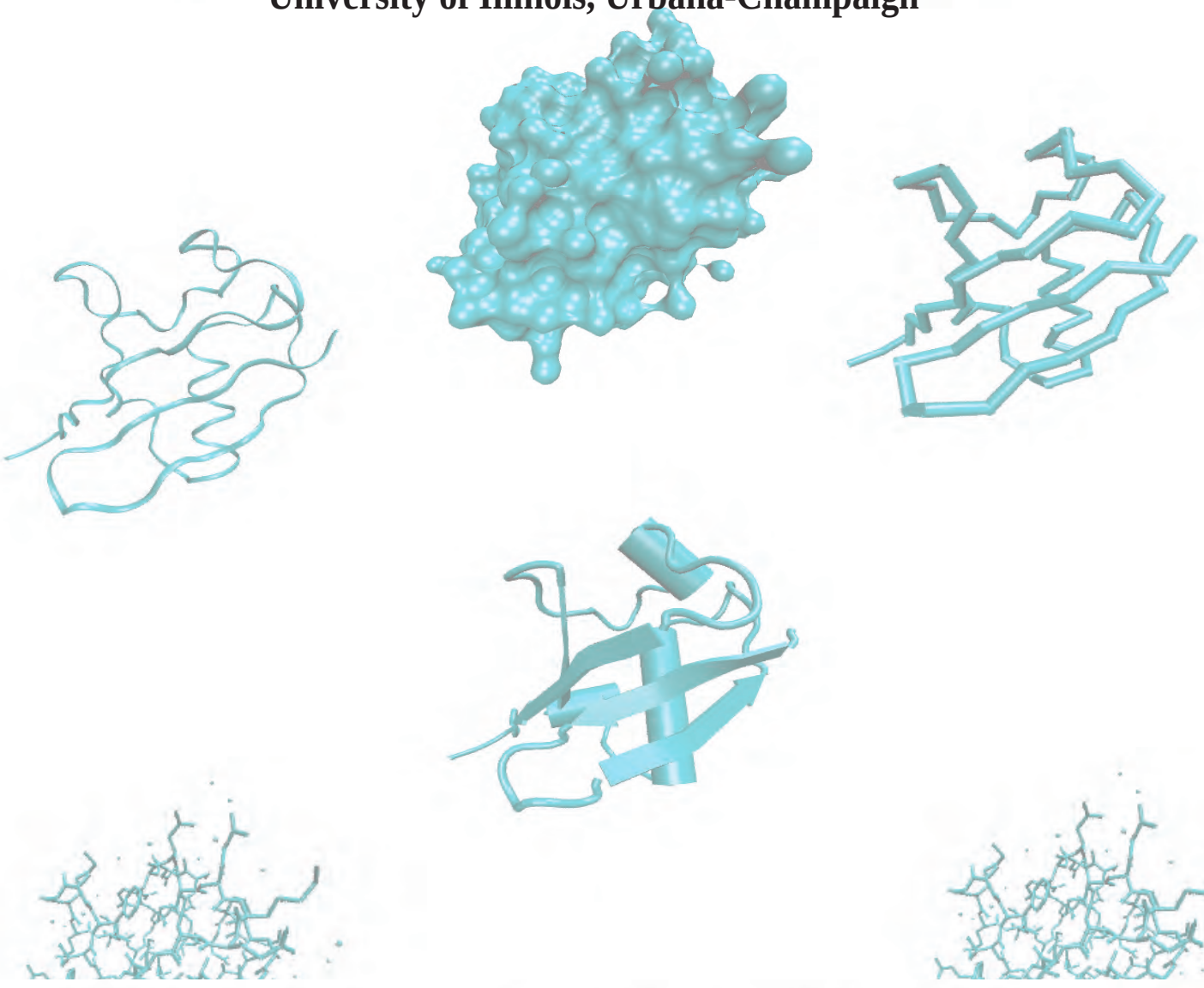
Summer School on Theoretical and Computational Biophysics

Theoretical and Computational Biophysics Group
University of Illinois, Urbana-Champaign



University of Illinois at Urbana-Champaign | Beckman Institute for Advanced Science and Technology

Theoretical and Computational Biophysics School

NIH Resource for Macromolecular Modeling and Bioinformatics

Modeling the molecular processes of biological cells is a craft and an art. Techniques like theoretical and computational skills can be learnt by training, but meaningful applications are achieved only with experience and sensitivity. A summer school in Theoretical and Computational Biophysics attempted to teach both the craft and art of modeling through learning by doing: nearly a hundred participants from all over the world came for two weeks to the Beckman Institute in Illinois to stretch proteins, pull water through molecular channels, mine genomic data, build their own computer cluster, and study their favorate biomolecules. After lectures and discussions in the morning, afternoon and evening were devoted to learning by doing, assisted through 300 pages of tutorials, in computer laboratories humming with computational biology software, e.g., VMD, NAMD, and GAMESS, and linked to NCSA's fast pentium machines. The school, funded by NSF and NIH, lasted two weeks, but will go on much longer: all school materials remain available on the web; participants will use BioCoRE to stay in touch and continue the scholarship and friendship experienced in Illinois.

Contents

Program

Locations
Morning lectures: Beckman Institute Auditorium
Coffee breaks: 1003 Beckman Institute
Afternoon and evening computer labs:
252 Everitt Lab / 406B1 Engineering Hall

Handouts
Running Simulations During the Afternoon Hands-on Sessions
Four Ways to Run NAMD at SS03

Mon, 6/2: *Introduction to Protein Structure and Dynamics (K. Schulten)*
07:30-12:00 Registration
08:30-09:00 Welcome, Opening Remarks, and Overview
09:00-10:00 Molecular Graphics Perspective of Protein Structure and Function
10:00-11:00 Molecular Dynamics Method (J. Phillips and J. Gullingsrud)
Coffee Break
11:30-12:30 Equilibrium Properties of Proteins
12:30-12:45 Daily Q & A
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
13:45-14:30 Overview of Technical Resources (T. Skirvin, K. Vandivort, R. Brunner)
[Beckman Institute Auditorium]
14:30-15:30 Hands-on -- Molecular Graphics Tutorial 1 (E. Villa, F. Khalili)
15:45-17:00 Hands-on -- Molecular Graphics Tutorial 2 (E. Villa, F. Khalili)
19:00-21:00 Free Session -- Model Your Own System (E. Villa, J. Gullingsrud, M. Sotomayor, M. Dittrich)

Tue, 6/3: *Statistical Mechanics of Proteins (I. Kosztin)*
09:00-11:00 Registration
09:00-10:00 Equilibrium and Nonequilibrium Properties of Proteins
10:00-11:00 Coherent Motion in Proteins: Temperature Echoes
Coffee Break
11:30-12:30 Simulated Cooling of Proteins
12:30-12:45 Daily Q & A
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- Molecular Dynamics Tutorial 1 (A. Aksimentiev, D. Lu)
15:45-17:00 Hands-on -- Molecular Dynamics Tutorial 2 (A. Aksimentiev, D. Lu)
18:00-20:00 Banquet [Beckman Institute Atrium] (closed event; nametags required)

Wed, 6/4: Steered Molecular Dynamics of Proteins (K. Schulten)
09:00-10:00 Introduction and Examples
10:00-11:00 Mechanical Proteins
Coffee Break
11:30-12:30 Determining Potentials
12:30-12:45 Daily Q & A
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- Molecular Dynamics Tutorial 3 (S. Park, M. Gao)
15:45-17:00 Hands-on -- Stretching Deca-Alanine (S. Park, M. Gao)
19:00-21:00 Free Session -- Model Your Own System (A. Aksimentiev, J. DeSouza, B. Isralewitz, J. Cohen)

Thu, 6/5: Simulating Membrane Channels (E. Tajkhorshid)
09:00-10:00 Introduction and Examples
10:00-11:00 Transport in Aquaporins
Coffee Break
11:30-12:30 Nanotubes
12:30-12:45 Daily Q & A
12:45 Summer School Photo
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- Water Channel 1 (F. Zhu, J. Cohen)
15:45-17:00 Hands-on -- Water Channel 2 (F. Zhu, J. Cohen)
17:30-19:00 Demonstration of Aquaporin channel and Haptic Device IMD (3 demos) [3151 BI]
19:00-21:00 Free Session -- Model Your Own System (D. Lu, F. Zhu)

Fri, 6/6: Quantum Chemistry of Proteins (T. Martinez)
09:00-10:00 Introduction and Examples
10:00-11:00 Ab Initio and Semiempirical Quantum Chemistry
Coffee Break
11:30-12:30 QM/MM Methods and Direct Dynamics
12:30-12:45 Daily Q & A
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- Introduction to QM Simulations (html, pdf) (M. Dittrich, S. Olsen)
15:45-17:00 Hands-on -- Computational Determination of Proton Affinities (M. Dittrich, S. Olsen)
19:00-21:00 Free Session -- Model Your Own System (C. Kanchanawarin, M. Gao)

Sat, 6/7
Bus Trip to Chicago (Optional, Not Funded by School, Sign up Early)

