



Computational Biology Workshops in 2004

First Announcement

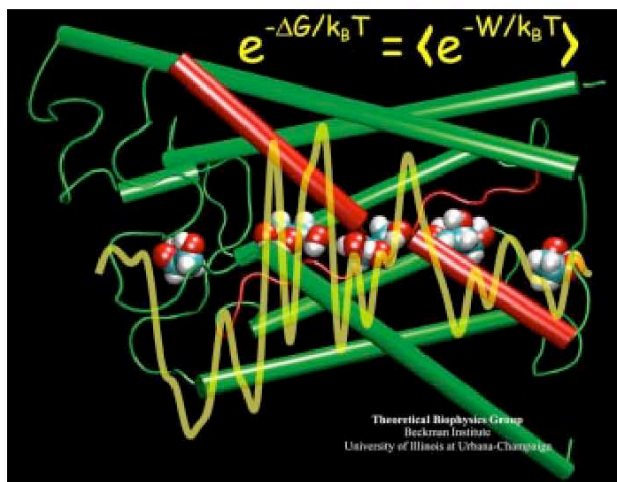
The IAS Professor-at-Large Klaus Schulten will conduct two workshops in the *Faculty of Life & Physical Sciences* in 2004.

June 7-12

"Introduction to Molecular Dynamics in Biological Systems"

June 14-19

"Computational & Theoretical Biophysics"



Free Energy of Glycerol Transport

Welcome



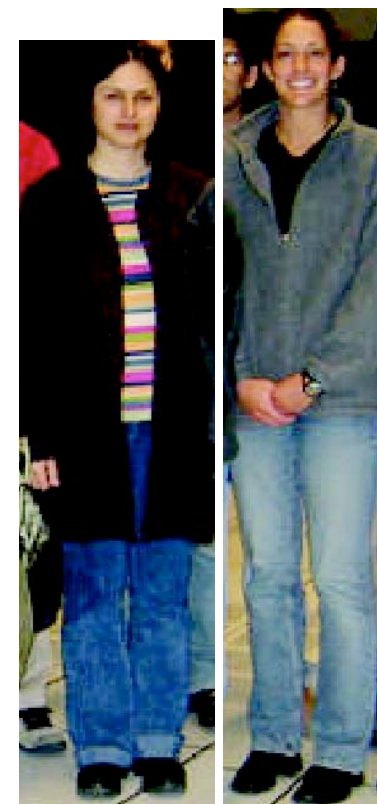
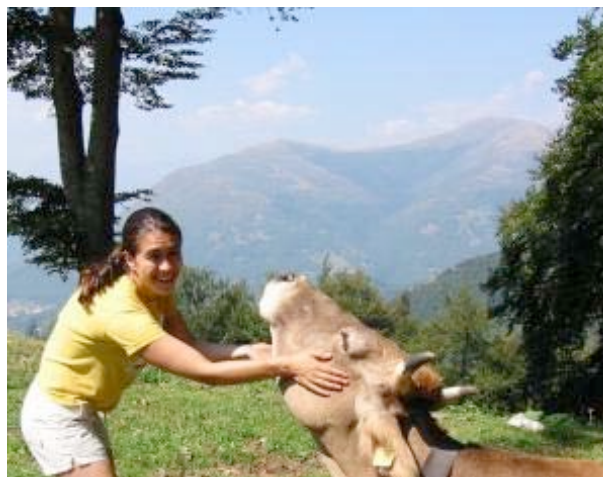
Theoretical and Computational Biophysics Group

