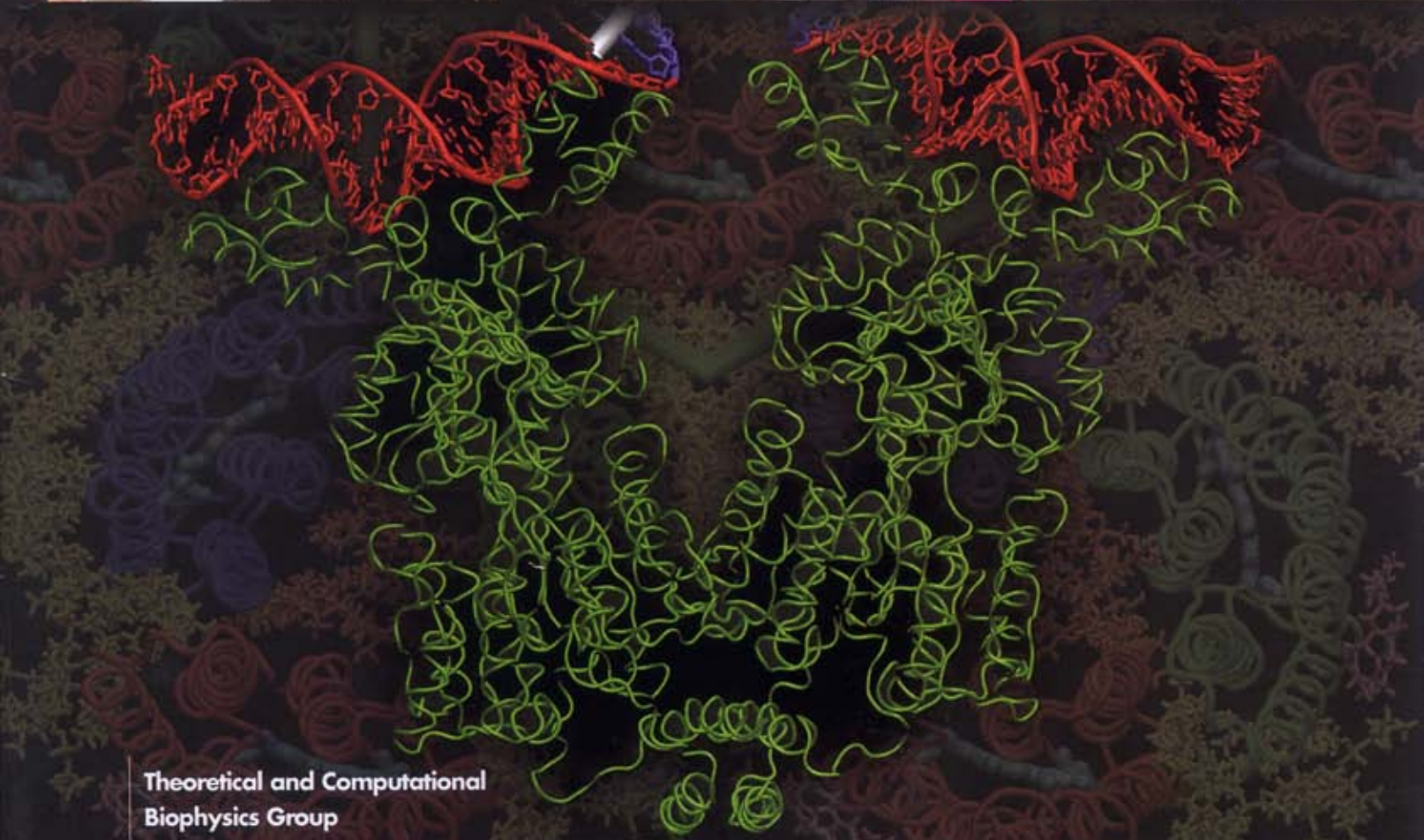
Theoretical and Computational Biophysics Workshops: Training for the New Discipline







Theoretical and Computational
Biophysics Group

Theoretical and Computational Biophysics Workshops: Training for the New Discipline

Contents

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1.

While the life sciences are perhaps the oldest area of human inquiry, the field is still evolving. Today quantitative and computational methods are joining traditional experimental methods, and the combination is opening new areas of research and enabling new discoveries.

"We see the life sciences transformed into a new discipline," says Klaus Schulten, the leader of the Theoretical and Computational Biophysics Group at the University of Illinois at Urbana-Champaign. "We have to take account of this change not just in research but also in education. What is in the research lab today is applied tomorrow in medicine and industry, so we have to train students to deal with quantitative information and computational methods."

Schulten's group, funded as a National Institutes of Health Resource for Macromolecular Modeling and Bioinformatics, is addressing this educational need through hands-on workshops, which have been supported by the National Institutes of Health, the National Science Foundation, and the National Center for Supercomputing Applications. Through these workshops, graduate students, postdocs, and other researchers are able to extend their skill-set to include computational simulation and modeling techniques using the NAMD and VMD software developed by Schulten's group.

2. Workshops combine theory with hands-on experience

"We really feel that you cannot teach just by lecturing; you have to teach through hands-on examples," explains Schulten. Therefore, the workshops combine lectures on concepts with the practical application of computational methods guided by tutorials that allow participants to explore the examples on their own under the watchful eyes of teaching assistants and lecturers.

"This is the most effective way of learning modeling techniques," says Emad Tajkhorshid, the assistant director of research for the NIH Resource.

After the 2003 workshop, the tutorials, along with all the required data and software, were loaded on laptop computers and provided for participants to use throughout the workshops taught in 2004-2005. This uniform computing environment allows the instructors and workshop participants to avoid obstacles caused by heterogeneous equipment.