Sun, 6/8
14:00-21:00 Free Session -- Model Your Own System

Mon, 6/9: Parameters for Classical Force Fields (Z. Schulten)
09:00-10:00 Introduction and Examples
10:00-11:00 Introduction to Classical Force Fields
Coffee Break
11:30-12:30 Methods of Parameterization
12:30-12:45 Daily Q & A
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- System Setup of HisH with the Molecular Modeling Package Moe
(R. Amaro, F. Autenrieth, R. Braun)
15:45-17:00 Hands-on -- Semiempirical Parameter Generation with Spartan
(R. Amaro, F. Autenrieth, R. Braun)
17:30-19:00 Demonstration of Aquaporin channel and Haptic Device IMD (3 demos) [3151 BI]
19:00-21:00 Free Session - Model Your Own System (G. Zheng, S. Kumar)

Tue, 6/10: Bioinformatics of Proteins (Z. Schulten)
09:00-10:00 Protein Structure Prediction and Function
10:00-11:00 Sequence and Structure Alignment Algorithms
Coffee Break
11:30-12:30 Sequence and Structural Analysis Tools on the Web
12:30-12:45 Daily Q & A
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- Bioinformatics Introduction on Class II tRNA Synthetases
(F. Autenrieth, B. Isralewitz, T. Pogorelov)
15:45-17:00 Hands-on -- Sequence and Structural Alignment Methods
(F. Autenrieth, B. Isralewitz, T. Pogorelov)
19:00-21:00 Free Session -- Model Your Own System (D. Hardy, F. Khalili)

Wed, 6/11: Simulation of Lipids (M. Klein); Parallel Computing (L. Kale)
08:55-09:00 Entries for Beauty Contest are due
09:00-10:00 Atomic Level Simulation of Membranes (M. Klein)
10:00-11:00 Coarse Grained Modeling of Lipid Phases (M. Klein)
Coffee Break
11:30-12:30 Introduction to Parallel Computing Issues (L. Kale)
12:30-12:45 Daily Q & A
12:45-12:50 Announcement of Beauty Contest Finalists
Lunch Break (12:50-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- Case Studies in Effective Parallelization of MD Simulations (L. Kale)
15:45-16:30 Optional - Introductory Lessons on Cluster Building ; Choose-up for Section 1, 2, or 3
(T. Skirvin, J. Stone, J. Phillips)
16:30-18:30 Optional - Hands-on -- Build Your Own Cluster 1 (T. Skirvin, J. Stone, J. Phillips) (5602 BI)
19:00-21:00 Free Session -- Model Your Own System (R. Braun, D. Brandon)

Thu, 6/12: Numerical Algorithms (T. Schlick, R. Skeel)
09:00-10:00 Force Evaluation, Integrators, and Propagators (Slides, Notes) (R. Skeel)
10:00-11:00 Optimization Techniques (T. Schlick)
Coffee Break
11:30-12:30 Monte Carlo Methods (T. Schlick)
12:30-12:45 Feedback Forms
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
14:30-15:30 Hands-on -- Numerical Laboratory (D. Hardy, R. Engle, J. Marriott, W. Wang)
15:30-17:30 Optional - Hands-on -- Build Your Own Cluster 2 (T. Skirvin, J. Stone, J. Phillips) (5602 BI)
17:30-19:30 Optional - Hands-on -- Build Your Own Cluster 3 (T. Skirvin, J. Stone, J. Phillips) (5602 BI)
15:30-17:00 NCSA Cave Tours (6 Tours) [3510 BI]
19:30-21:00 Beauty Contest [Beckman Institute Auditorium]
The certificate of the summer school will be handed out.

Fri, 6/13: Modeling Large Systems (K. Schulten)
09:00-10:00 Molecular Machines of the Living Cell
10:00-11:00 Light Harvesting in Photosynthesis
Coffee Break
11:30-12:00 ATP Synthase
12:00-12:15 Daily Q & A
12:15-12:45 Concluding Remarks
Lunch Break (12:45-13:30 Staff Meeting, 3169 BI)
13:00-14:30 NCSA Cave Tours (6 Tours) [3510 BI]
14:30-15:30 Hands-on -- Excitation Transfer (M. Sener, C. Kanchanawarin)
15:45-17:00 Hands-on -- Electron Transfer (M. Sener, C. Kanchanawarin)

Summer School Instructors

* L. Kale (UIUC)
* M. Klein (U. Penn)
* I. Kosztin (U. Missouri)
* T. Martinez (UIUC)
* T. Schlick (NYU)
* K. Schulten (UIUC)
* Z. Schulten (UIUC)
* R. Skeel (UIUC)
* E. Tajkhorshid (UIUC)

Participants

Sandeep Agnihotri	USA	Graduate Student	University of Illinois at Urbana Champaign Civil and Environmental Engineering
Ni Ai	USA	Graduate Student	University of Medicine & Dentistry of New Jersey Pharmacology
Karunesh Arora	USA	Graduate Student	New York University Chemistry
Walter Ash	Canada	Graduate Student	University of Calgary Biological Sciences
Ryan Bannen	USA	Graduate Student	University Wisconsin-Madison Biochemistry
Tj Brunette	USA	Graduate Student	UMass Amherst Computer Science Dept.
Don Burgess	USA	Associate Professor	Asbury College Chemistry and Physics
Richard Kramer Campen	USA	Graduate Student	Pennsylvania State University Geosciences
Pinaki Chakraborty	USA	Graduate Student	University of Illinois at Urbana-Champaign Theoretical and Applied Mechanics
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Eileen Faucher	USA	Graduate Student	University of Washington chemistry
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Kaden Hazzard	USA	Undergraduate	The Ohio State University Physics
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Jacob Sonne	Denmark	Graduate Student	Technical University of Denmark Department of Chemistry
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Scott Stagg	USA	PostDoc	Georgia Institute of Technology Biology
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Ioannis Tziligakis	USA	Graduate Student	University of Illinois Physics
Ana Vila Verde	Portugal	Graduate Student	University of Minho Physics

Jean-Marc Vuissoz	Switzerland	Research Scientist	university hospital of Bern Bern, Switzerland clinic of pediatry
Amy Waligorski	USA	Graduate Student	Duquesne University Chemistry and Biochemistry
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Xiaofei Wang	USA	Graduate Student	Princeton University Chemistry
Yanli Wang	USA	Graduate Student	University of Toledo Chemistry
Christopher Wassman	USA	Graduate Student	UC Irvine Information and Computer Science / Informatics in Biology and Medicine
Norbert Welsch	Germany	Graduate Student	Eberhard Karls Universit√§t T√ºbingen Germany Institut f√ºr Organische Chemie
Kirk Williams	USA	Graduate Student	Tulane University Molecular and Cellular Biology
Miriam Wodrich	USA	Graduate Student	University of York Biology
Guosheng Wu	USA	PostDoc	Eli Lilly and Company Computational Chemistry
Jiancong Xu	USA	Graduate Student	University of Utah Department of Chemistry (Henry Eyring Center for Theoretical Chemistry)
Deqiang (David) Zhang	USA	PostDoc	UCSD Chem & Biochem 0365
Jieru Zheng	USA	Graduate Student	Duke University Chemistry Department

Lectures

* 6/2: Introduction to Protein Structure and Dynamics (K. Schulten)
* Welcome, Opening Remarks, and Overview
* Molecular Graphics Perspective of Protein Structure and Function
* Molecular Dynamics Methods (Part 1)
* Molecular Dynamics Methods (Part 2)
* Equilibrium Properties of Proteins

* 6/3: Statistical Mechanics of Proteins (I. Kosztin)
* Equilibrium and Nonequilibrium Properties of Proteins
* Coherent Motion in Proteins: Temperature Echoes
* Simulated Cooling of Proteins

* 6/4: Steered Molecular Dynamics of Proteins (K. Schulten)
* Introduction and Examples
* Mechanical Proteins
* Determining Potentials

* 6/5: Simulating Membrane Channels (E. Tajkhorshid)
* Introduction and Examples
* Transport in Aquaporins
* Nanotubes

* 6/6: Quantum Chemistry of Proteins (T. Martinez)
* Introduction and Examples
* Ab Initio and Semiempirical Quantum Chemistry
* QM/MM Methods and Direct Dynamics

* 6/9: Parameters for Classical Force Fields (Z. Schulten)
* Introduction and Examples
* Introduction to Classical Force Fields
* Methods of Parameterization

* 6/10: Bioinformatics of Proteins (Z. Schulten)
* Protein Structure Prediction and Function
* Sequence and Structure Alignment Algorithms
* Sequence and Structural Analysis Tools on the Web

* 6/11: Simulation of Lipids (M. Klein); Parallel Computing (L. Kale)
* Atomic Level Simulation of Membranes
* Coarse Grained Modeling of Lipid Phases
* Introduction to Parallel Computing Issues
* Cluster Building

* 6/12: Numerical Algorithms (T. Schlick, R. Skeel)
* Force Evaluation, Integrators, and Propagators
* Optimization Techniques (Homework 1: Biphenyl Minimization)
* Monte Carlo Methods (Homework 2: Global Optimization)

* 6/13: Modeling Large Systems (K. Schulten)
* Molecular Machines of the Living Cell
* Light Harvesting in Photosynthesis
* ATP Synthase