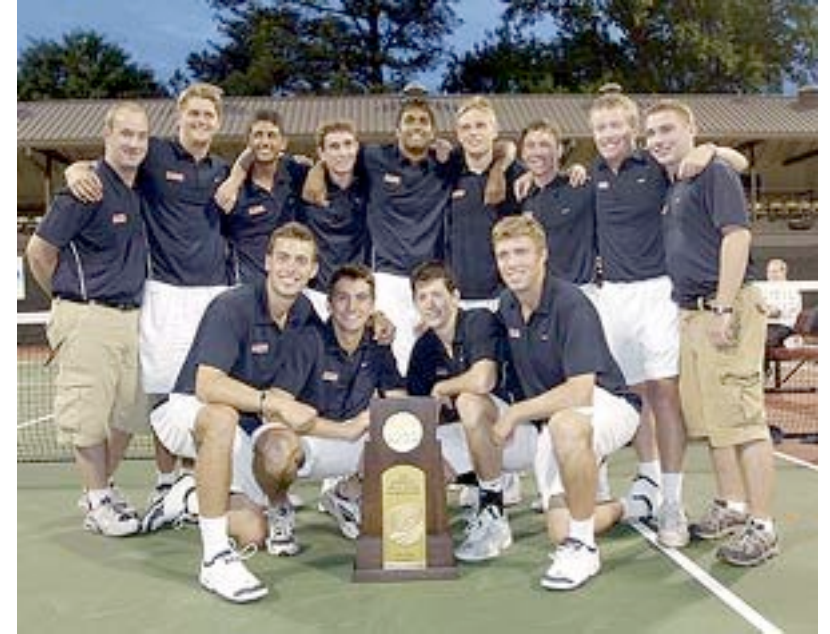
Professors Zan Luthey-Schulten
and Klaus Schulten

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](#))

12:30-12:45

Daily Q & A

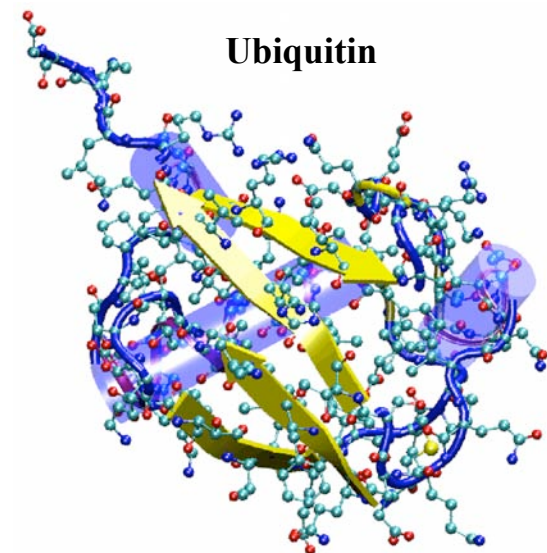
Lunch Break

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

Lunch Break

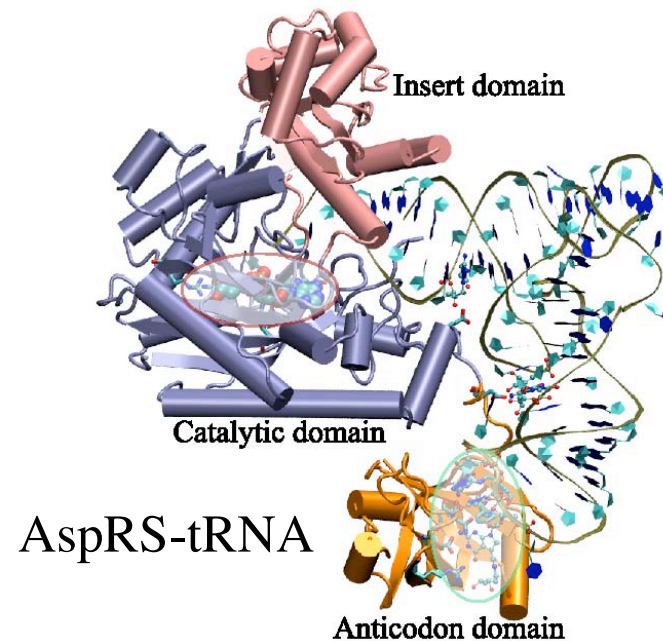
(12:45-13:30 Staff Meeting, 3169 BI)

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](#))

