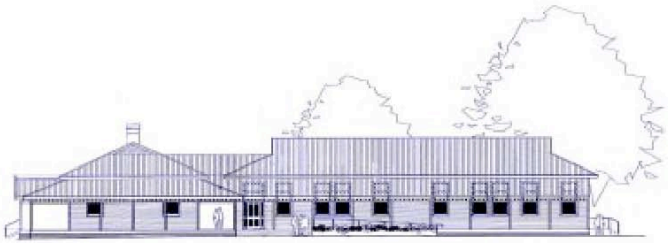


Institute of Advanced Studies

The University of Western Australia

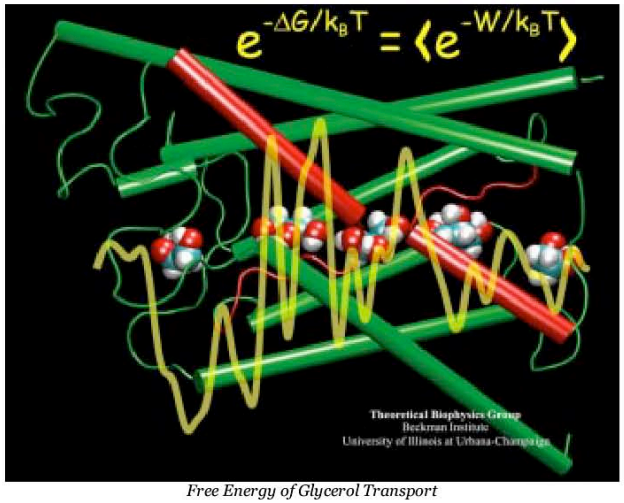
Computational Biology Workshops in 2004

First Announcement

The IAS Professor-at-Large Klaus Schulten will conduct two workshops in the *Faculty of Life & Physical Sciences* in 2004.

June 7-12
"Introduction to Molecular Dynamics in Biological Systems"

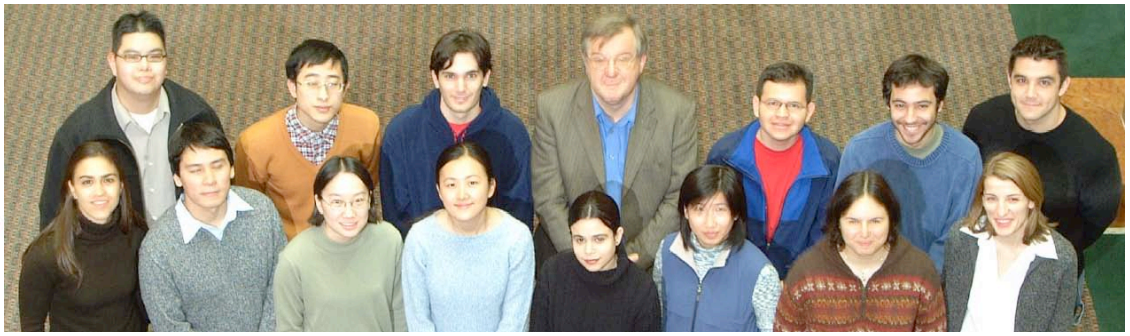
June 14-19
"Computational & Theoretical Biophysics"