Tutorials

* Mon, 6/2: Introduction to Protein Structure and Dynamics
* Molecular Graphics Tutorial - An introduction to VMD and its capabilities
* input files

* Tue, 6/3: Statistical Mechanics of Proteins
* Molecular Dynamics Tutorial - An introduction to NAMD and its capabilities
* input files

* Wed, 6/4: Steered Molecular Dynamics of Proteins
* Stretching Deca-Alanine Tutorial - An introduction to IMD and SMD simulations with VMD and NAMD
* input files

* Thu, 6/5: Simulating Membrane Channels
* Water Channel Tutorial - A tutorial simulating water diffusion and permeation through nanotubes
* input files

* Fri, 6/6: Quantum Chemistry of Proteins
* Introduction to Quantum Mechanics Simulations - An introduction to quantum mechanical (QM) simulation
* input files

* Mon, 6/9: Parameters for Classical Force Fields
* Determining Force Fields - Tutorial on determining new force field parameters to describe novel system components of a new molecule
* input files

* Tue, 6/10: Bioinformatics of Proteins
* Bioinformatics - Tutorial on using Bioinformatics to classify protein domains and align determined protein domains structurally
* input files

* Wed, 6/11: Simulation of Lipids; Parallel Computing
* Parallel Computing - Tutorial on Parallelizing MD Simulations
* charm input files
* logs input files
* NAMD2 input files

* Thu, 6/12: Numerical Algorithms
* Numerical Laboratory - A tutorial on numerical algorithms
* Cluster Building Tutorial - Tutorial on building your own computer cluster

* Fri, 6/13: Modeling Large Systems
* Excitation and Electron Transfer
* input files

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Monday, June 2 -- Ana Verde

I arrived in Urbana at 7 pm on Sunday (after being up for 24 hours straight), so I felt pretty tired on Monday. I was late for the first talk, because I thought that it began at 9am and not 8:30am. I thought it hadn't been a very good idea to start earlier on the first day, given that people would be more tired, but I also thought that the really tired ones (like me) wouldn't miss a lot by cutting the first class.

I liked the introduction about the potential of VMD, particularly the emphasis on "One can see many things just by looking", with which I agree entirely. I would have liked the speaker to have provided a definition of terms like "residue", "betastrand" and similar ones that I am unfamiliar with, not working with proteins. I managed to understand their significance as the lecture went on and as the speaker illustrated what he was saying with VMD images of proteins.

I thought the introduction to MD simulations was also very good. I didn't know anything about it and it provided clear information on the spatial and temporal scales accessible to MD, as well as more specific information regarding "tools" available in NAMD, like solvation.

The hands-on molecular graphics tutorial was a bit long so I couldn't finish it, but was very clear and easy to follow, and provided valuable information that we used in subsequent tutorials.

I thought the lectures were clear, and I was particularly happy about that, not being a native English speaker. There were some speakers in other days that spoke too fast and/or did not worry about being articulate. They don't remember that people who do not live in English speaking countries will have problems understanding them.

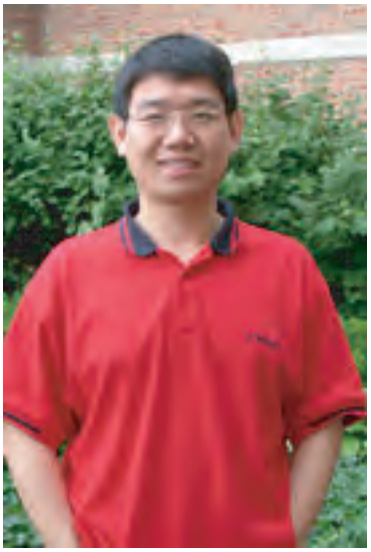
"The high point of this day was seeing how the speakers and the tutors at the hands-on sessions were willing to help us with everything. I felt that I would actually learn to do things and not just learn that they existed."

At the end of the day, I felt like I was drowning in information, but it's always like this in these schools, so I wasn't very worried.

The high point of this day was seeing how the speakers and the tutors at the hands-on sessions were willing to help us with everything. I felt that I would actually learn to do things and not just learn that they existed.

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Tuesday, June 3 -- Han Liang



Today I am quite excited because I am going to learn molecular dynamics, which is the core of this summer school. After learning about the great power of VMD yesterday, I really look forward to using NAMD today.

The lectures in the morning give us several vivid examples how molecular dynamics can help us to think and get quantitative results. During the lectures, many ideas just come into my mind: ha, maybe I can do this! The same calculations can be applied to my protein. That is cool!

The hands-on session is really fantastic! Following the tutorials, a system is easily set up. Although many details are still not fully understood, I can really sit down and play with MD! Before I came to Urbana, I really worried about whether I can learn MD in such a short time, especially being a newcomer. Now I feel much more confident and have so much motivation to do something.

"Now I feel much more confident and have so much motivation to do something."

At night, there is a great banquet! Another good point about the summer school is to see many many new faces and make many many friends. And Prof. Schulten gave very wise open remarks. I love some sentences and record them here: "The most important thing in science is to have fun! The number is not absolute; more important is to use one's brain to make sense of the numbers. When we do computational biology at least we don't kill anybody!" I will surely remember them in the rest of my life. This is really a wonderful day! Thank all your guys!

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Wednesday, June 4 -- Elif Ozkirimli

Today we went over steered molecular dynamics, in which I am very interested since I'm using a similar method to study my system. I was especially happy to learn more about how AFM works and about the comparison of forces in AFM and SMD; sometimes I need to be reminded that most of this computational work is motivated by experiments. The section on Jarzynski and umbrella sampling was exciting and new stuff, I should definitely read the paper.

The sun came out from behind the clouds for the first time since the summer school started and we had a very nice picnic lunch on the Quad; UIUC is pretty and lively after all!!

"UIUC is pretty and lively after all!"

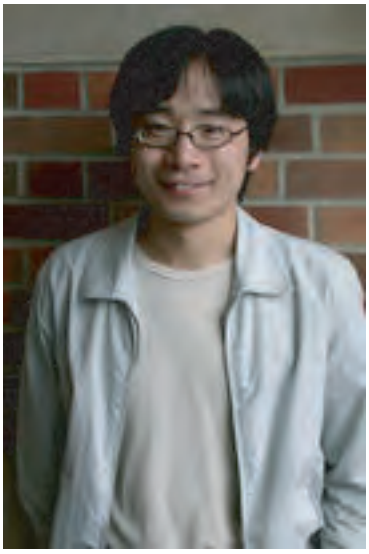
I was very excited about the IMD hands on session. SMD really works! Learning how to calculate the PMF was very useful, but I didn't have a lot of time to think about what I was doing while I was doing it. It would be very good if there were a few more questions to make us think through the process rather than just follow the directions. The questions that were there were pretty beneficial, though.

After a nice coffee and dessert break, we went to the evening session and worked some more. These evening sessions are very useful for me. They also give me a chance to check my jobs that are running back home. Then, the usual: going out with friends and enjoying the fun Champaign night life.

I really enjoyed all of my time here and learned many things not only from the lectures and hands-on sessions but also from all the other people. Thank you summer school team, you did a fabulous job.

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Thursday, June 5 -- Zhanwu Liu



Today Dr Emad Tajkhorshid gave lectures on the simulation of membrane protein. Membrane proteins are very important because many biological functions are performed at the membrane, but currently the knowledge of membrane proteins is rather limited. In the first lecture Emad introduced different types of membrane proteins, mainly different kind of channels. The second lecture focused on the real example of SMD simulation using the water channel AQP0, a wonderful work published in Science last year. Several important points for simulating a system were mentioned: One should be very familiar with the system. Not only should one examine the structure, but one should also check the literature and get new experimental information. He then introduced and compared strategies currently used for preparing lipid membrane systems, and answered how much one can learn from simulations.

"The stereo view creates an astonishing effect: I feel like I've become a small water molecule swimming in the protein."

In the AQP0 study, SMD was used to study the free energy change during transport. The analysis is based on the Jarzynski equation, in which the free energy change can be calculated from non-equilibrium processes. After a nice coffee and dessert break, we went to the evening session and worked some more. These evening sessions are very useful for me. They also give me a chance to check my jobs that are running back home. Then, the usual: going out with friends and enjoying the fun Champaign night life.

There is lot of fun in the research. In the movie shown in the lecture, it was very impressive to see the water molecules permeate through the channel in single file, with the orientation tuned to prevent proton transport. The third lecture and the afternoon hands-on session used nanotubes as a model for the channel. Nanotechnology is a hot topic, but I always thought it would be irrelevant for biological systems. It is surprising to see water molecules penetrating into the hydrophobic carbon nanotube. Now I believe nanotubes can be good models for biological systems. In the afternoon, we tried SMD using haptic devices. The stereo view creates an astonishing effect: I feel like I become a small water molecule swimming in the protein. The feedback haptic device gives the direct feeling of the force acting on the molecule; the device is very helpful to understanding details of simulations and constructing better systems to simulate.

In summary, this was a wonderful day. I learnt a lot of science and experienced a lot of fun. Nature is always beautiful at every level of magnification that I can really enjoy!

