Pavillion (E3)
K4 Krannert Ctr for Performing Arts (C5)

L

L1 La Casa Cultural Latina (D5)
L2 Labor & Indust Relations, Inst of (D3)
Large Animal Clinic—see V5
L3 Latina/o Studies (C4)
L4 Law Bldg (E3)
L5 Levis Faculty Ctr/Visitor Ctr (C5)
L6 Library (D4)
L7 Library & Information Science (C3)
L8 Lincoln Hall (D4)
L9 Loomis Lab (B5)

M

M1 Madigan Lab (D5)
M2 Mailing Ctr (F1)
M3 Management Information Div (C4)
M4 Materials Sci & Engr Bldg (B5)
M5 McKinley Health Ctr (E6)
M6 Meat Science Lab (E5)
M7 Merriam Lab (C4)
M8 Mechanical Engineering Bldg (B5)
M9 Mechanical Engineering Lab (B5)
M10 Medical Sciences Bldg (C5)
M11 Memorial Stadium (E3)
M12 Micro & Nanotechnology Lab (B4)
M13 Minority Student Affairs Academic Services Ctr (D5)
M14 Moorman Swine Rsch Farm (H3)*
M15 Morrill Hall (C5)
M16 Mumford Hall (D4)
M17 Mumford House (E4)
M18 Music Annex (D6)
M19 Music Bldg (D5)

N

N1 National Soybean Rsch Ctr (E5)
N2 Native American House (D5)
N3 Natural History Bldg (C5)
N4 Natural Resources Bldg (E4)
N5 Natural Res Studies Annex (G1)
N6 NCSA (A5)
N7 NCSA Petascale Computing Fclty (F1)
N8 Nevada St Computing Serv (D5)
N9 Newmark Lab (B4)
N10 Noble Hall (E3)
N11 North Campus Chiller Plant (A5)
N12 Noyes Lab (C5)
N13 Nuclear Engineering Lab (B5)
N14 Nuclear Physics Lab (E1)
N15 Nuclear Radiations Lab (B5)
N16 Nursing, School of (C5)

O

O1 Observatory (D5)
O2 Optical Physics & Engr Lab (B4)
O3 Oregon St Computing Serv (D6)

P

P1 Parking Structures (C3, A5)
P2 Parking Structure/Fire Substation (D5)
P3 Personnel Services Bldg (D2)
P4 Physical Plant Service Bldg (E1)
P5 Physiology Rsch Lab (H2)*
Plant & Animal Biotech Lab—see M1
P6 Plant Clinic (G4)
P7 Plant Sciences Lab (E5)
P8 Plant Services Bldg NE (B5)
P9 Plant Services Storage Bldg (B5)
P10 Police Training Institute (D3)
P12 Poultry Farm (F4)
P13 President's House (F6)
P14 Presidential Towers/University Inn (C3)
P15 Printing Services Bldg (D2)
P16 Printing Services Imaging Bldg (D2)
P17 Professional Arts Bldg (B4)
P18 Psychology Bldg (C4)
P19 Public Safety (B5)

R

R1 Rehabilitation Education Ctr (D1)
R2 Research Park (G2)
R3 Richmond Studio (A5)
R4 Roger Adams Lab (C5)

S

S1 Seitz Materials Rsch Lab (B5)
S2 Siebel Ctr for Computer Sci (B5)
Small Animal Clinic—see V5
Small Homes Council—see B8
S3 Smith Hall (D4)
S4 Social Work, School of (D5)
S5 Special Materials Storage Fclty (H1)*
S6 Speech & Hearing Clinic (C4)
S7 Spurlock Museum (C6)
S8 State Regional Ofc Bldg (H2)*
S9 Stock Pavilion (E4)
Student Services—see A22 or T9
S10 Structural Warehouse (B5)
S11 Superconductivity Ctr (B5)
S12 Survey Rsch Lab (C4)
S13 Surveying Bldg (D4)
S14 Swanlund Admin Bldg (C4)

T

T1 Taft House (E5)
T2 Talbot Lab (B4)
T3 Technology Commercialization Bldg (G4)
T4 Temple Hoyne Buell Hall (E4)
T5 Track & Soccer Stadium (F4)
T6 Transportation Bldg (B5)
T7 Turner Hall (E5)
T8 Turner Hall Greenhouses (E5)
T9 Turner Student Services Bldg (C4)

U

U1 Ubben Basketball Facility (F3)
U2 Undergraduate Library (D4)
U3 University High School (B5)
U4 University High School Gym (B5)
U5 University Press Bldg (E1)
Urban & Regional Planning—see T4
University Inn —see P14

V

V1 Vegetable Crops Bldg (D5)
V2 Vet Med Basic Sciences Bldg (G5)
V3 Vet Med Feed Storage Bldg (G5)
V4 Vet Med Surgery & Obstetrics Lab (G5)
V5 Vet Teaching Hospital (G5)
Visitor's Center—see L5
V6 Vivarium, Shelford (B4)
V7 Volatile Storage Bldg (E1)

W

W1 Waste Mgt Rsch Ctr (H1)*
W2 Water Survey Rsch Ctr (I2)*
W3 Women's Studies (C4)
W4 Wood Engineering Lab (E5)
W5 Wohlers Hall (D4)

UNIVERSITY RESIDENCE HALLS

Undergraduate Halls

Champaign Residence Halls
BR Barton (D3)
FR Forbes (D2)
GR Garner (D3)
HP Hopkins (E2)
IR Ikenberry (D3)
LN Lundgren (D3)
SC Scott (E2)
SN Snyder (E3)
TF Taft (E3)
VD Van Doren (E3)
WS Weston (D3)

Urbana North Residence Halls
AL Allen (D6)
BS Busey (D5)
EV Evans (D5)
LA Lincoln Ave (Shelden-Leonard) (D6)
Illinois Street
TW Townsend (C6)
WR Wardall (C5)

Urbana South Residence Halls
Pennsylvania Avenue
BB Babcock (E6)
BL Blaisdell (E6)
CR Carr (E6)
SD Saunders (E6)
Florida Avenue
OG Oglesby (E6)
TR Trelease (E6)

Graduate Halls

DN Daniels (B5)
SM Sherman (C3)

Family Housing

GG Goodwin/Green Apts (C5)
OD Orchard Downs Apts (East of F6)

Private Certified Housing

1P Armory House (D3)
2P Bromley Hall (C3)
4P Brown House on Coler (C6)
5P Christian Campus House (C6)
6P Europa House (C6)
7P Hendrick House (B6)
8P Illini Tower (D3)
9P Koinonia (C3)
11P Nevada House (D6)
12P Newman Hall (D4)
14P Presby House (C3)
15P Stratford House (C3)
16P University YMCA (D4)
17P Nabor House (D6)
18P Evans Scholars (D3)
19P Orthodox Christian Center (C2)
20P 312 House (C3)

8.5 x 11 legend prepared by Creative Services. Revised 9/09.

Theoretical and Computational Biophysics Group
20th Anniversary Symposium

Computational Biology of the Cell
The Next Decade

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image: model of the bacterial ribosome obtained by cryo-EM and MDFF

Beckman Institute, Rm 1025, Urbana, IL, 61802
University at Illinois at Urbana-Champaign
contact: Nancy Borngasser 217-244-8949 <nlborn@ks.uiuc.edu>