Free Energy of Glycerol Transport

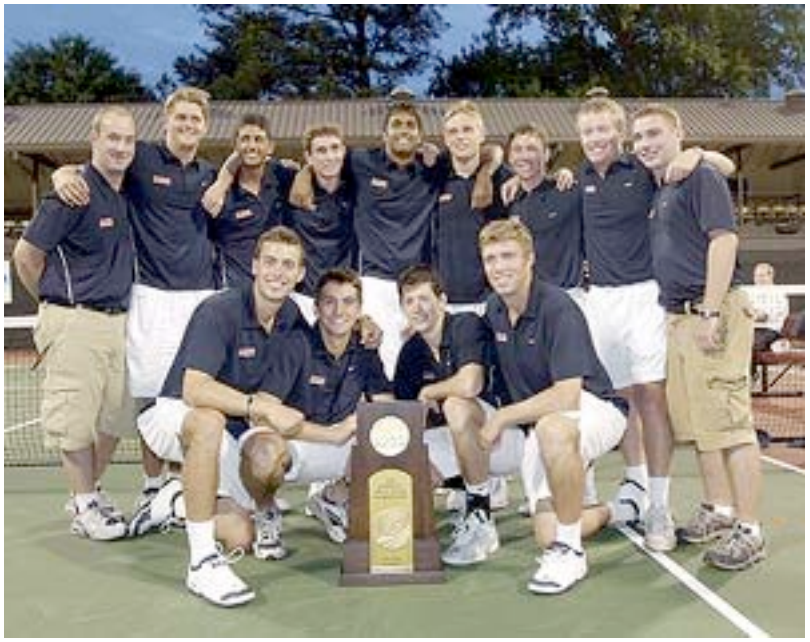
THE UNIVERSITY OF WESTERN AUSTRALIA
FACULTY OF Life and Physical Sciences

Welcome

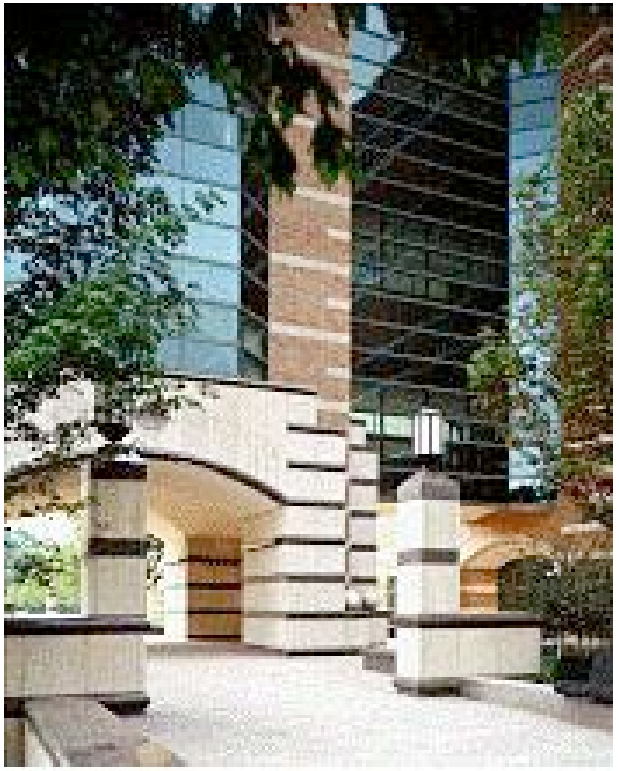


Theoretical and Computational Biophysics Group

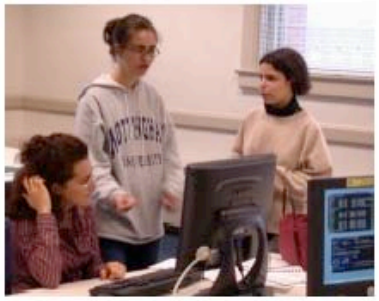
Professors Zan Luthey-Schulten
and Klaus Schulten
together with Rommie Amaro
Fatemeh Khalili
Elizabeth Villa



Our University



The Program



Theoretical and Computational Biophysics School 2004

Program

Location

All sessions will be in the Mathematics Lecture Room 2 (G19;
see map at http://maps.uwa.edu.au/crawley/display/10)
except the Mon, June 14 and Tue, June 15 (mornings only) "Model your own system" session for continuing participants; these sessions will be in the Institute of Advanced Studies (IAS) conference room as indicated in the program.