Friday, June 6 -- David Zhang

It has been a very fruitful week so far, and today's lecture was the last of the week. Prof. Todd Martinez gave lectures on QM/MM methods. Not surprisingly, many participants were not very interested in the lectures. I wasn't expecting much anyway. To be fair, I think Prof. Martinez did a good job in summarizing the different methods in QM. He was humorous and I laughed loud when he said "Chemists are the Fourier transform of Physicists."

I was again amazed by the devotion of the summer school organizers. Professor Klaus Schulten has been sitting on almost all the lectures. He didn't hesitate to stop the lecture to let us ask questions. When the first lecture ran late, he suggested us to have an early coffee break. Many of his group members were also present in the lecture room.

"I was again amazed by the devotion of the summer school organizers. Professor Schulten... didn't hesitate to stop the lecture to let us ask questions."

The weather wasn't very good. It was actually pretty clear in the morning when I left Hendrick House. But it started raining half way through the lectures, and was still raining heavily at lunch time. My plan was to go to the Thai restaurant to taste their beef shrimp noodle. Unfortunately I did not bring my umbrella (I later brought my umbrella in many days that wasn't raining). I waited in hope the rain would stop, but ended up skipping my lunch.

The rain did not stop when it was time for the afternoon hands-on session. We had to run over to the lab in the rain. The materials for the afternoon session wasn't about QM/MM at all. It would be nice if we could do some real QM/MM stuff. I guess it isn't trivial to prepare materials for such a practice, especially QM/MM itself is not a matured method. Still, I find the tutorial quite helpful. I have always used Antechamber in Amber to set up new systems. It is nice to learn how to do it in Charmm format. The tutorial provided most of the components of the topology file, and we only needed to fill out some missing parameters.

Dinner time I went to visit an old friend of mine here. He is an assistant professor, and he started his group three years ago. We had a long chat about almost everything from research to life. He gave me a tour of his lab. It seemed that he has already has a well established lab with lots of space.

By the end of the tour I found I was late for the evening session. My stomach complained strongly when I tried to head back to the computer lab. Instead, I headed to the Thai restaurant to taste the shrimp noodle. By the time I was back to the lab, I was 40 minutes late. All the doors to the Engineering Lab and Everitt Lab were locked, and I couldn't get in. I had to wait outside and finally I saw someone passing by. Out of desperation I asked if he had access to the building. Thank God, he let me in.

At the evening session I spent some time on finishing the tutorials. I then chatted with others in BioCoRE. Tomorrow some of us are going to Chicago, and we were very excited about it. The lab attendants were very helpful and let us stay for an extra half hour. Thanks, guys.

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Monday, June 9 -- Craig Jolley

By Monday morning everyone had returned from their weekend diversions safe and sound and we were ready to launch into a fresh new day in the world of computational biophysics

I'll have to admit that, as a newcomer to the field, the morning lectures were a little hard for me to follow -- the lectures during the second week of the summer school were generally more technical and advanced than those in the first week. The biggest things that I took away from the morning's lectures were a general "lay of the land" for empirical force field, and a deepened sense of how complicated this sort of research really is. After the first few days of the summer school, I had the impression that MD was going to be relatively easy -- just a matter of using the right software. Monday's lectures were the beginning of a new understanding of the level of creativity and finesse involved in MD.

During the mid-morning coffee break, I had a chance to speak with a post-doc at UIUC who works with systems similar to the one that I am studying. Possibly the most valuable thing about the summer school (for me) has been the opportunity to talk to more seasoned graduate students and post-docs who have provided me with a wealth of advice and ideas, at a more basic level than what I heard in the lectures.

"My own research has seen a lot of progress... primarily during the evening free sessions and informal conversations with other summer school students."

The weather was absolutely beautiful (a rare treat), so I digested the lectures while picnicking on one of the campus lawns with other summer school students.

The afternoon hands-on session dovetailed quite nicely with the morning lectures. I did struggle a bit, however, to really understand what I was doing -- the tutorial was so detailed and smooth that it allowed us to complete the exercise without fully understanding its conceptual foundations. It did succeed, however, in providing me with an impression of what tools are available and with a limited impression of how they are used.

The free session in the evening was especially productive; one of the computer lab TA's guided me in the use of VMD's "membrane" script to create a lipid

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Tuesday, June 10 -- Kirk Williams

It was a capstone of a beautiful two weeks. Officially it was an unofficial social gathering of 11 scientist to discuss our daily journals. Our journals would cover events over the course of two weeks. Rosemary, a senior graduate student in Dr. Schulten's group, explained to us how the summer school came about, how it worked, who are the major planners, and what was going on during each of the daily tutorials. It was made straight forward and simple, tell us some information about that you think the program did for you. With my objective in hand, my mission was clear: write, express, discuss, and report our thoughts of the day's activities.

Today's lecture, from Dr. Zan Schulten, focused on Bioinformatics of Proteins: Protein Structure Prediction and Function, Sequence and Structure Alignment Algorithms, and Sequence-Structure Analysis Tools on the Web. I had a Bioinformatics class, but evidently some of the things discussed there did not cover the topics that Zan focused on here. The lecture was great. I was able to fill in the gaps in my knowledge that I did not know existed and I was about to learn more about the Blosum Substitution Matrix, Structural Alignments and Hidden Markov Models (HMM). The daily question and answer period gave me a clearer understanding of the Smith-Waterman sequence-sequence alignment. I still can not see the difference between it and Needleman-Wunsch's matrix, but maybe I will catch the difference sometime soon. Although I heard of the topics before, it was unclear how Tracebacks worked and how Gap Penalties actually hurt your scoring and alignments. Overall, today's lectures were very informative, and it cleared up some misconceptions in my knowledge.

"I was able to complete the tutorial, understand my results, and begin to ask questions of my own research based on what was taught thus far."

The afternoon hands-on session was excellent. I was able to complete the tutorial, understand my results, and begin to ask questions of my own research based on what was taught thus far. From talking with others, they, like myself, have seen ways to incorporate and adapt VMD and NAMD to their research projects.

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Wednesday, June 11 -- Walter Ash

The day started rather typically - a faint glimmer of consciousness struggling to peel away layers of groggy sleep, motivated only by some vague sense that somewhere there might exist a ceramic object filled with bitter stimulant alkaloids in hot water...

Several minutes later, I (at this point a functional human being, thanks to the previously alluded to cup of coffee) arrived at the Beckman Institute building and took a seat in the shiny modern lecture theater. Today's agenda included a talk on lipid simulations by M. Klein (U. Penn), and an introduction to parallel scientific computing by L.V. Kale (UIUC).

"bitter stimulant alkaloids in hot water..."

The first presentation by M. Klein provided an introduction to biomembranes and lipids, including their relevance and methods used to study them at an atomistic level. A brief overview of biomembrane structure was presented, followed by a discussion of experiments used to characterize membranes and a comparison to theoretical treatments, which usually include only a very finite fraction of the complex systems (such as liposomes or oriented bilayers) studied by techniques such as NMR spectroscopy. A few case studies were presented, along with a description of some of the serious challenges still faced by scientists who model these systems.

The second lecture by M. Klein discussed coarse grained approaches to modeling biological membranes. These models, though lacking atomic detail, provide some qualitative insight into the behavior of phospholipids and other molecules interacting with membranes on time scales beyond those that are practical for atomic detail simulations. Several interesting studies on the self-assembly of phospholipid complexes (bilayers, monolayers, vesicles, etc), the behavior of water channel mimetics, and amphipathic bacteriocidal peptides were overviewed.

At this point, we headed out for our daily ration of coffee and doughnuts and (with the Beckman Institute's private garden as a pleasant backdrop) some reflection and discussion of the lecture material.

After coffee break, L.V. Kale gave a broad overview of parallel computing, followed by some case studies. Some of the challenges involved in setting up useful parallel computing platforms and designing efficient algorithms were discussed, with particular attention to problems that may arise, and some methods to overcome them. After a pleasant lunch break (tuna salad sandwich on rye) we performed some scalability tests on multiple processors using a mechanosensitive ion channel system (MscL) on the NCSA supercomputer. Finally we reconvened in the lecture hall for an overview of building inexpensive 'in-house' Linux clusters, and an opportunity to sign up for a 'hands-on' cluster building tutorial.

And after all of this, there was still plenty of time to walk to downtown Champaign for a coffee and a visit to the used bookstores and record shops.

Thursday, June 12 -- Shantenu Jha

"NAMD: Not (just) Another Meaningless Day!"

For those too lazy to read on, the summary: An action packed day, with three lectures (two lecturers today- Robert Skeel & Tamar Schlick), a hands on session, Cluster Building Sessions, Cave tours and the grandest event of them all- "The Beauty Contest"!

And now for those with nothing better to do, the details: The day began like most other days with lectures, and the suspense of when Tim would have the 'tickets to the nice lab' up for grabs (and you'll be surprised how literally the term 'grabs' should be taken!). [Personal note from the author: Creationists may loose faith, if they had the chance to observe how close we humans (or at least SS03 participants) can be to monkeys under the pressure of limited resources, i.e., tickets to the "nice" computers].

I'll refrain from discussing how the lectures were perceived as the SS03 organizers probably already have statistically more significant insight from the surveys.