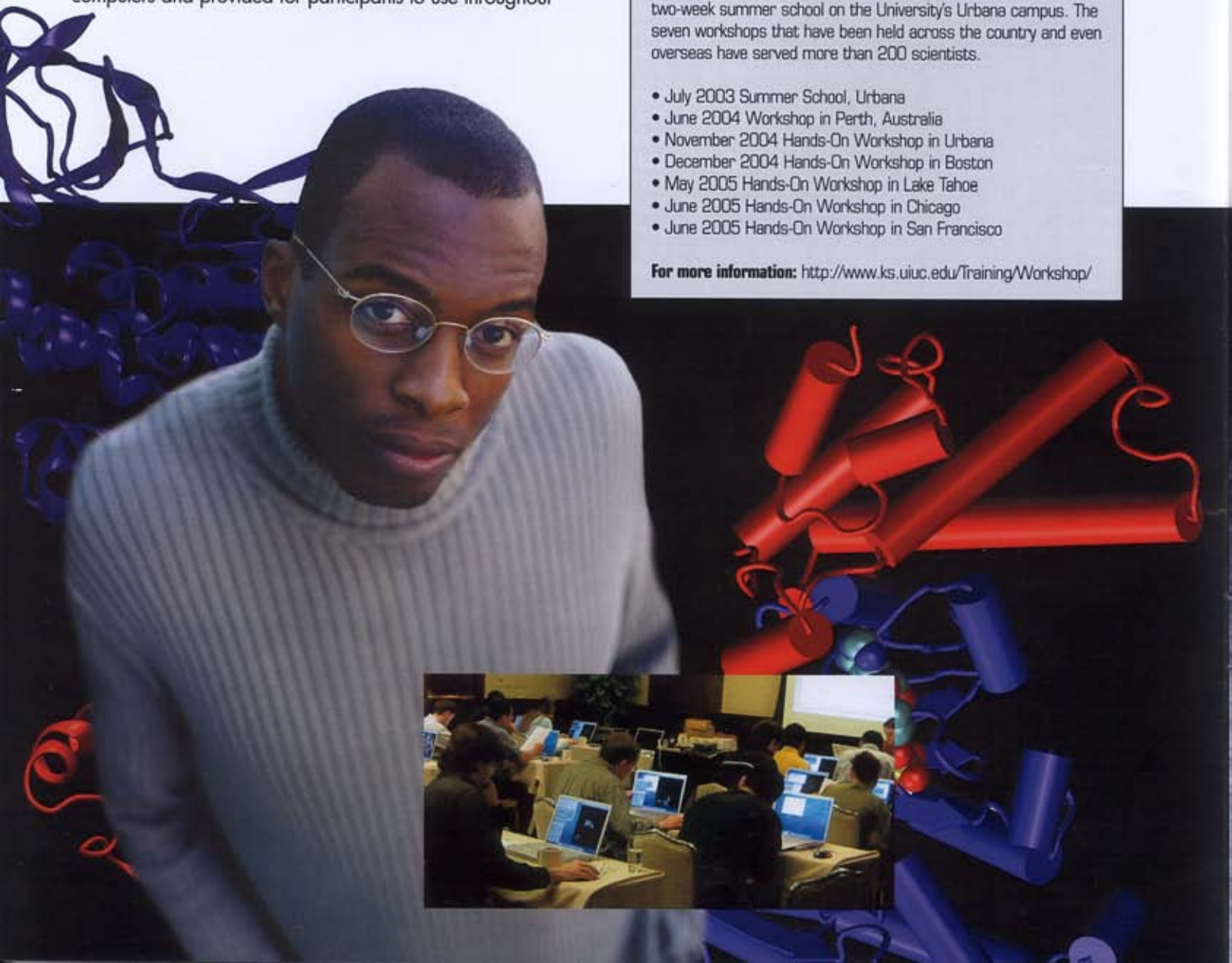
The laptops furnished to users also provide portability; by shipping the machines, the workshops can be (and have been) conducted at any location. This enables a wide range of scientists to participate in the workshops.

Hands-On Workshop Series

The Theoretical and Computational Biophysics Group at the University of Illinois launched its workshop series in 2003 with a two-week summer school on the University's Urbana campus. The seven workshops that have been held across the country and even overseas have served more than 200 scientists.

- July 2003 Summer School, Urbana
- June 2004 Workshop in Perth, Australia
- November 2004 Hands-On Workshop in Urbana
- December 2004 Hands-On Workshop in Boston
- May 2005 Hands-On Workshop in Lake Tahoe
- June 2005 Hands-On Workshop in Chicago
- June 2005 Hands-On Workshop in San Francisco

For more information: http://www.ks.uiuc.edu/Training/Workshop/



3. Lectures lay a firm foundation

The workshops begin every morning with lectures from experienced researchers, including Klaus Schulten, Zan Luthey-Schulten, and Emad Tajkhorshid. These lectures provide participants with a foundation in the theory behind computational simulation and modeling, examples of the research problems these techniques can effectively address, and descriptions of the use of the software developed by Schulten's group, NAMD and VMD. These programs are widely used in the life sciences community, with more than 60,000 registered users.

NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3D graphics. Together, NAMD and VMD form a powerful simulation and visualization environment that is used by tens of thousands of scientists around the world.


Klaus Schulten


Zan Luthey-Schulten


Emad Tajkhorshid

"I try to be as practical as possible," says frequent instructor Tajkhorshid, pointing out that the lectures employ numerous examples to connect the topics to real-world research. "I try to walk participants through one concrete project – how we set up a simulation, how we looked at a system, and how we analyzed the results."

Typical lecture schedule

Day 1: Introduction to Protein Structure and Dynamics
- Molecular Graphics Perspective of Protein Structure and Function
- Molecular Dynamics Methods

Day 2: Statistical Mechanics of Proteins
- Equilibrium Properties of Proteins
- Using NAMD
- Simulated Cooling of Proteins
- Temperature Echoes

Day 3: Introduction to Bioinformatics
- Evolution of Protein Structure
- Sequence and Structure Alignment Algorithms
- Bioinformatics of Aquaporins

Day 4: Parameters of Classical Force Fields
- Introduction and Examples
- Introduction to Classical Force Fields
- Methods of Parameterization

Day 5: Simulating Membrane Channels
- Introduction and Examples
- Transport in Aquaporins
- Nanotubes

4. Self-directed tutorials provide first-hand experience

The tutorials are the core of the workshop experience. Building on the foundation established through the lectures, the interactive tutorials guide workshop participants through activities that familiarize them with the basics of the NAMD and VMD software and through examples of how to apply the techniques they have learned. The tutorials guide students through tasks that approximate actual research activities.

Because the tutorials are self-directed, students can work at their own pace and focus on topics that most closely correspond to their own research interests.