Handouts

Hands-on Sessions (html ,pdf)
Mac Primer (html ,pdf)
Unix Primer (html ,pdf)

Collaborative Exercises

To be posted

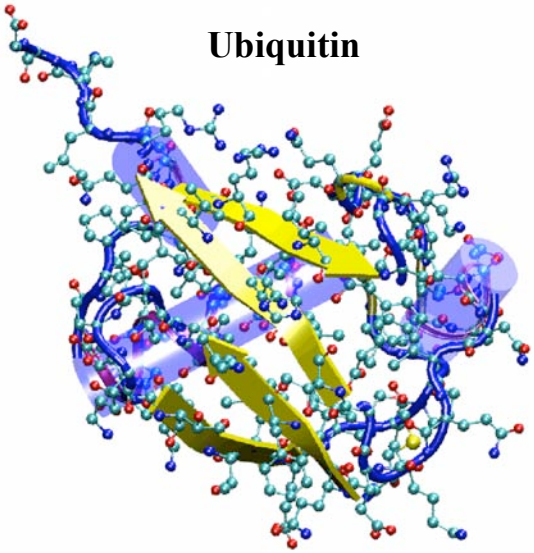
Mon, 6/7: *Introduction to Protein Structure and Dynamics*

09:00-9:30
Opening Remarks (pdf)

9:30-11:00
Molecular Graphics Perspective of Protein Structure and Function (pdf)

Coffee Break

11:30-12:30
Molecular Dynamics Method (part 1 - pdf; part 2 - pdf)


Ubiquitin

12:30-12:45
Daily Q & A

Lunch Break

14:00-14:45
Overview of Hands-on Sessions (E. Villa, F. Khalili)

15:00-18:00
Hands-on -- Molecular Graphics Tutorial (html, pdf) (E. Villa, F. Khalili, R. Amaro)

Tue, 6/8: *Introduction to Bioinformatics*

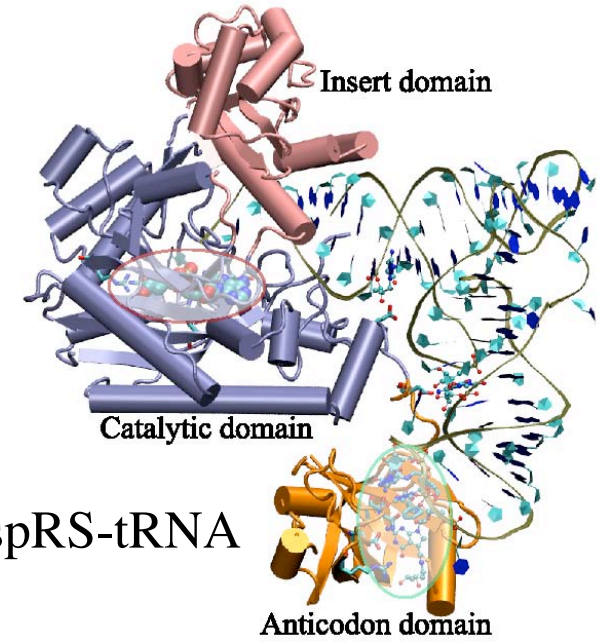
09:00-10:00
Sequence and Structure Alignment Algorithms (pdf)

10:00-11:00
Evolution of Protein Structure (pdf)

Coffee Break

11:30-12:30
Bioinformatics of tRNA Synthetase (pdf)

12:30-12:45
Daily Q & A



AspRS-tRNA

Lunch Break
(12:45-13:30 Staff Meeting, 3169 BI)

14:30-16:00
Sequence Alignment Algorithms (html, pdf) (R. Amaro, E. Villa, F. Khalili)

16:00-18:00
Evolution of tRNA Synthetases (html, pdf) (R. Amaro, E. Villa, F. Khalili)

Wed, 6/9: *Statistical Mechanics of Proteins*

09:00-10:00
Equilibrium Properties of Proteins (pdf)