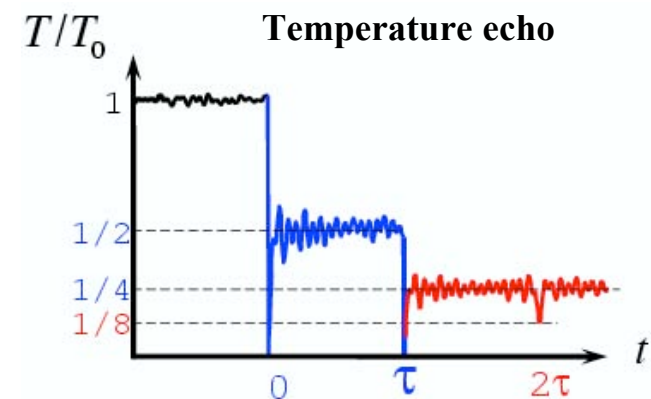
12:30-12:45

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

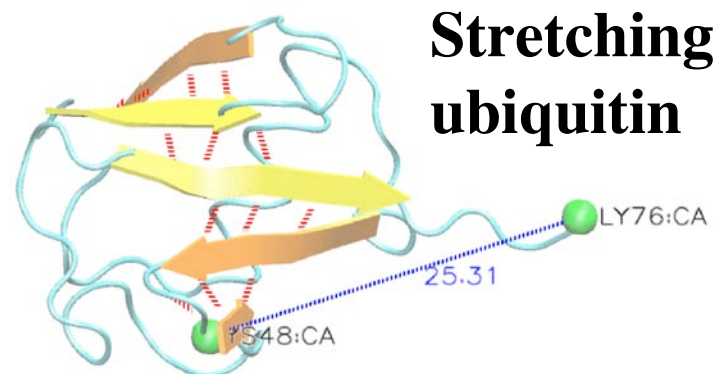
Daily Q & A

Lunch Break

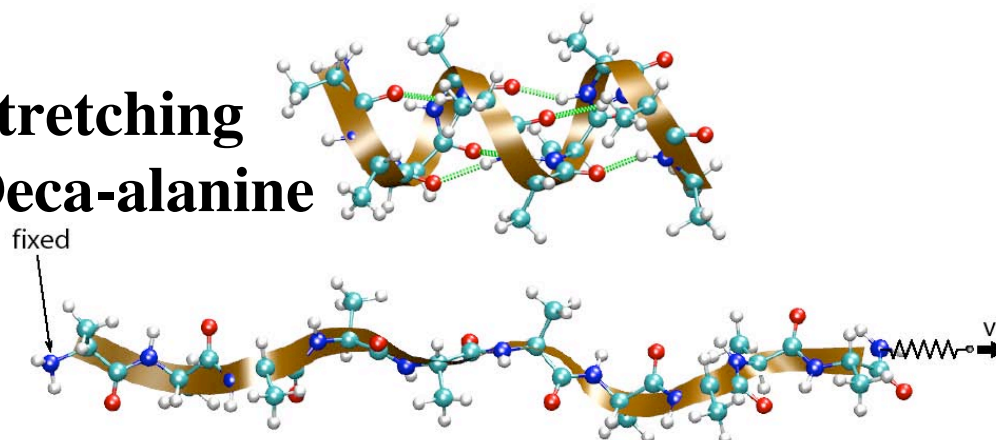
(12:45-13:30 Staff Meeting, 3169 BI)

14:00-18:00

Hands-on -- Molecular Dynamics Tutorial ([html](#), [pdf](#)) (E. Villa, F. Khalili, R. Amaro)