The first tutorials were developed for the workshop held in the summer of 2003. Graduate students in the group tackled this task because their level of expertise was not so far removed from that of the workshop participants. The experience of learning the software and techniques was fresh in their minds, so they could anticipate the needs and questions of the participants. As a result, the tutorials are accessible and user-friendly.

"The tutorials are based on what we would have wanted to know, what we wish someone had told us," says graduate student and workshop assistant Elizabeth Villa.

The tutorials are continually improved based on feedback from workshop participants. "We take great care in asking the participants for their evaluations, using their feedback to refine and improve," Schulten says. "The high quality and the successful execution is due to the tutorials being developed through the workshops over the past few years." New tutorials are regularly added to respond to learners' needs.

The tutorials are posted online, allowing participants to extend their learning beyond the workshops and enabling other learners to participate.

Tutorials

All of the tutorials developed by the Theoretical and Computational Biophysics Group at the University of Illinois are available online at http://www.ks.uiuc.edu/Training/Tutorials/.

- Aquaporins with the VMD MultiSeq Tool
- VMD Molecular Graphics
- NAMD Tutorial
- Parameterizing a Novel Residue
- Evolution of Protein Structure Aspartyl-tRNA Synthetase
- Sequence Alignment Algorithms
- Topology File Tutorial
- Stretching Deca-Alanine
- Simulation of Water Permeation through Nanotubes

5. Experienced mentors share their knowledge

Researchers are trailblazers; they tackle novel problems, test novel techniques, and arrive as fresh discoveries. The generous trailblazers led by Schulten then share their knowledge with others.

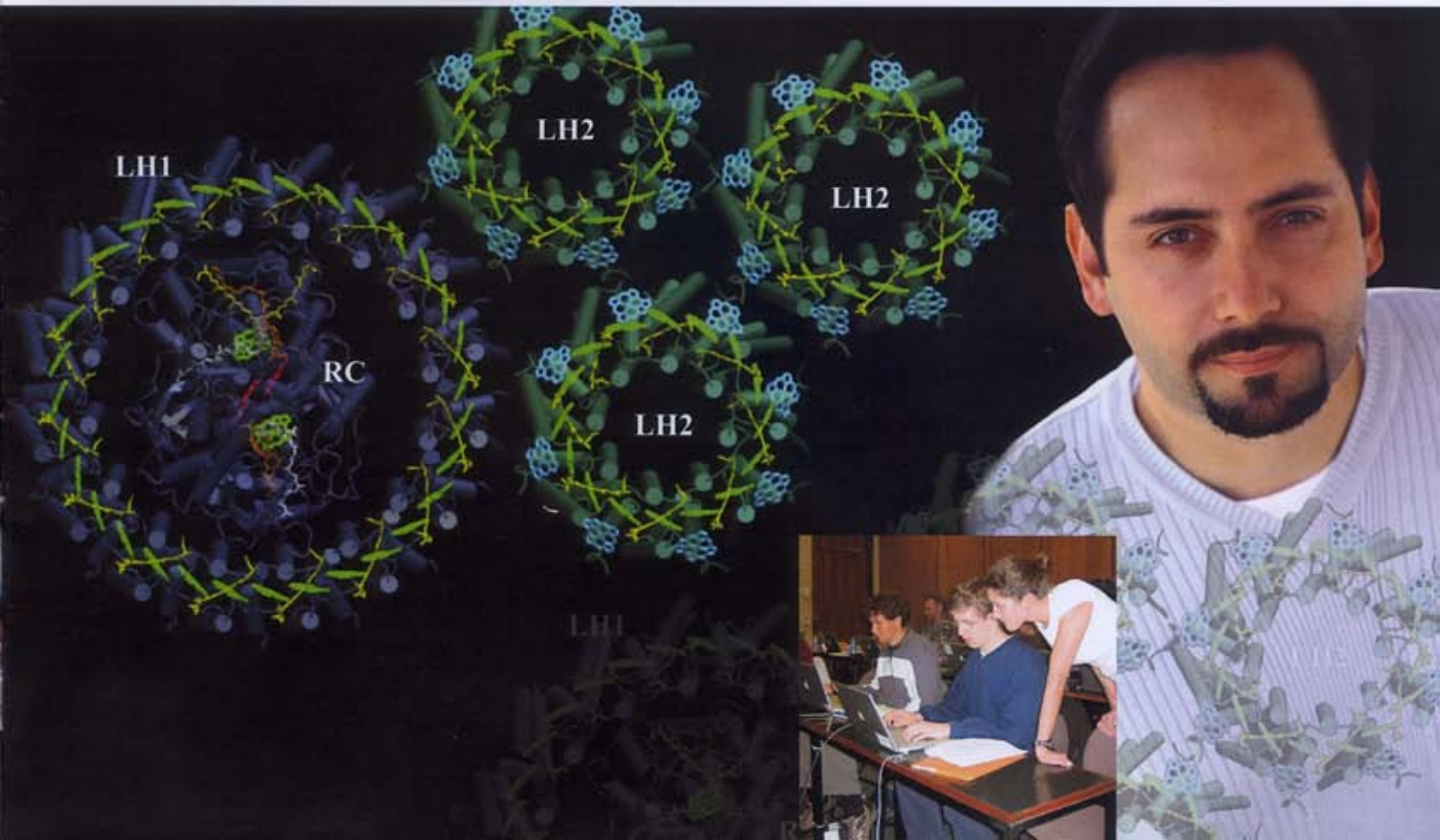
"I really felt that the learning curve was just too steep," says Luthey-Schulten, a professor of chemistry at the University of Illinois as well as a researcher with the University's Institute for Genomic Biology and the Beckman Institute for Advanced Science and Technology. "Even if you publish papers and tell people how you addressed a problem and got your results, people really need to come and sit next to you and try it themselves with the tools."

And that's just what happens during the workshops. The lectures are given by researchers with expertise in the theory, techniques, and software. The tutorials have been developed and refined by graduate students with first-hand experience conducting computational simulations and visualizing biomolecular systems using NAMD and VMD. And these same graduate students are available during the workshops to answer participants' questions and provide additional support.

"Modelling and computer simulation is an emerging field and it's growing quickly; there is more and more need for and interest in visualization and simulation," Tajkhorshid says. "It's really rewarding to see how effective the workshops are and how much practical knowledge you are transmitting to people who really need it."