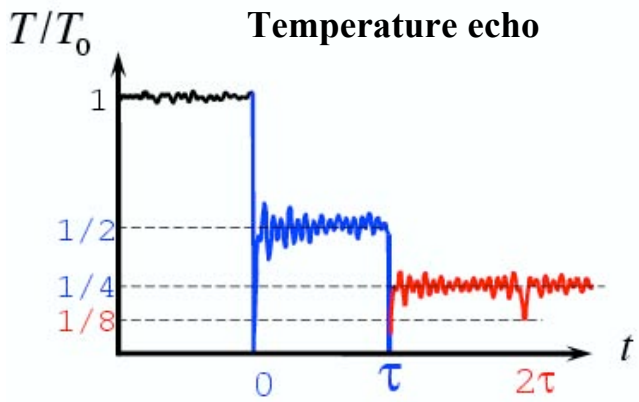
10:00-11:00
Nonequilibrium Properties of Proteins (pdf)

Coffee Break

11:30-12:30
Simulated Cooling of Proteins (pdf)

12:30-12:45
Daily Q & A

Lunch Break



14:00-18:00
Hands-on -- Molecular Dynamics Tutorial (html, pdf) (E. Villa, F. Khalili, R. Amaro)

Thu, 6/10: *Steered Molecular Dynamics of Proteins*

09:00-10:00
Introduction and Examples (pdf)

10:00-11:00
Mechanical Proteins (pdf)

Coffee Break

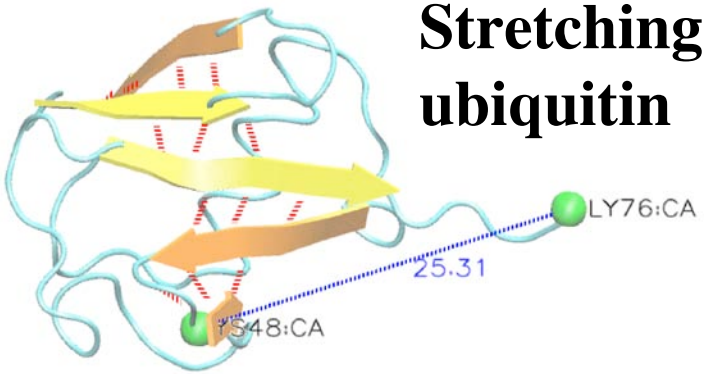
11:30-12:30
Determining Potentials (pdf)

12:30-12:45
Daily Q & A

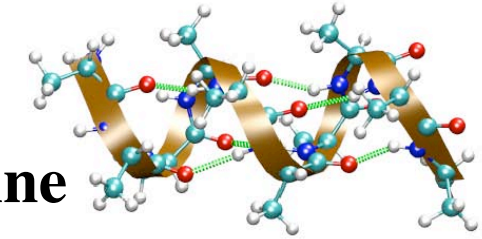
Lunch Break
(12:45-13:30 Staff Meeting, 3169 BI)

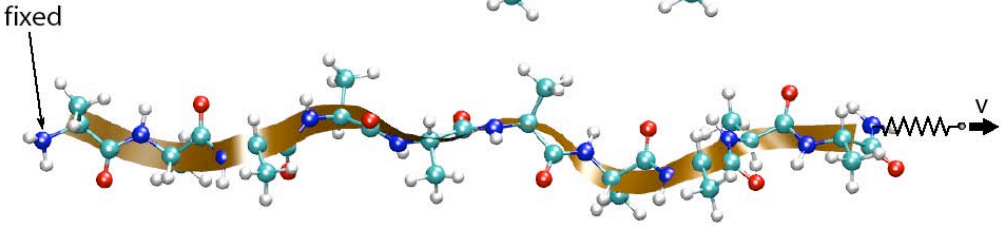
14:00-18:00
Hands-on -- Molecular Dynamics Tutorial (html, pdf) (E. Villa, F. Khalili, R. Amaro)

Stretching ubiquitin



Stretching Deca-alanine





Fri, 6/11: *Modeling Large Systems*

09:00-10:00
Molecular Machines of the Living Cell (pdf)

10:00-11:00
Light Harvesting in Photosynthesis (pdf)