Klaus's insightful suggestion to SS03 participants to not steal the four copies of Tamar Schlick's book, resulted in most people using Tamar Schlick in person to clear their doubts and not resorting to illicit version(s) of Tamar Schlick in print! Consequently Q&A session and particularly the coffee break seemed to generate more than normal activity around the last speaker (TS). Further circumstantial evidence in support of the above hypothesis was the greater intensity required in Melih Sener's break-breaking braying to produce the desired effect.

The last of the morning events was the General Q&A, when SS03 organizers would gather en masse to collectively dodge questions from the participants! On a less facetious note, the general Q&A session was as always very useful. Lunch time and people's intellectual apetite gave way to real apetite. However SS Organizing team had to wait that just little longer, for one could see them dutifully heading of for their penultimate staff meeting (yupee!). [Thanks you folks once again for all the hard work. BTW, what happens to all the unusued SU's on NCSA?]

Participants diverged for different activities in the afternoon. I for one didn't get the time to go for the hands-on sesssion getting ready for the evening's presentation. Some folks had a cluster building session, some a cave tour and a select few had both. People converged around 7-ish for the evening's event.

One could write pages on the evening's event, but as they say a picture is world a thousand words, (with the often skipped fineprint: only if accompanied by a few meaningul words), so I'll refer you to the photos. But in short, it was a creative, well organized, fun, easy-going evening, with what I thought also included some good science too (in spite of Elizabeth's drilling the finalists that the good science was optional), reinforcing the general impression that the Schulten group works hard and plays hard too! [Way to go folks!] We also got to know how Klaus likes to describe his German accent! [for those who missed it and didn't skip their elementary trignometry course, the answer is: 1/Cos(C)]. I'm sure those present and who haven't been permanently brain-damaged by Barry's 'awful' witticism, it was a great time. [BTW: what happened to the original prizes- the four signed books?]. Thanks to Marcos and Tim too for the evening's effort.

It should be mentioned, though not in passing, that the evening really took off after the contest. I counted at least 40 people assosciated with SS03 at the "Cowboy Monkey". I guess the details of the brazen bacchanalia are best left out...

Diary of the 2003 Summer School on Theoretical and Computational Biophysics

Friday, June 13 -- Kramer Campen

Every now and then (more often and I think it's a bit physiologically dangerous) you (you in this context meaning only me) like to go to lectures of material which starts in a place you know, describes tools and then moves onto places about whose existence you were completely unaware. I collect these sorts of experiences because they invigorate my faith in the ability of science to explain the natural order of things: the ability of humanity to better understand the sort of world in which we live.

Which is all by way of saying that this is what happened to me in the lecture this morning. I felt as if I were starting with all sorts of materials I understood (or at least had seen before) which were then thrown together and shown (using tools of which I was unaware) to have interesting collective properties and an ability to stabilize in the presence of noise: ideas which must be generally important in biophysics but which seem to have received far too little attention thus far (possibly because of a lack of good tools - but now we've got them and, maybe, just maybe, the world awaits).

Shortly after the lectures I headed up to the NCSA cave. I came into biophysics/biophysical chemistry sideways (Russian Literature/Geology undergrad,MS in ice core chemistry/snow physics) current PhD on bacterial biophysics (how bacteria stick to mineral surfaces). This whole background is by way of noting that I usually think (because I was a Geologist long before I was a Chemist/Physicist) that I visualize 3-D data pretty well. Even with this background it was pretty obvious that the cave could be a great help in seeing the subtle, dynamic structural feature of biomolecules that might be critical for function. To make the environment truly immersive, I only wonder what would be the the sort of music you might expect to hear inside a biomolecule.

The tutorial this afternoon nicely complements the stuff that was discussed this morning. It's an interesting last note to the course and goes into the topics engaged in enough detail to make me feel like I'm "learning while doing".

This is the final note so I suppose I should add as well that I was making a list during lunch this afternoon about the ideas for future research projects that might spring from the course. I stopped when I'd filled a hand written page (I've already got a long list of things to do for this PhD so I figured more and I might just get a bit depressed). But the point is that this is the sort of environment that you all managed to create: a place where people might enter and coming out thinking about their work in a whole collection of new ways.

"People come out
thinking about their work
in a whole collection of new ways."

Evaluation

		Poor	Fair	Good	Very Good	Excellent
	N	%	%	%	%	%
Day 1 Lecture: Molecular Graphics and Molecular Dynamics	35			8.6%	42.9%	48.6%
Day 1 Tutorial: VMD Tutorial	35		2.9%	5.7%	25.7%	65.7%
Day 2 Lecture: Nonequilibrium Analysis of Molecular Dynamics	35		5.7%	11.4%	42.9%	40.0%
Day 2 Tutorial: NAMD Tutorial	35		2.9%	5.7%	28.6%	62.9%
Day 3 Lecture: Steered Molecular Dynamics	35			17.1%	14.3%	68.6%
Day 3 Tutorial: Stretching Deca-Alanine	34		2.9%	8.8%	32.4%	55.9%
Day 4 Lecture: Simulating Membrane Channels	35			8.6%	31.4%	60.0%
Day 4 Tutorial: Simulating Nanotubes	33		3.0%	6.1%	36.4%	54.5%
Day 5 Lecture: Overview of Quantum Chemistry	34	11.8%	17.6%	29.4%	17.6%	23.5%
Day 5 Tutorial: Computing Proton Affinities	33		18.2%	18.2%	21.2%	42.4%
Day 6 Lecture: Determining Classical Force Fields	34	2.9%	11.8%	17.6%	44.1%	23.5%
Day 6 Tutorial: CHARMM Parameters for non-standard residues	33	3.0%	9.1%	21.2%	39.4%	27.3%
Day 7 Lecture: Bioinformatics	34	8.8%	11.8%	23.5%	38.2%	17.6%
Day 7 Tutorial: Sequence and Structure Alignment	34	5.9%	11.8%	29.4%	23.5%	29.4%
Day 8 Lecture: Simulating Membranes	34		2.9%	8.8%	47.1%	41.2%
Day 8 Lecture: Parallel Computing	34	2.9%		14.7%	44.1%	38.2%
Day 8 Tutorial: Parallel Computing Performance Analysis	34	2.9%	14.7%	32.4%	29.4%	20.6%
Day 9 Lecture: Force Evaluation, Integrators, & Propagators	33		15.2%	15.2%	39.4%	30.3%
Day 9 Lecture: Optimization and Monte Carlo Techniques	34	2.9%	11.8%	29.4%	32.4%	23.5%
Day 9 Tutorial: Numerical Analysis	30	16.7%	13.3%	26.7%	16.7%	26.7%
Day 10 Lecture: Modeling the Photosynthetic Unit	33			3.0%	27.3%	69.7%
Day 10 Tutorial: Electron and Excitation Transfer	22			9.1%	36.4%	54.5%
Cluster Building Overview Lecture	31	3.2%		9.7%	32.3%	54.8%
Cluster Building Hands-on Sessions	29			3.4%	20.7%	75.9%

Survey#	Day 1 Lecture: Molecular Graphics and Molecular Dynamics
4	A very nice lecture - I already had some limited expertise with VMD, but I did pick up a few tricks. I learned a great deal from the lecture on MD, with which I had much less experience - I found it be well-structured and suited to my level.
5	Beautiful.
8	It was a very important lecture.
9	A few more technical details about equilibration may help.
13	Wonderful. I learned a lot of new things.
15	Learning VMD was very useful. Having access to TCL scripts & language would have been very useful.
18	A nice broad overview of what we would be learning, and the types of problems tackled by biophysicists.
20	I needed a better introduction to the material, how it fit together, etc. Reviewing the schedule did not help. I needed more explanation, a better overview, and an overall description of the "big picture".
23	Impressive. VMD is a nice program.
32	Good intro.
37	Good lecture & good tutorial. Our lab has VMD, but we normally use it just for graphics in papers, PowerPoint, etc. I found out that VMD has many more applications that we can now use in our lab.

Survey#	Day 1 Tutorial: VMD Tutorial
4	Nice for getting everyone on the same page; I learned the most form bits on scripting.
5	Good example system.
9	Many functionalities of VMD were not included (e.g. isosurface). Since the tutorial was very long, they might deserve a separate tutorial.
13	Wonderful. However, some people use Amber coordinate & parameter files. Perhaps someone should be on hand to explain how to use NAMD w/Amber param/tops.
15	I think it was needed (??) that was the software we were using @ SS03. But a lot of us use this software in our research. Possible access to our software (charm, Amber, DL-POLY) would have been more productive.
18	It was very nice. Even as a solid-state physicist, VMD's power and Tcl/Tls scripting will be useful.
20	I have used VMD extensively but still learned a lot. I came here to learn about NAMD & its capabilities & feel that thru the tutorials, I accomplished this. The TAs were great!
23	Really helpful to set up a NAMD run. If instructors could give more explanation on different parameters it'll be great.
26	Nice tutorial however the participant should know VMD on this level prior to attending the summer school.
31	Very detailed. The only thing I think is maybe we should setup NAMD a little more.
32	Good intro.
56	Very, very good. Need more on how to write TCL.
58	My only complaint is that I needed about 30 more minutes! (to finish)
69	Only slightly too long for the available time. Very clear and very well thought out.