The graduate students find that the workshops are a learning experience not just for those attending the workshops, but also for those assisting with them. During the workshops, the TAs field novel questions and see problems from new perspectives as they help the participants.

And the questions don't stop when the workshop ends. The partnerships between the mentors and mentees continues as the participants carry their new skills back to their own labs, to be applied to their own research. As questions arise, many will contact their TAs for advice and assistance.



6. Participants from diverse backgrounds gain new skills

The more than 200 students who have so far participated in the workshops come from diverse backgrounds and have a wide range of research interests. Many are graduate students or post-doctoral researchers, while others have more established careers. Most come from academic and research institutions, but some are from industry. Some are computationally oriented life scientists, while many others are experimentalists who are eager to gain computational skills to guide their future work. And of course the participants come from across the country and around the world.

"The diversity of the participants really reflects the degree to which the community needs computational tools and modeling," says Tajkhorshid.

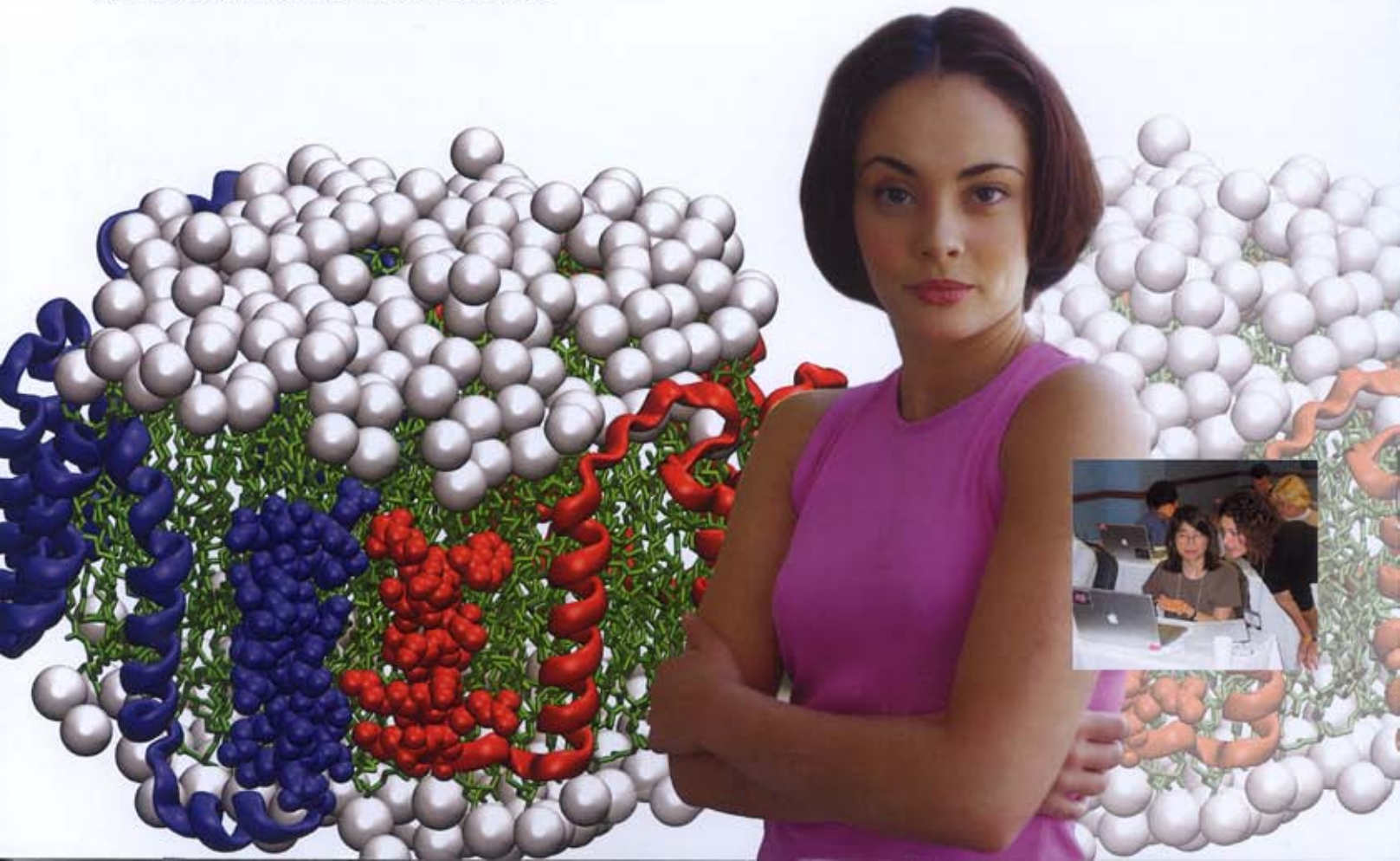
Some of the attendees arrive at the workshops with specific research issues with which they need assistance. Perhaps they have been trying to do computational research and have been stymied by technical roadblocks or simply by a lack of time to devote to acquiring the necessary skills. After the workshop, they return to their own labs able to apply the techniques they learned and to transfer them to other researchers.

"We wanted people to be able to start from scratch and end up being able to run a simulation," says Villa, a graduate student who has assisted at several workshops. The goal is to have the participants master the techniques required to set up and run a simulation, and to apply these techniques to their own research interests.

"This is a much faster, more systematic way of bringing students up to speed," Schulten says.

At the end of each day during each workshop, the participants were asked to evaluate the lectures and tutorials. And on the final day of each workshop, the students were asked to complete a more comprehensive evaluation of the workshop as a whole. The workshops have been highly praised by participants, who overall find them relevant, useful, and well-organized.

"When they leave the workshop, they really feel that they've become new kinds of scientists," Schulten says.



7. Providing clustering skills to enable computational research

The Theoretical and Computational Biophysics Group complements its simulation and modeling workshops with workshops on the basics of cluster computing. After all, once researchers have gained computational skills, they need compute systems on which to conduct computational studies.

These cluster computing workshops familiarize users with the basics of designing, building, and deploying clusters of off-the-shelf PC components. In addition to the discussion of the ABC's of clustering, the workshop also includes the opportunity for participants to build a small PC cluster and to test their own applications.