**Stretching
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](#))

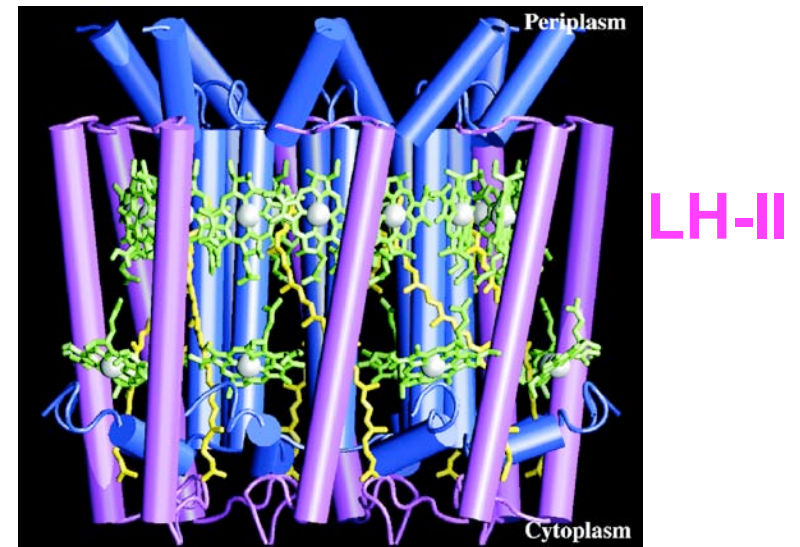
12:00-12:15

Daily Q & A

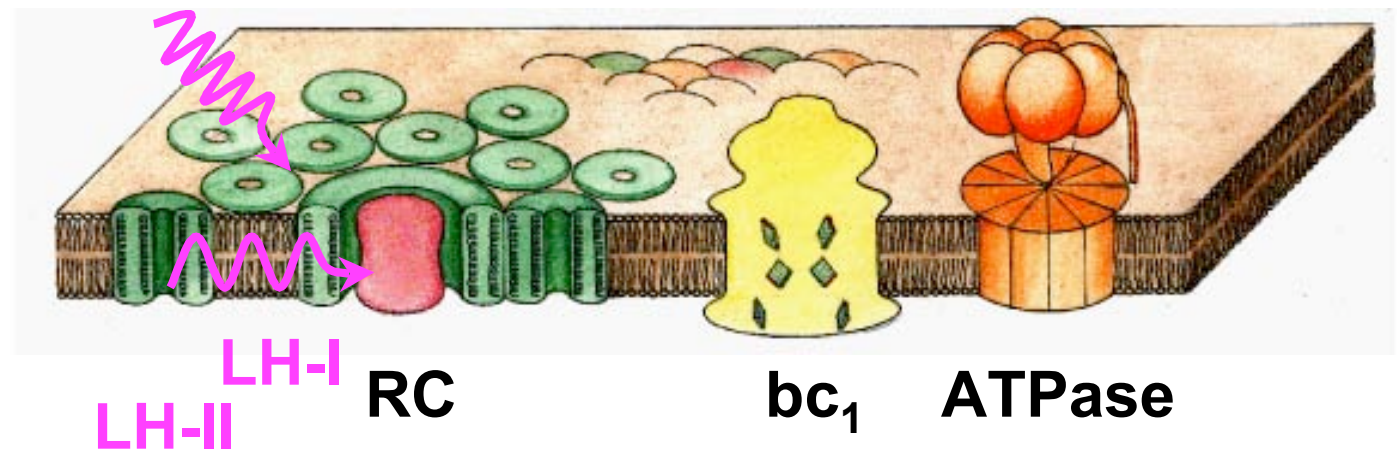
Lunch Break

14:00-18:00

Hands-on -- Stretching Deca-Alanine ([html](#), [pdf](#)) (E. Villa, F. Khalili, R. Amaro)



Photosynthetic unit of purple bacteria



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](#))