Survey#	Day 2 Lecture: Nonequilibrium Analysis of Molecular Dynamics
4	Also a very nice lecture - I especially enjoyed the temperature quench echoes.
5	Very nice talk, but is "temperature echo" phenomenal useful?
13	This was new to me. I used it well and understood it.
18	Effects reminding us that thermodynamics is not the god of all microscopic dynamics - this was great! I love seeing kinetics and coherence.
20	Again, I could have used a better "road map" of how things complimented each other. But, the specifics were clearly presented.
32	Temp. Echo seemed cute but not interesting or relevant. The cooling was interesting.
37	The lecture was informative.
54	I wish the equations were not skipped that fast. Since this was a school in theoretical biophysics I was expecting a bit emphasis on the theory and more careful look at some equations.

Survey#	Day 2 Tutorial: NAMD Tutorial
4	This was possibly the best tutorial in the SS - informative, well-organized, and easy to follow.
5	Good example to show, although seems useless for real simulation.
9	Some technical details (e.g. what PME parameters to use? What're the coupling contrasts, which are needed for the LD?) should be explained more thoroughly.
13	Great. More explanation needed on what the scripts do and a good reference on Tcl would be great.
18	A nice tutorial, but running MD simulations can only be so much fun. Seeing the results was very good though.
20	It was great to have such an in depth NAMD tutorial. The TAs were excellent - a huge help, very knowledgeable, & eager to help.
23	Learnt a lot.
36	I felt this tutorial was extremely well written.
37	The tutorial taught me a lot - it combined VMD and NAMD so we could see how they could be used together. Also, we found that we can use NAMD w/the CHARMM force field so we can run our simulations w/NAMD rather than CHARMM.
41	Tutorial is very good, but long, maybe shorten a bit.
56	Very, very good.
58	Very good, but I didn't get through it all. Maybe put this over 2 days next time.
69	Very clear and very well thought out. An invaluable tool for new NAMD users.

Survey#	Day 3 Lecture: Steered Molecular Dynamics
4	Three good ones in a row! I especially enjoyed the biology of mechanical proteins.

5	Excellent theory lecture and show.
9	To my opinion, the lecture should've included more on umbrella sampling on the expanse of (???) SMD examples.
10	Very interesting!
13	Awesome!
15	Needed more detail & comparison to umbrella sampling.
18	As a facility for hypothesis testing, this seems to be an extraordinary tool for augmenting our chemical intuition. I can't help but be scared when I see how hard some things are yanked - practitioners must be careful not to pull the system to the point where the bonds should break, but the potential does not allow. This warning should have been emphasized!
20	I did not understand this lecture on its own. However, the tutorial helped. I'm not sure how I'd fix this. It would have helped to get the notes before the lecture to follow along & take notes on. (For all lectures this would have helped tons).
23	The fun part. The first time to know the new kind of MD.
32	Nicely motivated and historically informative presentation.

Survey#	**Day 3 Tutorial: Stretching Deca-Alanine**
4	Basically a continuation of Tuesday's tutorial; I only wish we hadn't had to cut so much of it.
5	From this tutorial I learnt a lot!
13	Awesome! No change, only more understanding of the math --> equations.
18	Calculating free energies is extremely important for giving thermodynamics interpretations of a system. However, we must be precise when talking about free energies. Really, all points that project to a point (?) a reaction path should be included in the averaging process inherent in calculating free energies. This is hard to do and often is not helpful. Thus, we are always looking at free energies (?) to the reaction path. Explaining this and quantifying it are crucial to understanding what one is comparing and how to interpret it.
20	This was cool - I understood a lot more by doing.
23	Its good to experience SMD and view its
37	This tutorial was very interesting - I liked being able to watch the stretching of peptide.

Survey#	**Day 4 Lecture: Simulating Membrane Channels**
1	Good.
4	I enjoyed the bit on aquaporins - especially with 3D glasses.
5	Excellent talk. Membrane proteins are important.
10	Too simple.
13	This area was new to me, but I learned a lot. I can not make a good suggestion on how to improve it.
18	I liked how this exemplified replacing complex systems with simpler ones in order to elucidate the fundamental mechanisms of a process.

20	This was better organized & much clearer to me than the other lectures this week. Still, having the slides beforehand would have increased my understanding.
23	Nice lecture and helpful to my own research.
26	Too many examples.
32	Emad's presentation was carefully composed and informative. The slides were beautifully illustrative. He did a superb job.
37	The lecture was really good. I learned a lot from this lecture, and the speaker made the material understandable for people that are not familiar w/membrane channels.
58	Very interesting and great pictures.

Survey#	**Day 4 Tutorial: Simulating Nanotubes**
4	Also, excellent - I was impressed by the part where we modified the vdw radius of carbon.
5	Very intuitive tutorial, especially the change of water behavior after changing non-bond parameters.
9	I'd rather work on a real (small) membrane protein. The charge effects were very good!
10	Sounds not bad, yet still don't know what I can do with it? :(
13	This was a new area to me.
15	Was fun, but I didn't know how much I really learned from exercise.
20	Another great tutorial that complimented the lecture very well. As usual, the TAs were a great asset.
23	Good. If I get a sample answer to the questions in the tutorial it will help me more.
58	This tutorial was really fun.

Survey#	**Day 5 Lecture: Overview of Quantum Chemistry**
4	I felt like I was trying to drink out of a fire hose - too much information too fast.
5	Not well organized.
10	What did he say? I can't help sleeping during the section. Everything was in text-book. And I finished that course just 3 month ago!
11	May need some more detail/or basic concept.
13	This area and lecture I am familiar with . . . however, not everyone understood the lecture as much as I did. Therefore, more explanation would be needed.
15	Needed more detail. Lecturer went very fast to cover a large subject. More detail in less topics would be better. More info on QM/MM systems.
18	Very nice overview. I would have liked very much to see each method described more rigorously, but this is clearly impossible with the time constraint given to Prof. Martinez.
20	This was the worst! The speaker went on and on for 3+ hours without giving us a break. It was a completely unreasonable amount of information. Also, it was poorly presented. He tried to go too in depth instead of giving a good overview. He ended up getting nothing across to the audience.

23	Nice to know how to calculate FF parameter using QM.
24	Anyone who hadn't already learned QM simulation methodology would have been lost. It would have been more useful to show many examples of how QM is applied to biomolecules.
26	Either you know everything in the lecture on beforehand else you understand nothing.
32	Poorly organized --> the overall structure.
36	I felt the lecturer was great. He was through but at the same time kept the topic simple.
41	Interesting but very hard to understand for non-chemist/physicist.
54	I was pleased to see that the speaker does not hesitate to go into more formal and theoretical material but two days after the lecture I realized that I haven't acquired any practical knowledge that could help me with my own system.
56	Far too much detail --> did not have good feel for overview. Too many acronyms.
58	Excellent overview!
69	The speaker tried to convey too much information in a short time. The speaker also spoke very fast, which sometimes made it hard to understand.
70	It is very difficult to go through all the topics and even only mention all the important things in q.c. in just 2-3 hours. I think that there should have been more time given for this part and more examples considered (for those non-physicists among us :-)

Survey#	**Day 5 Tutorial: Computing Proton Affinities**
4	Much more helpful than the lecture, but I still didn't manage to finish it.
13	This was great, but a little thought challenging.
18	Skipped last half, but first was fun.
20	I was so turned off by the lecture that I completed very little of this tutorial because I had no clue what I was doing & was just clicking buttons.
37	This definitely made me appreciate QM methods more!
69	The tutorial was well thought out and very clear. However, it was very long if one tried to set up the input files instead of using the sample files provided. Overall, I worked (around) 8 hours on this tutorial and I didnít finish.

Survey#	**Day 6 Lecture: Determining Classical Force Fields**
4	This wasn't too well-suited to my (beginner) level - the first 20 minutes or so were very helpful.
10	This was a very interesting lecture. Very useful & very helpful. Although the lady was not very good at lecturing.
15	Very helpful. Again more info on the technical side of how this is done for charm & amber.
20	This was better than Friday, but only slightly. It seems that there must be a better way to introduce this material.
23	Very clear.
32	Nice presentation.

37	This lecture & the tutorial that went w/it was very helpful. I am presently working on parameterizing some new residues for the CHARMM force field, & the lecture assured me that I was using a correct method to do it.
54	I don't know why the speaker had to present other's work. This made her unsure and resulted in many sentences like "they have done this" and "they observed that".
69	R. Amaro spoke too fast, which made it difficult to understand her at some points.

Survey#	Day 6 Tutorial: CHARMM Parameters for non-standard residues
4	Nice as a tar, but at the end I wasn't quite sure what I'd accomplished. Not terribly clear.
5	A good try.
9	In the background, a practical approach could help (e.g. when working with this ligand, we have used X-STD** level of theory etc.)
13	OK, we did not really develop parameters, or really edit the files. That would have been great.
15	Good project, but would like the scripts.
20	I did not attend but am happy to have this info for later reference in case I need to learn to do this. I haven't used CHARMM.
23	Great help from Markus. Thank you very much!
24	Very useful for people who may have to parameterize a force field.
32	Useful. Nice to see this level of detail.
69	The tutorial was not clear enough at certain points: in p. 6 and p. 10 it indicates that the structures in the files correspond to the end of step 2, which is not true. More instructions regarding commands in VMD should have been given. I did not understand the point of comparing bond (?) and lengths obtained using MOE (non-minimized structure). I did not finish this tutorial; partly because it was not clear enough and partly because it was a bit long. The overall ideas in it is very good, but the tutorial itself needs to be improved.