"We would like to help people avoid the mistakes we made with our first cluster," says Jim Phillips, a senior research programmer in the TCB group and one of the cluster workshop instructors.

To that end, Phillips and co-instructor Tim Skirvin, the administrator of the TCB group's in-house clusters, introduce workshop participants to the potential limiting factors that might influence what type of hardware they should install. Do they have a limited amount of space? If so, dual-core processors might allow them to pack more computational punch into a smaller footprint. Is memory bandwidth crucial to their applications? Maybe an SMP system is the way to go. A research group that is considering adding a cluster to its lab needs to consider how much space is available, how much current the cluster will draw, how the hardware will be cooled, etc.

"One of the nice things about clusters is that you build them to do your specific tasks well," Phillips said. A research group can tailor their cluster to their application and to work with any constraints they face.

Cluster Workshops

Cluster workshops have been held on the campus of the University of Illinois at Urbana-Champaign on Sept. 22-23, 2005, and Nov. 10-11, 2005.

8. Appendix A: Sample agenda

This sample agenda shows the program for the workshop held June 26-30, 2005 in San Francisco, California.

Sun, 6/26: Introduction to Protein Structure and Dynamics, *K. Schulten*

08:30-09:00 Breakfast
09:00-09:30 Opening Remarks
09:30-10:40 Molecular Graphics Perspective of Protein Structure and Function
Coffee Break
11:00-11:50 Molecular Dynamics Method
11:50-12:00 Daily Q & A
Lunch Break
14:00-14:45 Overview of Hands-on Sessions
15:00-15:30 Molecular Graphics Tutorial
Coffee Break
15:45-18:00 Molecular Graphics Tutorial (continued)

Mon, 6/27: Statistical Mechanics of Proteins, *K. Schulten*

08:30-09:00 Breakfast
09:00-10:00 Molecular Dynamics with NAMD
10:00-10:40 Equilibrium Properties of Proteins
Coffee Break
11:00-11:50 Nonequilibrium Properties of Proteins
11:50-12:00 Daily Q & A
Group photo
Lunch Break
19:00-20:30 Molecular Dynamics Tutorial
Coffee Break
20:45-23:00 Molecular Dynamics Tutorial (continued)

Tue, 6/28: Introduction to Bioinformatics, *Z. Luthey-Schulten*

08:30-09:00 Breakfast
09:00-10:00 Introduction to Bioinformatics: Sequence, Structure, and Alignment
10:00-10:40 Evolutionary Concepts in Bioinformatics
Coffee Break
11:00-11:50 Application of Bioinformatics
11:50-12:00 Daily Q & A
Lunch Break
14:00-16:30 Evolution of Protein Structure - Aspartyl tRNA Synthetase
Coffee Break
16:45-18:00 Sequence Alignment Algorithms/Bioinformatics Study of Aquaporins

Wed, 6/29: Parameters for Classical Force Fields, *E. Tajkhorshid*

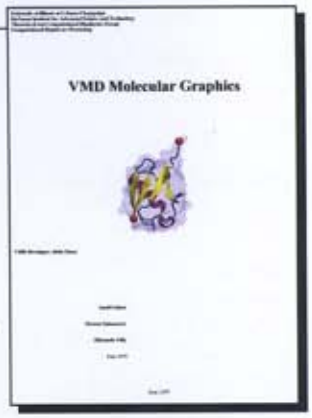
08:30-09:00 Breakfast
09:00-10:00 Introduction to Classical Force Fields
10:00-10:40 Force Fields Parameterization
Coffee Break
11:00-11:50 Applications
11:50-12:00 Daily Q&A
Lunch Break
19:00-21:00 Parameterizing a Novel Residue
Coffee Break
21:15-23:00 Topology File Tutorial

Thu, 6/30: Simulating Membrane Channels, *E. Tajkhorshid*

08:30-09:00 Breakfast
09:00-10:00 Introduction and Examples
10:00-10:40 Transport in Aquaporins
Coffee Break
11:00-11:50 Nanotubes
11:50-12:00 Daily Q&A
Lunch Break
14:00-15:30 Nanotubes/IMD
Coffee Break
15:45-18:00 Stretching Deca-alanine/Open tutorial work time

9. Appendix B: Sample tutorials

VMD Molecular Graphics

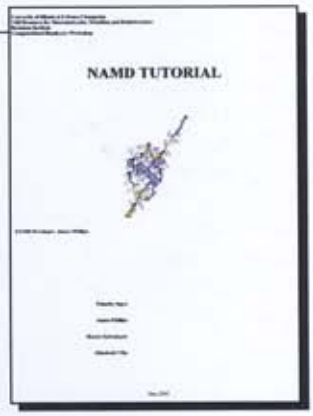


This tutorial, available online at http://www.ks.uiuc.edu/Training/Tutorials/#vmd, introduces new users to VMD and its capabilities. It can also be used as a refresher course for the occasional VMD user wishing to employ this program more productively.

The tutorial covers the basics of molecular graphics representations and will introduce everything you need to know to generate nice graphics. The tutorial also walks scientifically oriented users through the essentials of scripting in VMD, which provides powerful, easy-to-use tools that cannot be offered by a simple graphical user interface.

The examples in the tutorial focus on ubiquitin—a small protein with interesting properties.

NAMD



This tutorial, available online at http://www.ks.uiuc.edu/Training/Tutorials/#namd, provides a first introduction to NAMD and its basic capabilities. It can also be used as a refresher course for the non-expert NAMD user.

The tutorial covers the initial steps of a molecular dynamics simulation, that is, minimization and equilibration of the system. The tutorial then goes on to introduce typical simulation techniques and the analysis of equilibrium properties. Finally, the tutorial deals with steered molecular dynamics and the analysis of unfolding pathways of proteins.

The examples in the tutorial focus on ubiquitin—a small protein with interesting properties.

