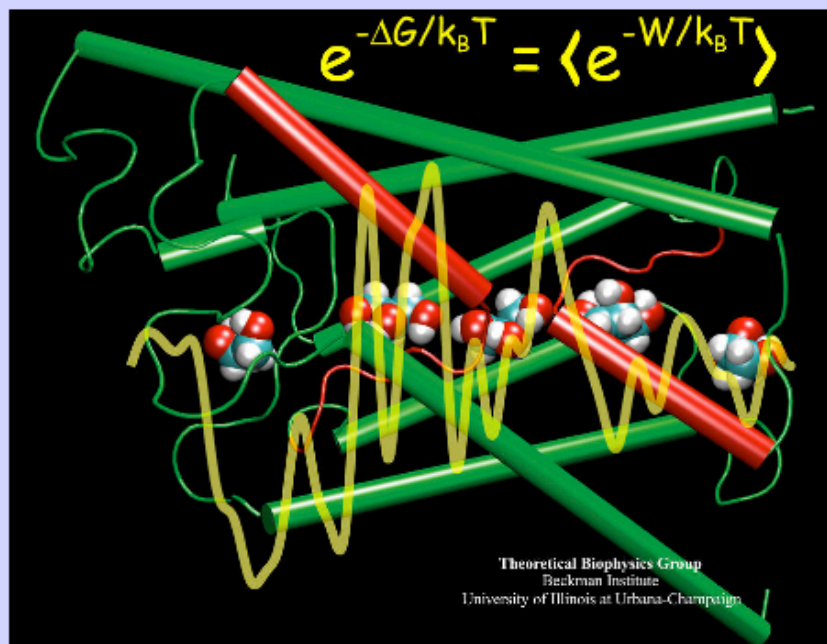


Summer School on Theoretical and Computational Biophysics



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.

Computational Approaches for Simulation of Biological Systems

June 2 - 13, 2003

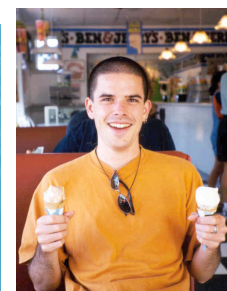
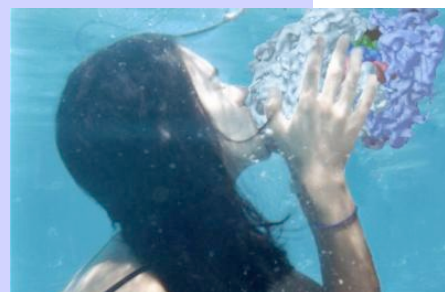
Theoretical & Computational
Biophysics Group
University of Illinois
Beckman Institute
405 N Mathews Ave
Urbana, IL 61801
217/244-2212
sumschool03@ks.uiuc.edu

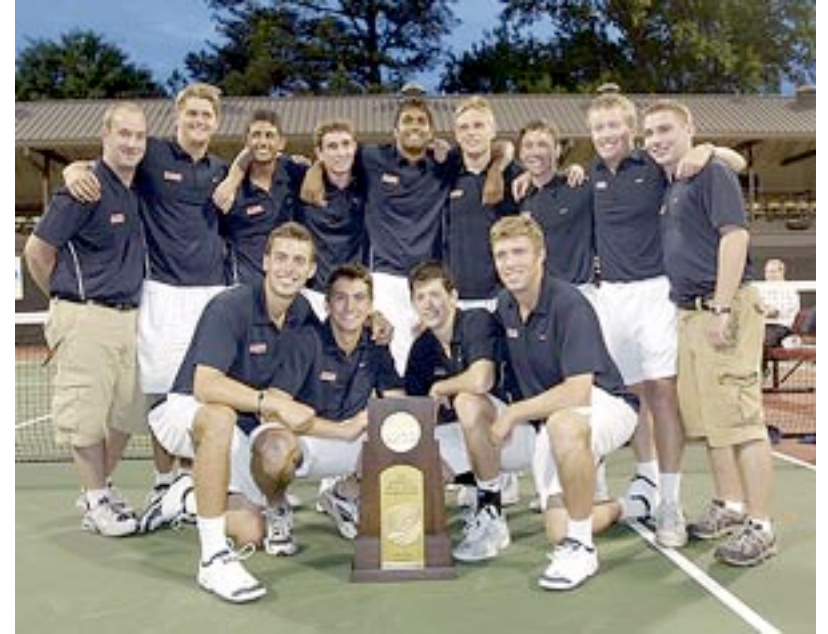
Local Resources

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)

Welcome





Our University

The Program

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

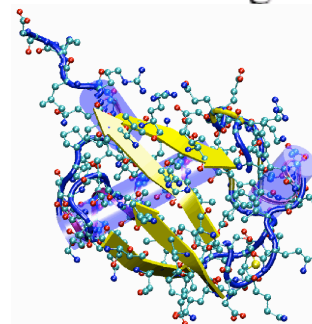
Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

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)



Ubiquitin

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

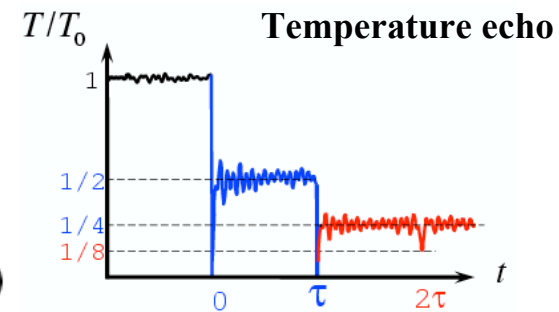
12:30-12:45 Daily Q & A

Lunch Break (12:45-13:30 Staff Meeting, 3151 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