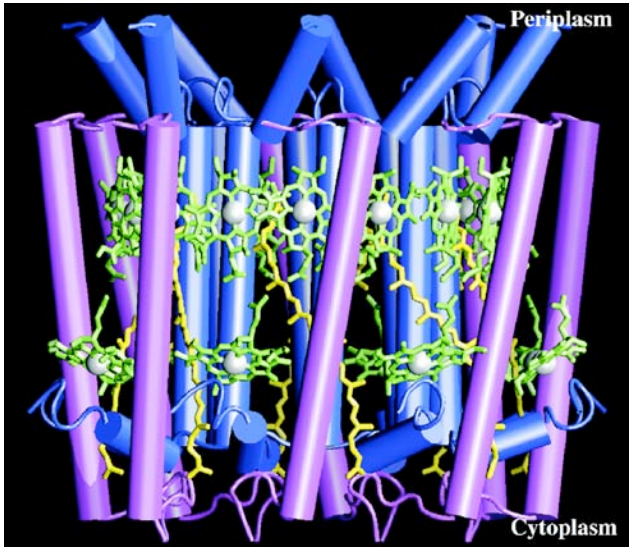
Coffee Break

11:30-12:00
ATP Synthase (pdf)

12:00-12:15
Daily Q & A

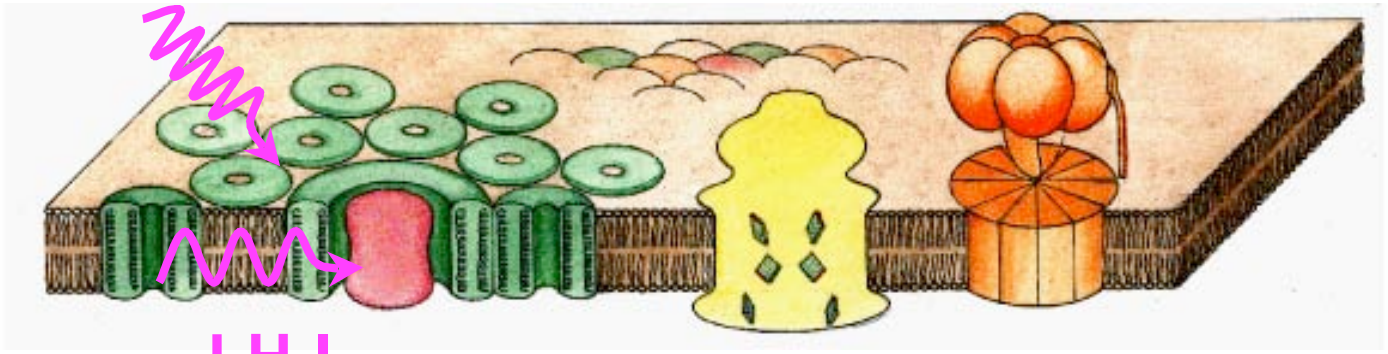
Lunch Break

14:00-18:00
Hands-on -- Stretching Deca-Alanine (html, pdf) (E. Villa, F. Khalili, R. Amaro)