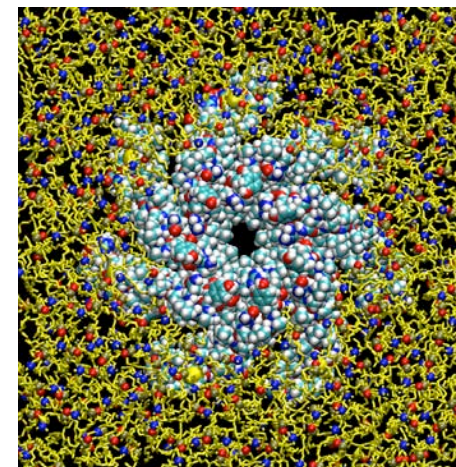
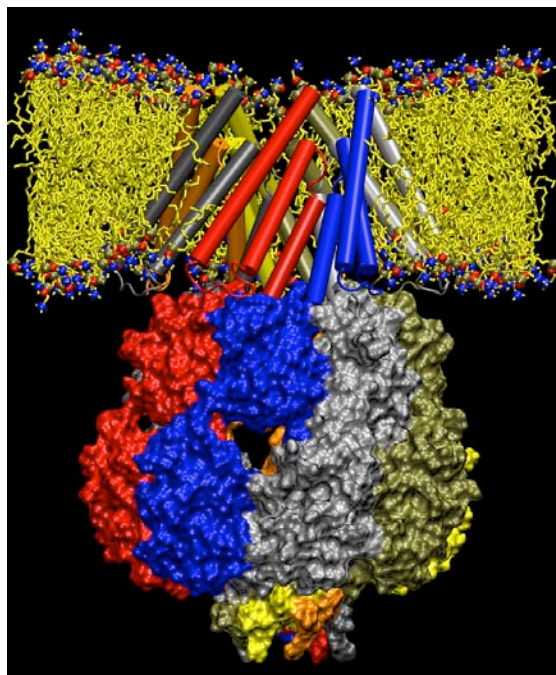
10:00-11:00

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)

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)

All Participants

12:30-12:45

Daily Q & A

Lunch Break

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

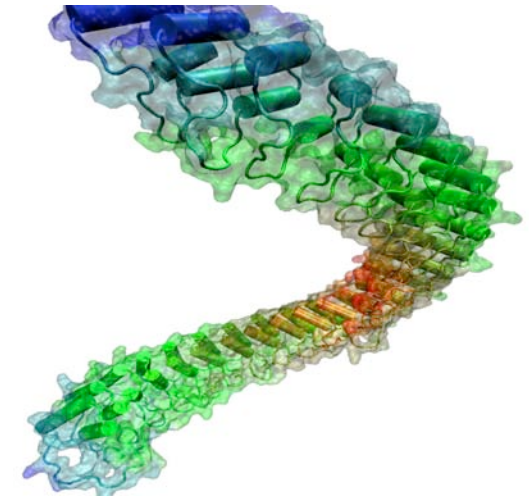
Nonequilibrium Properties of Proteins ([pdf](#))

Coffee Break

11:30-12:30

Simulated Cooling of Proteins ([pdf](#))

Ankyrin stretching



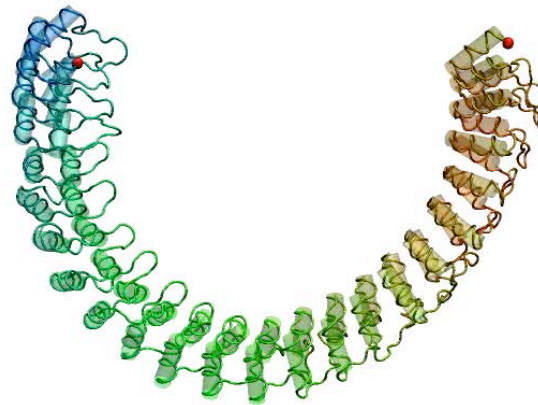
Continuing Participants

9:00-12:30

IAS Conference Room

Model your own system

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

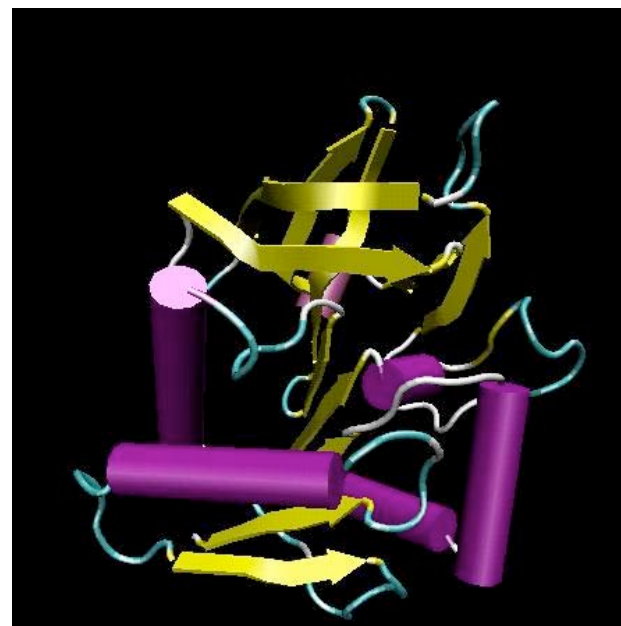
14:30-15:30

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)