Appendix C: Instructors and teaching assistants

Instructors:

Rommie Amaro	University of Illinois at Urbana-Champaign
Laxmikant Kale	University of Illinois at Urbana-Champaign
Michael L. Klein	University of Pennsylvania
Ioan Kosztin	University of Missouri
Zan Luthey-Schulten	University of Illinois at Urbana-Champaign
Todd J. Martínez	University of Illinois at Urbana-Champaign
Patrick O'Donoghue	University of Illinois at Urbana-Champaign
James Phillips	University of Illinois at Urbana-Champaign
Tamar Schlick	New York University
Klaus Schulten	University of Illinois at Urbana-Champaign
Robert D. Skeel	University of Illinois at Urbana-Champaign
Tim Skirvin	University of Illinois at Urbana-Champaign
Emad Tajkhorshid	University of Illinois at Urbana-Champaign
Elizabeth Villa	University of Illinois at Urbana-Champaign

Teaching Assistants:

Rommie Amaro	University of Illinois at Urbana-Champaign
Anton Arkhipov	University of Illinois at Urbana-Champaign
Jordi Cohen	University of Illinois at Urbana-Champaign
Eduardo R. Cruz Chu	University of Illinois at Urbana-Champaign
James Gumbart	University of Illinois at Urbana-Champaign
Fatemeh Khalili-Araghi	University of Illinois at Urbana-Champaign
Patrick O'Donoghue	University of Illinois at Urbana-Champaign
Elijah Roberts	University of Illinois at Urbana-Champaign
Marcos Sotomayor	University of Illinois at Urbana-Champaign
Elizabeth Villa	University of Illinois at Urbana-Champaign

Top row, left to right: Anton Arkhipov, Elijah Roberts, JC Gumbart, Jordi Cohen. Bottom row, left to right: Rommie Amaro, Elizabeth Villa, Eduardo Cruz-Chu.

10. Appendix D: Workshop participants

Urbana, Illinois / July 2003

Name	Institution
Sandeep Agnihotri	University of Illinois at Urbana-Champaign
Ni Ai	University of Medicine & Dentistry of New Jersey
Karunesh Arora	New York University
Walter Ash	University of Calgary
Ryan Bannen	University of Wisconsin-Madison
TJ Brunette	University of Massachusetts, Amherst
Don Burgess	Asbury College
Richard Kramer Campen	Pennsylvania State University
Pinaki Chakraborty	University of Illinois at Urbana-Champaign
Eric Chancellor	Vanderbilt University
Chia-en Chang	University of Maryland
Yixin Chew	University of Illinois at Urbana-Champaign
Jason de Joannis	Emory University
Matthew Diamond	Mount Sinai School of Medicine
Richard Evans	University of Illinois at Urbana-Champaign
Eileen Faucher	University of Washington
Philip Fowler	University College London
Ran Friedman	Tel Aviv University
Emmanuel Giodice	Mount Sinai School of Medicine
Genetha Gray	Sandia National Laboratories
Sergei Grudinin	Forschungszentrum Juelich
Anton Guliaev	Lawrence Berkeley National Laboratory
Randall Hall	Louisiana State University
Scott Hampton	University of Notre Dame
Bong-Gyoon Han	Lawrence Berkeley National Laboratory
Melinda Harrison	Duquesne University
Kaden Hazzard	Ohio State University
Jerome Henin	Universite Henri-Poincare
Michael Hoffmann	University of Paderborn
JuHyun Huh	Pohang University of Science and Technology
Timothy Isgro	University of Illinois at Urbana-Champaign
Ask Frode Jakobsen	University of Southern Denmark
Henry Jakubowski	College St. Benedict/St. John's University
Lorant Janosi	University of Missouri, Columbia
Shantenu Jha	University College London
Craig Jolley	Arizona State University
Mohammad Kaazempur-Mofrad	Massachusetts Institute of Technology
Tsutomu Kawatsu	Duke University
Dongwook Kim	Pohang University of Science and Technology
Taeho Kim	University of Toronto
Gemma Kinsella	Trinity College Dublin
Christophe R. Koudella	University of Cambridge
Olga Kravchenko	University of California at Davis
Jer-Lai Kuo	University of Pennsylvania
Han Liang	Princeton University
Jianping Lin	Duke University
Zhanwu Liu	University of Pittsburgh
Anne Loccisano	Duquesne University
Gustavo E. Lopez	University of Puerto Rico at Mayaguez
Gun Ma	University of Notre Dame
James MacDonald	Birkbeck College, University of London
Christopher Maupin	University of Utah
Jason McCoy	University of Wisconsin, Madison
William Moser	Illinois Wesleyan University
Sarah Mueller	Duquesne University
Parag Mukhopadhyay	University of Calgary
Navaratnam Namachchivaya	University of Illinois at Urbana-Champaign
Surendra Singh Negi	School of Health Information Sciences
Steve Nielsen	University of Pennsylvania
Patrick O'Donoghue	University of Illinois
Vanessa Ortiz	University of Pennsylvania
Elif Ozkirimli	Purdue University
Sterling Paramore	University of Utah
Ognjen Perisic	University of Illinois at Chicago
Tatiana Prytkova	Duke University
Yamini Purohit	University of Illinois at Urbana-Champaign
Zhen Qin	University of Utah
Jasmina Sabolovic	Institute for Medical Research and Occupational Health
Gayle Schulte	Pfizer
Elad Segev	Hebrew University of Jerusalem
Anurag Sethi	University of Illinois
Deniz Sezer	Cornell University / Cornell Medical School
William Sheffler	Brown University
Jacob Sonne	Technical University of Denmark
Marcos Sotomayor	University of Illinois at Urbana-Champaign
Scott Stagg	Georgia Institute of Technology
Thomas Steinbrecher	Universitaet Freiburg
Jin Tao	Rutgers
Ioannis Tziligakis	University of Illinois
Ana Vila Verde	University of Minho
Jean-Marc Vuissoz	University Hospital of Bern (Switzerland)
Amy Waligorski	Duquesne University
Jin Wang	Citigroup/SUNY at Stony Brook
Xiaofei Wang	Princeton University
Yanli Wang	University of Toledo
Christopher Wassman	University of California at Irvine
Norbert Welsch	Eberhard Karls Universität Tübingen Germany
Kirk Williams	Tulane University
Miriam Wodrich	University of York
Guosheng Wu	Eli Lilly and Company
Jiancong Xu	University of Utah
Deqiang (David) Zhang	University of California at San Diego
Jieru Zheng	Duke University