LH-II

Photosynthetic unit of purple bacteria



LH-I
LH-II
RC
bc_1
ATPase

Mon, 6/14: *Introduction to Protein Structure and Protein Bioinformatics*

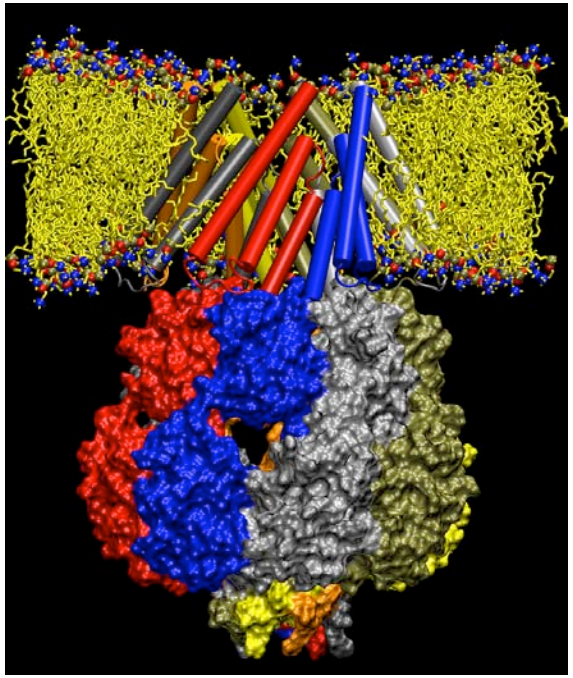
New Participants

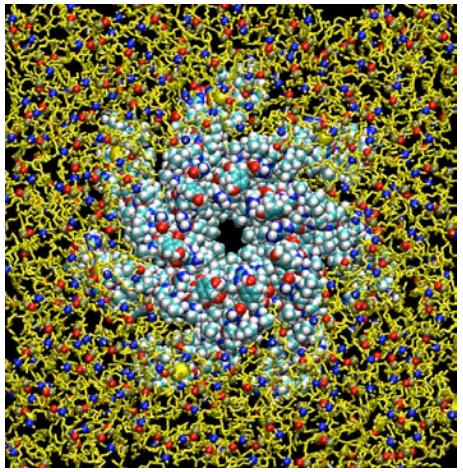
09:00-10:00
Molecular Graphics Perspective of Protein Structure and Function (pdf)

10:00-11:00
Introduction to Bioinformatics

Coffee Break

11:30-12:30
Evolutionary Analysis of Aquaporins (pdf)





Mechanosensitive channel MscS - a bit too large, yet.

Continuing Participants

9:00-12:30

IAS Conference Room
Model your own system with assistance from teaching assistants (E. Villa, F. Khalili, R. Amaro)

All Participants

12:30-12:45
Daily Q & A

Lunch Break

New Participants

14:00-14:30
Overview of Hands-on Sessions (E. Villa, F. Khalili, R. Amaro)

14:30-16:30
Molecular Graphics Tutorial (html, pdf) (continuing participants, E. Villa, F. Khalili, R. Amaro)

16:30-18:00
Bioinformatics of Aquaporins (html, pdf) (continuing participants, E. Villa, F. Khalili, R. Amaro)

Continuing Participants

14:00-18:00

Tue, 6/15: *Introduction to Protein Dynamics*

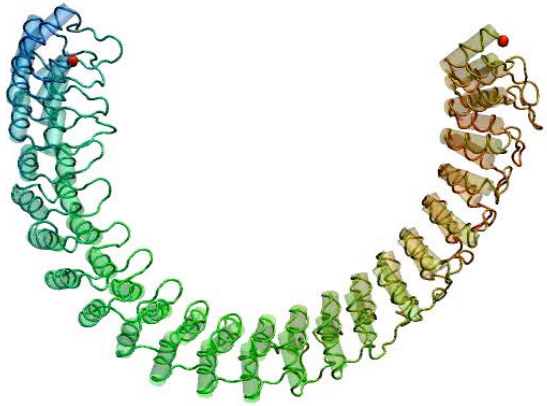
09:00-10:00
Equilibrium Properties of Proteins (pdf)

10:00-11:00
Nonequilibrium Properties of Proteins (pdf)

Coffee Break

Ankyrin stretching

11:30-12:30
Simulated Cooling of Proteins (pdf)



Continuing Participants

9:00-12:30

IAS Conference Room
Model your own syst**New Participants**

14:00-18:00

All Participants Molecular Dynamics Tutorial (html, pdf) (continuing participants, E. Villa, F. Khalili, R. Amaro)

12:30-12:45
Daily Q & A

Continuing Participants

Lunch Break

14:00-18:00
Model your own system with assistance from teaching assistants (E. Villa, F. Khalili, R. Amaro)

Wed, 6/16: *Parameters for Classical Force Fields*

09:00-10:00
Introduction and Examples (pdf)

10:00-11:00
Introduction to Classical Force Fields (pdf)