HisH



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

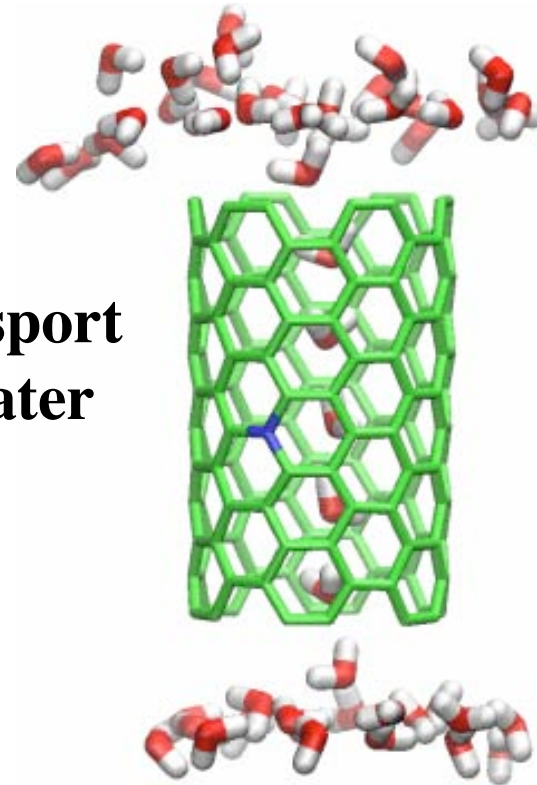
14:00-15:00

Bioinformatics of Aquaporin ([html](#), [pdf](#)) (E. Villa, F. Khalili, R. Amaro)

15:00-18:00

Nanotubes ([html](#), [pdf](#)) (E. Villa, F. Khalili, R. Amaro)

**Transport
of water**



Fri, 6/18: *Selected Participant Presentations*

09:00-11:00

"Model your own System" Presentations

Coffee Break

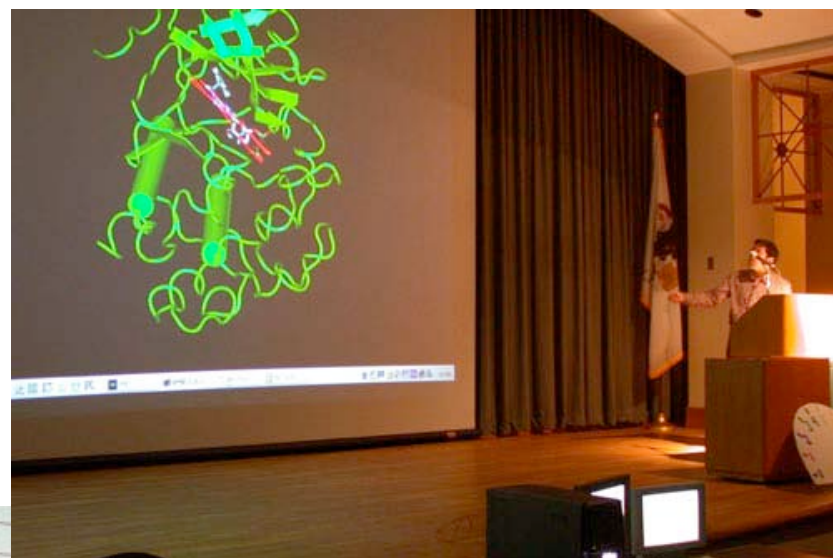
11:30-12:00

"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**