Perth, Australia / June 2004

Name	Institution
Mark Abraham	Australian National University
Hernan Alonso	Australian National University
Denis Ballantyne	Curtin University of Technology
David Chandler	Curtin University of Technology
Ben Corry	University of Western Australia
Paul Ellery	Curtin University of Technology
Joel Gilmore	University of Queensland
Sara Hackett	University of Western Australia
Marta Hallay-Suszek	Warsaw University
Joyanne Kelly	University of Western Australia
Abigail Klopper	University of Western Australia
Michael Le Page	University of Western Australia
Allan McKinley	University of Western Australia
Grischa Meyer	University of Western Australia
Mahsa Mooranian	University of Western Australia
Corrine Porter	University of Western Australia
Ben Powell	University of Queensland
Jennifer Riesz	University of Queensland

Jason Schmidberger	University of Queensland
Mahjooba Sidiqi	University of Western Australia
Donald Thomas	University of Western Australia
Julian Vivian	University of Western Australia
Jackie Wilce	University of Western Australia
Mathew Wilce	University of Western Australia

Urbana, Illinois / November 2004

Name	Institution
Vasyl Aleksenko	Michigan Technological University
Bogdan Barz	University of Missouri-Columbia
Violeta Beleva	Los Alamos National Laboratory
Nitin Bhardwaj	University of Illinois at Chicago
Michael Bradley	Washington University
Baoqiang Cao	University of Cincinnati
Yong Jiang	Emory University
Harindar Keer	University of California, Irvine
Heike Meiselbach	Friedrich-Alexander-Universitat, Institute for Biochemistry
Murtaza Mogri	University of California, San Diego
Lacramioara Negureanu	Louisiana State University
Rene Nome	University of Chicago
Ole Olsen	Novo Nordisk
Soumya Patnaik	Air Force Research Laboratory
Laura Rowe	University of Kentucky
Goundla Srinivas	University of Pennsylvania
Seiichiro Tanizaki	Michigan State University
Anne Tuukkanen	University of Helsinki
Ioannis Tziligakis	University of Illinois
Michael Yonkunas	University of Pittsburgh
Wanhua Zhao	Louisiana Tech University

Boston / December 2004

Name	Institution
Marcela Aliste	Georgia Institute of Technology
James Apgar	Massachusetts Institute of Technology
Gokhan Caliskan	Johns Hopkins University
Leyla Celik	University of Aarhus
Blake Charlebois	University of Toronto
Christopher Glosser	Southern Illinois University
John Ip	Dell, Inc.
Basak Isin	University of Pittsburgh
Ekta Khurana	University of Pennsylvania
Seung Lee	Massachusetts Institute of Technology
Edward Lyman	University of Pittsburgh
Shane Nelson	University of Wyoming
Lina Nilsson	University of Washington
Steve Presse	Massachusetts Institute of Technology
John Robinson	University of Alabama at Birmingham
Edina Rosta	Eotvos University, Hungary
Gaurav Sharma	Northeastern University
Arvind Sivasubramanian	Johns Hopkins University
Nuri Temiz	University of Pittsburgh School of Medicine
Marty Ytreberg	University of Maine

Lake Tahoe / May 2005

Name	Institution
Anton Burykin	University of Southern California
Andrea Catte	University of Alabama at Birmingham
Kevin Facemeyer	University of Nevada
Jesus Fernandez	Cajal Institute of Neurobiology
Samuel Flores	Yale University
Biff Forbush	Yale University, Cellular and Molecular Physiology
Kim Gunnerson	University of Washington
Mark Harder	Oregon State University
Ville Kaila	University of Helsinki
Karina Martinez	Mayorga University of Arizona
Justin McDowell	Florida A&M University
Anna Modzelewska	International Institute of Molecular and Cell Biology
Elad Project	Tel Aviv University
Shahid Qamar	Arizona State University
Jared Schrader	Northwestern University
Jufang Shan	St. Jude Children's Research Hospital
Alejandro Valbuena	Cajal Institute of Neurobiology
Robert Wiese	University of Nevada
Ying Yin	University of Illinois
Huamin Zhang	Purdue University

Chicago / June 2005

Name	Institution
Robert Bryce	University of Alberta
Christohper Calderon	Purdue/Princeton
Julio Cordero	University of Virginia
Naranbaatar Dashdorj	Purdue University
Laura Domínguez-Dueñas	Universidad Nacional Autónoma de México
Assaf Ganoth	Tel Aviv University
Alexander Karpikov	Yale University
Chien-Tsun Kuan	Duke University Medical Center
Pick-Wei Lau	University of Arizona
Chunhui Li	Northwestern University
Arpita Mitra	Washington University
Ersin Emre Oren	University of Washington
Reid Ormseth	Air Force Research Laboratory
Deepangi Pandit	New Jersey Institute of Technology
Sheldon Park	University of Pennsylvania
Vojislava Pophristic	University of the Sciences in Philadelphia
Andrew Shih	University of Pennsylvania
Arne Strand	Howard Hughes Medical Institute
Valeria Vasquez	University of Virginia
Sharon Weldon	Illinois State University

San Francisco / June 2005

Name	Institution
Bo Yang Baker	University of California, San Francisco
Christopher Chang	National Renewable Energy Laboratory
Gerardo Cisneros	National Institute of Environmental Health Sciences
Frank Cochran	Stanford University
Coray Colina	University of North Carolina
Matthew Downton	Simon Fraser University
Donald Engel	University of Pennsylvania
Haixiao Gao	Howard Hughes Medical Institute
Leo Kinarsky	University of Nebraska Medical Center
Piotr Koprowski	University of California, Berkeley
Noriyuki Kurita	Toyohashi University of Technology
Deborah Kuzmanovic	Geo-Centers/U.S. Army
Dmitry Lupyan	Mount Sinai School of Medicine
Neelan Marianayagam	University of California, Berkeley
Jeffrey Miller	Sangamo BioSciences, Inc.
Irina Moreira	Faculdade de Ciências da Universidade do Porto
Eric Peterson	California Institute of Technology
Birgit Schiott	Aarhus University
Darren Segall	California Institute of Technology
Su-Hsiu Wu	University of Rhode Island

12. Appendix E: Evaluation highlights

Urbana, Illinois / July 2003

- More than 87 percent of those participants who evaluated the summer school workshop said the experience broadened their understanding of concepts and principles of computational and theoretical biophysics.
- More than 80 percent believed the workshop improved their ability to carry out original research in computational and theoretical biophysics
- More than 50 percent said the workshop significantly improved their computational skills.
- More than 85 percent said the workshop taught them techniques that were directly applicable to their careers.
- More than 87 percent felt the workshop was relevant to their research.
- More than 95 percent said the hands-on tutorials were a crucial part of the learning process.