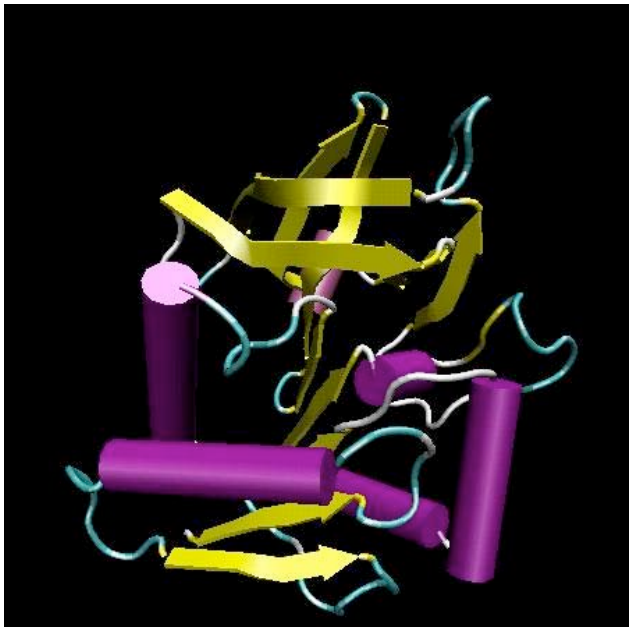
Coffee Break

11:30-12:30
Methods of Parameterization (pdf)

12:30-12:45
Daily Q & A

Lunch Break

HisH



14:30-15:30
System Setup of HisH with the Molecular Modeling Package Moe (html, pdf) (R. Amaro, E. Villa, F. Khalili)

15:45-17:00
Semiempirical Parameter Generation with Spartan (html, pdf) (R. Amaro, E. Villa, F. Khalili)

Thu, 6/17: *Simulating Membrane Channels*

09:00-10:00
Introduction and Examples (pdf)

10:00-11:00
Transport in Aquaporins (pdf)

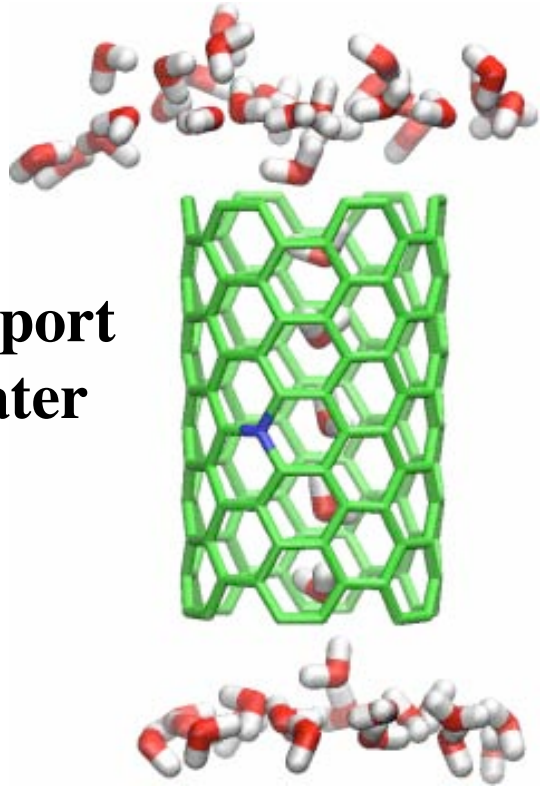
Coffee Break

11:30-12:30
Nanotubes (pdf)

12:30-12:45
Daily Q & A

12:15-12:45
Concluding Remarks

Lunch Break



14:00-15:00
Bioinformatics of Aquaporin (html, pdf) (E. Villa, F. Khalili, R. Amaro)

15:00-18:00
Nanotubes (html, pdf) (E. Villa, F. Khalili, R. Amaro)

