University of Illinois at Urbana-Champaign
Theoretical and Computational Biophysics Group
National Center for Supercomputing Applications

Hands-on Course in Computational Biology

Workshop Outcome Report

http://www.ks.uiuc.edu/

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Introduction

The Hands-on Course in Computational Biology was held at the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign, during the week of November 8 - 12, 2004. Sponsored by the Theoretical and Computational Biophysics Group (TCBG) and the National Center for Supercomputing Applications (NCSA), the workshop explored physical models and computational approaches used for the simulation of biological systems and the investigation of their function at an atomic level.

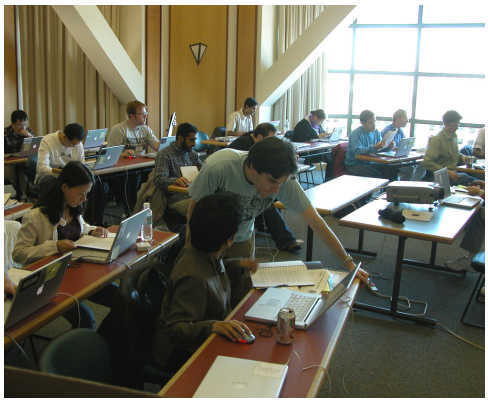

Figure 1: Workshop participants proceed through a tutorial on Apple G4 Laptops in room 5269 of the Beckman Institute

Participants attended lectures and took part in hands-on tutorial sessions. Following morning lectures on theory by TCBG professors, participants would proceed through tutorials on pre-configured Apple laptops in the afternoon computer lab managed by TCBG graduate students. In total, there were twenty-one participants from all over the United States and other countries. The workshop was 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.

1 Participant Profiles and Statistics

There were twenty-one participants in the workshop. Each individual applied for a seat, and was selected from a pool of 57 applicants.

Figure 2: Participants of the workshop

The average profile of a participant was a life sciences graduate student pursuing a doctorate at a university in the United States. About a quarter of participants were already in possession of a doctorate, whereas less then ten per cent were working towards an undergraduate degree. Overall the group was internationally diverse, with varying backgrounds in biology, chemistry, and physics. A distribution of education is provided in Table 1 and of industry in Table 2.

Current Educational Standing	**Number**
Doctorate	4
Graduate Student	14
Undergraduate Student	2
Non-student Academic	1
Total	21

Table 1: Breakdown of participants and their current educational standing.

Location	Number
Education	18
Government	2
Industry	1

Table 2: Distribution of types of participant work locations.

In order to gauge the performance of the workshop, lecture and tutorial surveys were distributed every day. The surveys asked participants to rate the relevance of lectures and tutorials, and to provide comments on each. Using a combination of a five-point relevance scale (5-Strongly agree, 4-Agree, 3-Unsure, 2-Disagree, 1-Strongly disagree), with space for comments, the intention was to gain as much critical feedback as possible.

Figure 3: Participants not only proceeded through the tutorials, but critically evaluated the tutorials every day.

On the final day, a general evaluation survey was given to assess the overall quality of the workshop. The survey contained a series of five-point scale questions on the items listed in the first column in Table 3. The final comment section included open-ended questions asking for suggestions to improve the workshop. A brief synopsis of the results from this survey are available in Table 3.

Survey Question Category	**Average**	**Mode**	**Percent Positive***
Outcome	4.3	5	81%
Lectures	4.5	5	92%
Hands-on Tutorials	4.6	5	88%
Environment & Technical Resources	4.6	5	91%
Communication & Dissemination	4.5	5	92%
General Organization	4.7	5	96%
Overall Satisfaction	4.7	5	96%

Table 3: A brief synopsis of survey results from workshop participants. Based on a five-point scale (5-Strongly agree, 4-Agree, 3-Unsure, 2-Disagree, 1-Strongly disagree), participants rated the quality of various aspects of the workshop in a survey conducted on the final day. *Percent Agreeing or Strongly Agreeing that a workshop attribute was positive.

2 Agenda

Below is the agenda for the workshop.

Mon, 11/8: Introduction to Protein Structure and Dynamics Klaus Schulten

09:15-09:40 Opening Remarks
09:45-10:40 Molecular Graphics Perspective of Protein Structure & Function
*B*reak
10:50-11:50 Molecular Dynamics Method
11:50-12:00 Daily Q & A
*L*unch
14:00-14:40 Overview of Hands-on Sessions
14:45-18:00 Molecular Graphics Tutorial
(R. Braun, M. Gao)

Figure 4: Klaus Schulten

Tue, 11/9: Introduction to Bioinformatics Zan Luthey-Schulten

09:00-10:00 Sequence Structure and Alignment
10:00-10:40 Evolution of Protein Structure
*B*reak
11:00-11:50 The Biology and Bioinformatics of tRNA Synthetase and Aquaporins
11:50-12:00 Daily Q & A
*L*unch
14:00-18:00 Evolution of Protein Structure: tRNA Synthetases
Time permitting: Bioinformatics of Aquaporins
(P. ODonoghue, J. Yu)

Figure 5: Zan Luthey-Schulten

Wed, 11/10: Statistical Mechanics of Proteins Klaus Schulten

09:00-10:00 Equilibrium Properties of Proteins
10:00-10:40 Nonequilibrium Properties of Proteins
*B*reak
11:00-11:50 Simulated Cooling of Proteins
11:50-12:00 Daily Q & A
*L*unch
14:00-18:00 Molecular Dynamics Tutorial, Deca-alanine Tutorial
(M. Dittrich, T. Isgro)