Perth, Australia / June 2004

- 100 percent of the participants who responded said the workshop broadened their understanding of concepts and principles in computational and theoretical biophysics
- 95 percent said the workshop improved their ability to carry out original research in computational and theoretical biophysics
- 85 percent said the workshop significantly improved their computational skills
- 65 percent believed the experience taught techniques that were applicable to their careers
- 70 percent thought the workshop was relevant to their research
- 100 percent said the hands-on tutorials were an important part of the learning process

Urbana, Illinois / November 2004

- More than 76 percent of the participants who responded said the workshop broadened their understanding of concepts and principles in computational and theoretical biophysics
- Over 86 percent said the workshop improved their ability to carry out original research in computational and theoretical biophysics
- More than 64 percent said the workshop significantly improved their computational skills
- 94 percent believed the experience taught techniques that were applicable to their careers
- Over 82 percent thought the workshop was relevant to their research
- 100 percent said the hands-on tutorials were an important part of the learning process

Boston / December 2004

- Nearly 95 percent of the participants who responded said the workshop broadened their understanding of concepts and principles in computational and theoretical biophysics
- Almost 90 percent said the workshop improved their ability to carry out original research in computational and theoretical biophysics
- More than 83 percent said the workshop significantly improved their computational skills
- 100 percent believed the experience taught techniques that were applicable to their careers
- 97 percent thought the workshop was relevant to their research
- Almost 95 percent said the hands-on tutorials were an important part of the learning process

Lake Tahoe / May 2005

- 92 percent of the participants who responded said the workshop broadened their understanding of concepts and principles in computational and theoretical biophysics
- 93 percent said the workshop improved their ability to carry out original research in computational and theoretical biophysics
- 71 percent said the workshop significantly improved their computational skills
- 86 percent believed the experience taught techniques that were applicable to their careers
- 85 percent thought the workshop was relevant to their research
- 85 percent said the hands-on tutorials were an important part of the learning process

Chicago / June 2005

- 100 percent of the participants who responded said the workshop broadened their understanding of concepts and principles in computational and theoretical biophysics
- 85 percent said the workshop improved their ability to carry out original research in computational and theoretical biophysics
- 80 percent said the workshop significantly improved their computational skills
- 95 percent believed the experience taught techniques that were applicable to their careers
- 95 percent thought the workshop was relevant to their research
- 100 percent said the hands-on tutorials were an important part of the learning process

San Francisco / June 2005

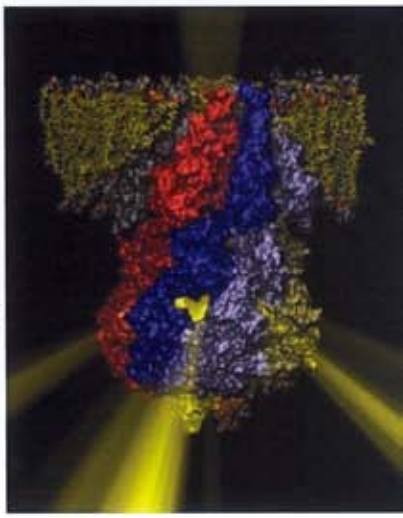
- 100 percent of the participants who responded said the workshop broadened their understanding of concepts and principles in computational and theoretical biophysics
- 84 percent said the workshop improved their ability to carry out original research in computational and theoretical biophysics
- 34 percent said the workshop significantly improved their computational skills
- 89 percent believed the experience taught techniques that were applicable to their careers
- 89 percent thought the workshop was relevant to their research
- 95 percent said the hands-on tutorials were an important part of the learning process

"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."

"Possibly the most valuable thing 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."

"The 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."

13. Appendix F: Sample announcement



This announcement was distributed to publicize the most recent workshop, held in San Francisco in June 2005.

The workshop will explore 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 and membrane proteins, mechanisms of molecular motors, trafficking in the living cell through water and ion channels, and signaling pathways. 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 and steered molecular dynamics simulations.

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 in the morning will be followed by hands-on computer labs in the afternoon in which students will be able to set up and run simulations. Enrollment limited to 20 participants.

Appendix G: Tutorial authors

Bioinformatics and Sequence Alignment
Felix Autenrieth
Barry Isralewitz
Zan Luthey-Schulten
Taras Pogorelov
Anurag Sethi

Bioinformatics of Aquaporins
Brijeet Dhaliwal
Fatemeh Khalili
Zan Luthey-Schulten
Emad Tajkhorshid
Elizabeth Villa

Evolution of Protein Structure - Aspartyl-tRNA Synthetase
Rommie Amaro
Brijeet Dhaliwal
Zan Luthey-Schulten
Patrick O'Donoghue

NAMD Tutorial
Timothy Isgro
James Phillips
Marcos Sotomayor
Elizabeth Villa

Parameterizing a Novel Residue
Rommie Amaro
Brijeet Dhaliwal
Zan Luthey-Schulten

Simulation of Water Permeation Through Nanotubes
Jordi Cohen
Emad Tajkhorshid
Fangqiang Zhu

Appendix H: Related websites

The Theoretical and Computational Biophysics Group
http://www.ks.uiuc.edu/

Visual Molecular Dynamics (VMD)
http://www.ks.uiuc.edu/Research/vmd/

NAMD, Scalable Molecular Dynamics
http://www.ks.uiuc.edu/Research/namd/

2003 Workshop Tutorials
http://www.ks.uiuc.edu/Training/SumSchool/labs.html

2004-2005 Workshop Tutorials
http://www.ks.uiuc.edu/Training/Tutorials/workshoptutorials/index.html

Appendix I: Laptop configuration

The computers used for the hands-on workshops were 21 Apple PowerBook G4 laptops:
- Apple G4 1.33 GHz processors
- 768 MB RAM
- 60 GB hard drive
- 15.1 inch display

The software configuration included:
- VMD 1.8.3a21
- NAMD 2.5
- Mathematica 5.0
- MatLab 6.5.1.200223

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