Survey#	Day 7 Lecture: Bioinformatics
4	A very good overview of a field about which I knew very little.
5	Learnt a lot.
10	What to say? Bioinformatics is too far from my research. :-(
13	Wonderful! More basic explanation.
18	This extremely exciting field should have been given more attention.
20	The info that was presented was good. However, I got the impression that we were only seeing the speaker's favorite tools. I would have preferred a more general overview.
23	Useful links.
26	I've never had any bioinformatics before and I didn't understand anything.
31	This was good just not quite as good as Klaus's lecture so I give it a 4.
32	Basic concepts (e.g. Hidden Markov Methods) not explained at all. Too much knowledge assumed.
37	The lecture & tutorial were informative, & they both taught me a little about protein sequence alignment. I don't deal w/proteins in my research, but knowledge is always useful!

41	Maybe a bit off topic, but not bad (???)
46	I lacked knowledge on the subject to be able to fool the lectures. Bored.
56	Would like to have heard more about homology modeling and other Bioinformatics-based structure prediction techniques (e.g. MODELLER).

Survey#	Day 7 Tutorial: Sequence and Structure Alignment
4	Very interesting. Working out the matrix by hand was a little tedious but it helped greatly in improving my understanding. Possibly as good as the NAMD tutorial.
5	Good practice.
10	It's funny to play with it. (Because I'd never played before).
13	Awesome!
18	Better if this focused on why algorithms work and what we can learn than rote application of techniques. Still quite nice.
20	This was OK. It gave a good intro to how bioinformatics works. However, web tools change so quickly that I am not sure how relevant this was. But, it fit with the lecture perfectly, probably the best of any other lectures - hands on pairing.
23	Structure alignment so nice.
24	This was new material to me and it was nice to put in my own protein and examine homologous structures. I even found a protein very similar to my own that I had not seen in my primary literature.
36	I felt this tutorial was extremely informative.
39	Some parts of the tutorial seem out of order.
56	No info on MODELLER! MOE very good package however (although not free). Appreciated references in material.
69	p. 27, question I did not understand why pairs ATI/AD (?) in the less evolutionary related, and not pairs (? ñ another pair sequence). This should be made more clear.

Survey#	Day 8 Lecture: Simulating Membranes
4	Fascinating. Very pertinent to my own work.
9	This was more of a "conference" lecture. A more practical approach ("this is how you do it with NAMD") could benefit us more.
18	Clear, thorough introduction.
20	This was well organized & at the right level for the audience. I was disappointed not have a hands-on with this. To give it a 5, would have wanted the notes prior to the lecture to follow along & take notes.
32	First lecture was good. Second lecture should have focused more on methodology and not so much on "results".
37	Very interesting lecture. I learned something about coarse-grain simulations, and I thought it was very interesting that these types of simulations could be used for membrane systems.
54	It was good to have a guest speaker. He brought a different flavour to the kinds of problems addressed and methods used to deal with them.
56	Perhaps more detail on simulating membranes with the NAMD2 in addition to the reduced model.

Survey#	Day 8 Lecture: Parallel Computing
4	As a (???) I lacked the background knowledge to get much out of it.
10	Useful!
18	I enjoyed the nice performance analysis tools, but have spent too much time writing and benchmarking parallel code to really get excited about this.
20	This was well done for the majority of the group who doesn't have much/any parallel computing . For me, I didn't learn anything new.
23	Great. Very clear. And interesting.
31	I do computer science this lecture seemed too fast in the interesting parts & too slow in the easy parts. I still liked the concept of this lecture but it could have been much better done.
32	Entertaining and informative lecture. Very nice.
36	My job was queued on the super computing system but never ran.
37	The lecture was very useful. The lecture gave me a better picture of the advantages & problems w/parallelization.
56	Very charismatic speaker. Good material although too much for 1 hour.
58	Very good talk, but the speaker went too fast through the lecture.

Survey#	Day 8 Tutorial: Parallel Computing Performance Analysis
4	Illustrative.
9	A table was enough for performance. Instead, a brief introduction to Charm++ (how to write a code on a parallel system) would be more interesting.
10	Not very useful.
13	This subject could have been presented better with more case studies and & explanation. Do not rush over the topic.
15	I don't know if this was needed. Possible just a handout to describe the basics is all that is needed.
18	I enjoyed the nice performance analysis tools, but have spent too much time writing and benchmarking parallel code to really get excited about this.
20	Unfortunately, Platinum was not behaving (it left jobs in the queue even though there were plenty of available processors) so this was difficult to complete. The basic idea was good though. I have extensive parallel computing experience, & thus did not feel that I was missing out on a lot by not completing this tutorial. I think it was good for beginners.
23	Experience the difference it parallel computing.
24	Everybody knows that parallelization does not scale perfectly. It might have been more interesting to write a small program which ran parallel (perhaps calculating some sort of integral or something).
31	The program didn't work well on the SUNS.
37	This was a useful tutorial, but since so many people were submitting their jobs, I couldn't finish the whole thing. (I guess that really can't be helped, though).
58	The queue got really full for NCSA jobs, and we didn't get to run all our jobs in the afternoon.
69	Section 2: Projections: Needs more information explaining what weíre seeing: definition of ìload imbalanceî; should say why weíre visualizing te[19, 39-39.5] and t t[38.52-65.93] (? Misc symbols?). Point 6.g) should say ìentering the window a lotî!

Survey#	Day 9 Lecture: Force Evaluation, Integrators, & Propagators
4	I really didn't understand a thing.
10	I like it very much myself. But other said it was too simple. :-(
11	May need some more background.
18	Nice to see things I've read editorialized and see the formalism.
20	I was disappointed that so many of the math details were glossed over. But, it was clearly a welll thought out and very organized lecture. Again, a 5 if the slides were available previous to the lecture.
32	Extremely informative lecture. Lots of detail was covered.
54	There is no way to make a popular theoretical lecture. It ends up being boring to both the people who know what is going on and people who don't. I think in lectures like this one should be ready to sacrifice a big part of the audience and present more recent results.
56	Very good linking lecture material to NAMD2 code & parameters.
58	Good lecture, but maybe give this topic more time next time.

Survey#	Day 9 Lecture: Optimization and Monte Carlo Techniques
4	More concrete examples of MC implementation would have been nice.
5	Good talk.
10	Interesting.
11	Could be better if we have the pdf slide. The note is 95 page, a little bit too much to print out.
18	Nice, but would have been much better if it had went into some real substance, say (1) Real MC algorithms and their details, (2) Detailed analysis and theory of optimization. The talk was very slow-paced.
20	First of all, I have a PhD in continuous optimization. So, I had nothing to gain from such a beginning lecture. However, I think it got some good points across. The Monte Carlo lecture was poor. The writing on the slides was small & difficult to see. I was extremely disappointed that Tamar spent so much time on random number generators. I know she does neat stuff with DNA and would have like to hear about that. I was so looking forward to this & was severely disappointed.
24	A little too general; not enough specific information on the methods or exactly why minimization is useful in bio simulations.
26	Level too low.
31	I don't believe the examples used in this talk related to the optimization method shown. I believe these scheduling algorithms are solved by a more computation method. I also thought the talk should have explained more of the biological uses of optimization.
32	Too basic, and general.
54	I do not see the point of going over textbook information. I was expecting to learn more about the research in the speaker's group and how she integrates the mathematical methods she talked about with her scientific research.
56	Too much detail on random number generators. Would like to have heard details of the MC DNA model (e.g. is atomistic/reduced etc). Would like to have optimization linked to NAMD2 i.e. discuss more minimization algorithms used in NAMD2.

Survey#	Day 9 Tutorial: Numerical Analysis
4	The fly in the summer school ointment. The instructions were opaque, the examples were baffling, and I wasn't sure what I was supposed to have learned from it, or what the point of it was.
9	This tutorial completely lacked explanations and background. Maybe we were spoiled by the high level of details in the other tutorials, but I still think this isn't enough for introduction.
10	That was the 'fun' part. I think it was a very special tutorial!
18	I didnít feel like as much was learned from this as the other tutorials.
20	It was cool to see the capabilities of mathematica (I usually use maple &/or matlab). Also, the tutorial was well set-up to get good & specific lessons to the students. I learned a lot.
23	Very helpful.
31	This was a waste of time that could have been much better done. Teach a little about the perl script, teach a little about mathematica. Tell us what we were doing.
37	This tutorial was interesting. I didn't really understand initially what I was supposed to be seeing w/the exercises, but the TAs gave very good explanations, so I was finally able to understand by the end.
41	Tutorial is hard to understand.
46	The tutorial was unclear and I was too tired to ask for explanations.
58	Strange bug in the computer(s) that wouldn't allow editing of mathematica notebooks. This happened to several of us in the Engr. Lab :(
69	Not nearly enough information to understand what was being visualized. The computational part was OK, and the concepts addressed sounded interesting and useful, from what I could understand afterwards by talking to other students. It was a pity that I couldnít understand better what was going on.