Figure 6: Klaus Schulten

Thu, 11/11: Parameters for Classical Force Fields Zan Luthey-Schulten

09:00-10:00 Introduction and Examples
10:00-10:40 Introduction to Classical Force Fields
*B*reak
11:00-11:50 Methods of Parameterization
11:50-12:00 Daily Q & A
*L*unch
14:00-15:30 System set-up of HisH
15:30-18:00 Semiempirical Parameter Generation with Spartan
(P. ODonoghue, F. Khalili-Araghi, C. Kanchanawarin)

Figure 7: Zan Luthey-Schulten

Fri, 11/12: Simulating Membrane Channels Emad Tajkhorshid

09:00-10:00 Introduction and Examples
10:00-10:40 Transport in Aquaporins
*B*reak
11:00-11:50 Nanotubes
11:50-12:00 Daily Q & A
*L*unch
14:00-15:00 Bioinformatics of Aquaporins
15:00-18:00 Nanotubes
(J. Cohen, D. Lu)

Figure 8: Emad Tajkhorshid

3 Laptop Specifications

The computers used for the hands-on computer lab were Apple PowerBook G4 Laptops. Each laptop was configured by TCBG staff to create an optimal computing environment.

3.1 Hardware

The Apple PowerBook G4 laptops had the following hardware specifications:

- Apple G4 1.33 GHz processor
- 768 MB RAM
- 60 GB hard drive
- 15.1 inch display

Figure 9: Apple G4 Laptop

3.2 Software

The laptops were configured with the following software packages:

VMD 1.8.3a21*
NAMD 2.5*
Mathematica 5.0
MatLab 6.5.1.200223
Spartan '02 v1.0.7a
* indicates software packages developed by TCBG

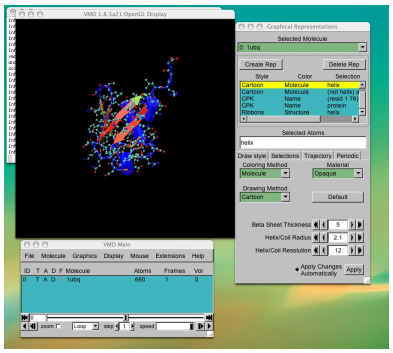

Figure 10: VMD is an example of the software. Here steps from the VMD tutorial are displayed.

4 Documents

Various documents were used throughtout the hands-on workshop. The bulk of documents were tutorials, which provided step-by-step instructions on how to use paticular software packages when evaluating certain biological systems.

4.1 Tutorials

Below is a list of tutorials used for the workshop:

VMD Molecular Graphics
Evolution of Protein Structure
Aquaporins
NAMD
Stretching Deca-Alanine
Parameterizing a Novel Residue
Simulation of Water Permeation through Nanotubes

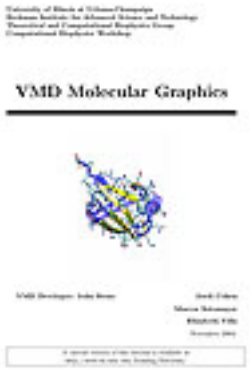

Figure 11: VMD Molecular Graphics Title Page

4.2 Supplementary Material

Supplementary materials were provided to gain familiarity quickly with the computers provided for the workshop. The titles are listed below:
Hands-on Session
UNIX Primer
Mac Primer

4.3 Websites

The following websites provided information and access to the tutorials for the workshop:
http://www.ks.uiuc.edu/Training/Tutorials/
http://www.ks.uiuc.edu/Training/Workshop/Urbana/

5 Anonymous Participant Comments

This was truly an outstanding workshop and experience. I commend all of those that worked very hard to provide such a complete, well-organized and excellent environment. Coming into the workshop having worked with NAMD and VMD I have to say it was very much challenged by the topics.
(General Evaluation, Question 1, Form 2)

I really enjoyed it. I hope I can stay longer.
(General Evaluation, Question 1, Form 12)

Very good job!
(General Evaluation, Question 1, Form 14)

The level of the talk was good considering the various background knowledge people have.
(Day 1, Form 3)

The handout is clear and self-explanatory. The hands-on approach also is very pedagogical. The TAs are friendly and knowledgeable.
(Day 1, Form 16)

I find the multiple sequence alignment feature incorporated in the VMD very smooth and well integrated. I will look forward for it. TA was very helpful and open for discussion.
(Day 2, From 19)

Well discussed. Well explained.
(Day 3, From 18)

Excellent tutorial! Excellent TAs!
(Day 4, Form 17)

The lecture today was excellent. It was lucid and included many practical hints and suggestions that were great.
(Day 5, Form 7)

Lecture created strong link between structure and function. On the whole, it was great.
(Day 5, Form 17)

This tutorial served as a good illustration of what you can learn from a simplified model. The use of auto IMD to view the consequences of changing atomic parameters was a nice illustration of Dr. Tajkhorshid‘s point that we should try things that you can only do in simulation (i.e. changing charge and VdW parameters) in order to understand the system better.
(Day 5, Form 3)

EXCELLENT
(Day 3, Form 1)