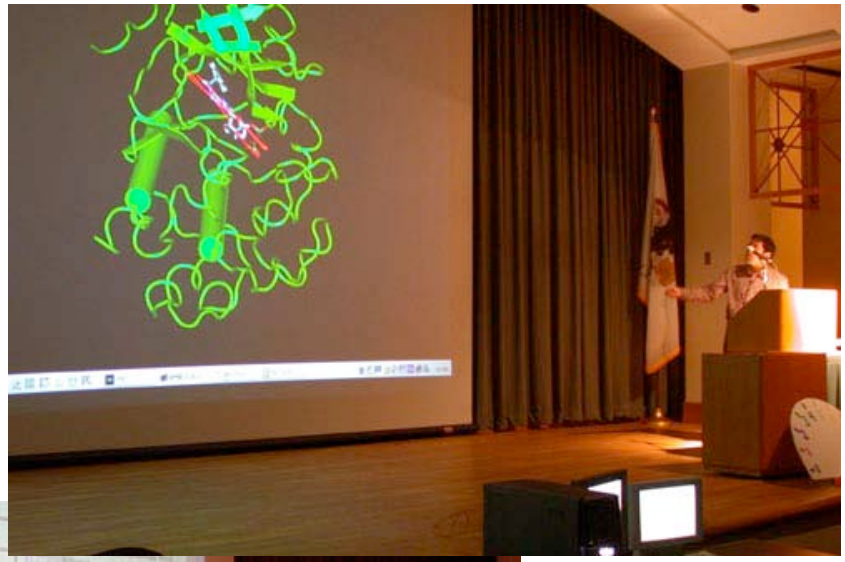
Fri, 6/18: *Selected Participant Presentations*

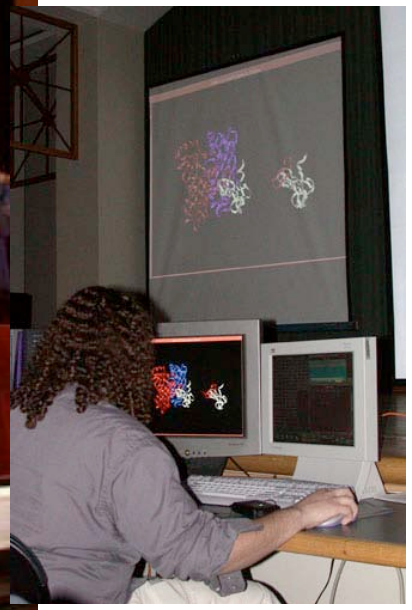
09:00-11:00
"Model your own System" Presentations

Coffee Break

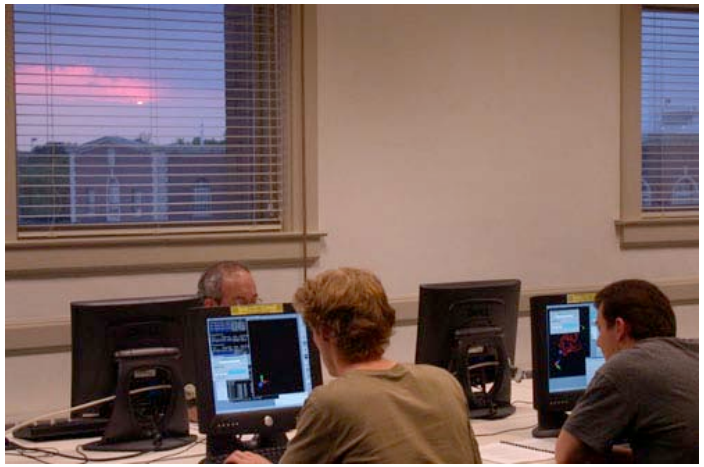
11:30-12:00
"Model your own System" Presentations
12:30-12:45
Closing Remarks

Lunch





General



- The summer school is a volunteer effort
- The main focus are the hands-on sessions
- The aim is to get you to do computational biology
- The lecturers / teaching assistants provide tutorials for you
- The optimal course is that you help each other

- Model your system (Friday, June 18: Beauty Contest)

- Please give us feedback to improve lectures and tutorials
- Please give us feedback to encourage more schools

Thank you University of Western Australia

Special thanks to:

Terri-ann White (IAS)

Jackie Wilce

Syd Hall

UWA Institute of Advanced Studies
Milka Bukilic

Let's enjoy two weeks of scholarship and collegiality