Survey#	Day 10 Lecture: Modeling the Photosynthetic Unit
4	The absolute high point of the lectures, in my opinion.
18	This was an amazing lecture emphasizing a growing interest in biology and science in general - putting things into the big picture. Models to guide intuition and calculate large systems were combined with molecular dynamics, quantum chemistry (computational HFIDFT and perturbation theory - very nice!), and biological function.
20	This was much better organized. The points were clear & the purpose of the lecture was well-stated. Again, having the slides before to take notes from would have made this a 5.
24	Klaus is a riot.
32	Beautiful lecture. Shows how MD can be coupled with simple physical models.
39	Probably the most exciting presentation. The presenter showed his real love and devotion toward the subject.
41	(??) Schulten gives very funny lectures.
56	Very good example of utility of modeling.
58	Very interesting!

Survey#	Day 10 Tutorial: Electron and Excitation Transfer
4	Excellent.

31	Unknown, but it looks well written
58	I liked having the option of skipping to the parts in the tutorial. Ex: the note on p. 5.

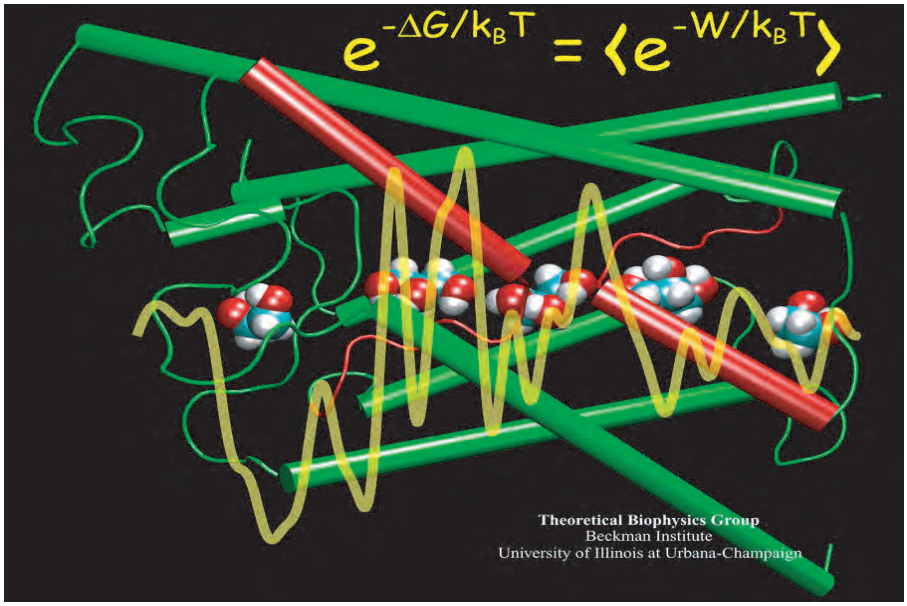
Survey#	Cluster Building Overview Lecture
4	Fast-paced and not too dry. Disabused me of some misconceptions about clusters.
5	Excellent.
10	The guys sound like the ones who care more about how much to spend on building a cluster. We NEED more technology details.
13	I will build a cluster in a few days!
20	Well-organized, clearly presented, relevant info.
23	Nice presentation.
31	It covered the topic very well.
32	Informative.
37	Very good lecture. The speakers gave us a good overview of what to consider when building a cluster, problems that arise, etc.
46	It was fun! And also an experience how a good team and cooperation is important to fulfill a goal.
56	Does not need any more detail. Maybe include more web links to allow us to follow up after.

Survey#	Cluster Building Hands-on Sessions
4	Very nice, well-organized and instructive.
5	Excellent practice. Feel much better about cluster.
10	Very interesting.
13	Wonderful, great session by Tim & the guys.
15	This was great.
20	I learned a lot from this & feel that I could do it myself.
23	Another fun part of the whole summer school.
24	It was very useful to have all of the components needed laid out on the table and to learn how they interact. The TA's were very good at answering general questions.
32	Useful.
37	I really liked this & had fun with the session. I don't know if I could completely build my own cluster yet, but I got a good idea of what is involved & what I would need to do.
56	Very good! Seems trivial but gives confidence that one will be able to (perhaps) build a small cluster.

58	I enjoyed this & feel pretty comfortable building my own cluster.

General Comments (appended somewhere on form, not in response to a particular question).
I enjoyed the Summer School a lot. I should admit I was not expecting such a wonderful organization. The selection of topics was diverse and interesting (with possible exception of DNA). I was also very pleased with the interaction between the lab instructors and the participants. I want to express my gratitude to everybody who worked to make this summer school satisfying both scientifically and socially. Thank you.
General comment: It would be better if the SS would start two weeks later, because some universities still have finals going on at that time. My final coincided with SS03 and I had to work on them and send them by mail that took some time that I'd prefer to spent work on SS03 projects.

Summer School on Theoretical and Computational Biophysics

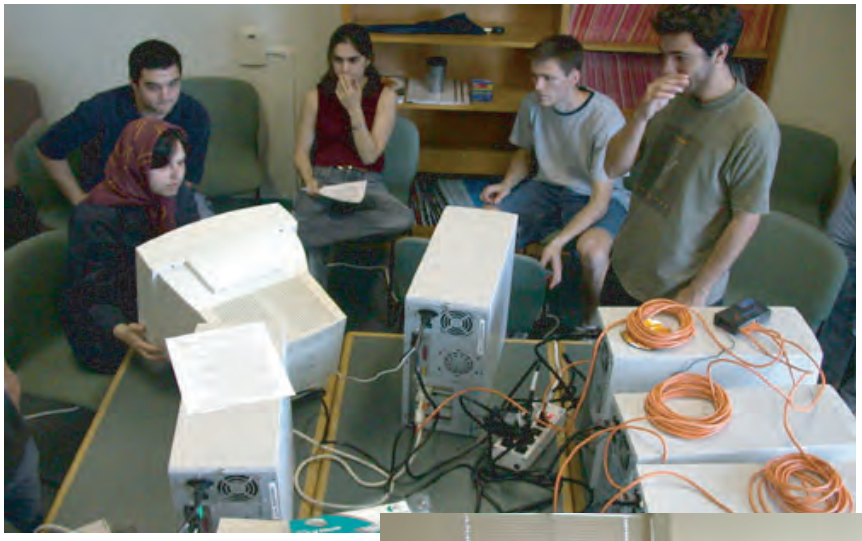


Free Energy of Glycerol Transport

The summer school will explore a wide range of physical models and computational approaches used for the simulation of biological systems and the investigation of their function at an atomic level. The course will be based on case studies including the properties of membranes, mechanisms of molecular motors, trafficking in the living cell through water and ion channels, signaling pathways, visual receptors, and photosynthesis. Relevant physical concepts, mathematical techniques, and computational methods will be introduced, including force fields and algorithms used in molecular modeling, molecular dynamics simulations on parallel computers, steered molecular dynamics simulations, and combined quantum mechanical - molecular mechanical calculations.
The workshop is designed for graduate students and postdoctoral researchers in computational and/or biophysical fields who seek to extend their research skills to include computational and theoretical expertise, as well as other researchers interested in theoretical and computational biophysics. Theory sessions will be followed by hands-on computer labs in which students will be able to set up and run simulations.

Photo Gallery

Photo Gallery



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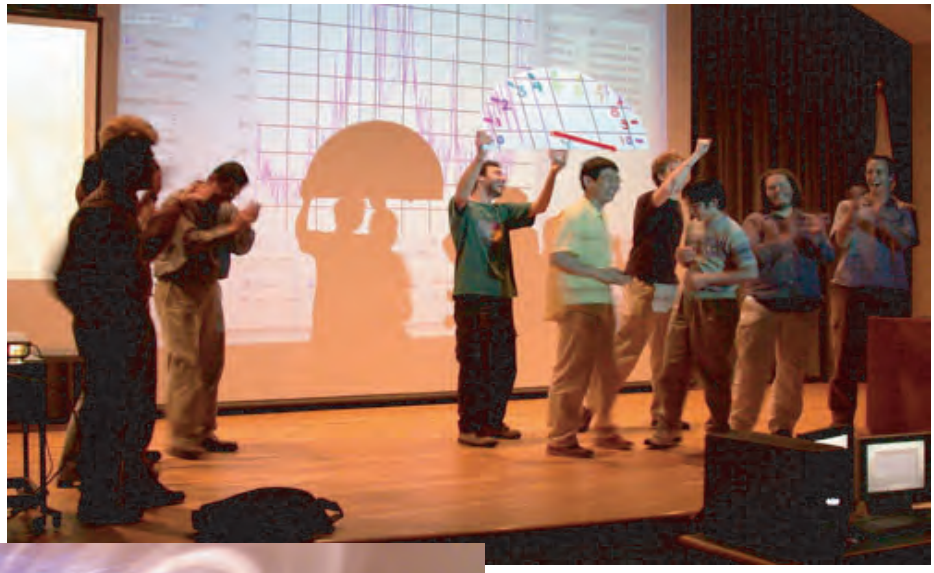

Photo Gallery