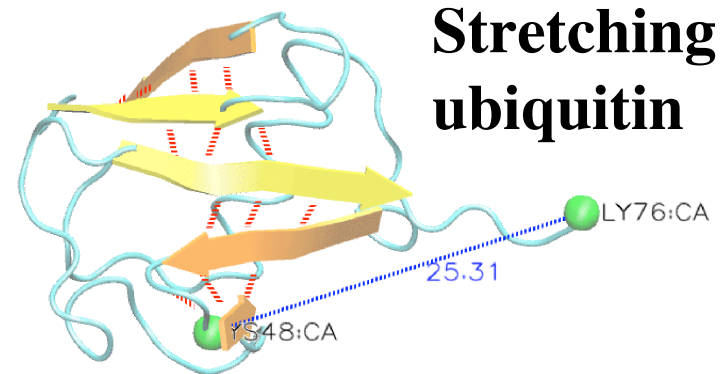
12:30-12:45 Daily Q & A

Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

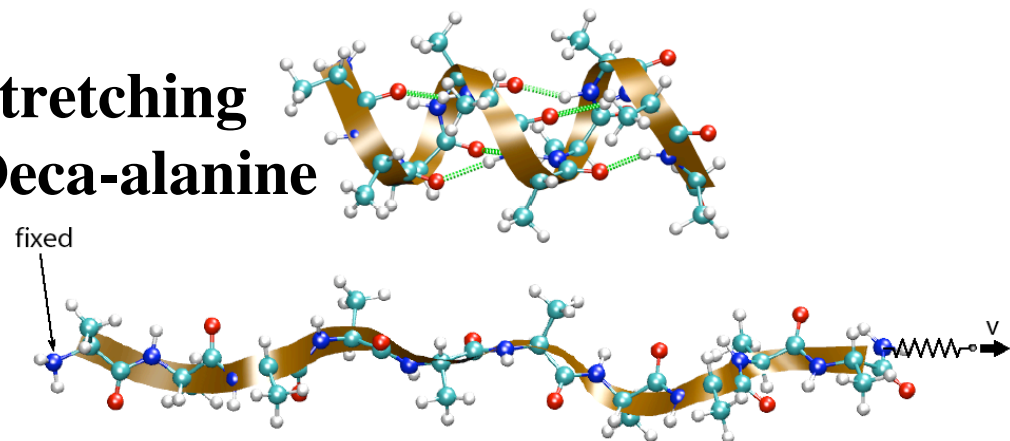
14:30-15:30 Hands-on -- Molecular Dynamics Tutorial 3 (S. Park, M. Gao)

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)



**Stretching
Deca-alanine**



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 Group Photo

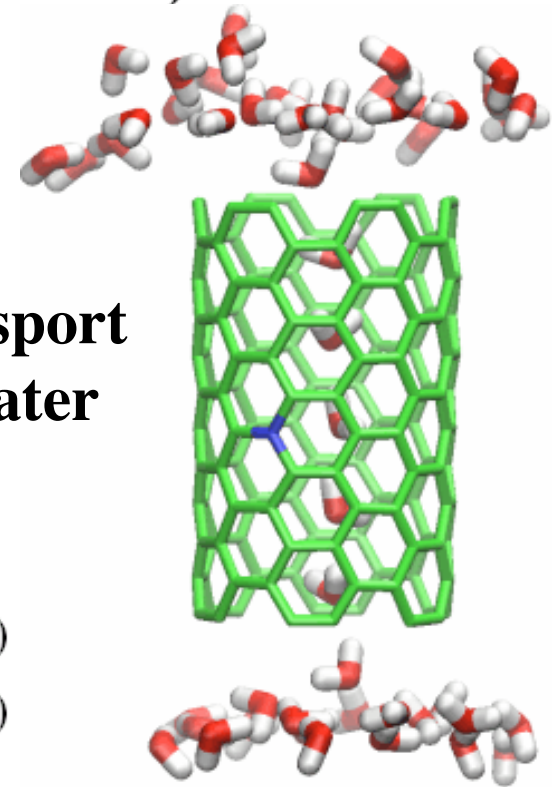
Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

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)

19:00-21:00 Free Session -- Model Your Own System (D. Lu, F. Zhu)

**Transport
of water**



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

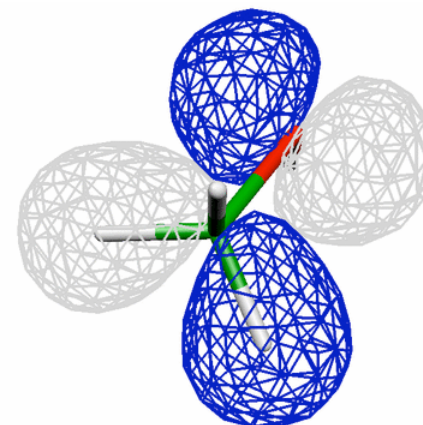
12:30-12:45 Daily Q & A

Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

14:30-15:30 Hands-on -- Introduction to QM Simulations (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)



Chicago, Chicago ...

Sat, 6/7

Bus Trip to Chicago (Optional, Not Funded by School, Sign up Early)

Sun, 6/8



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

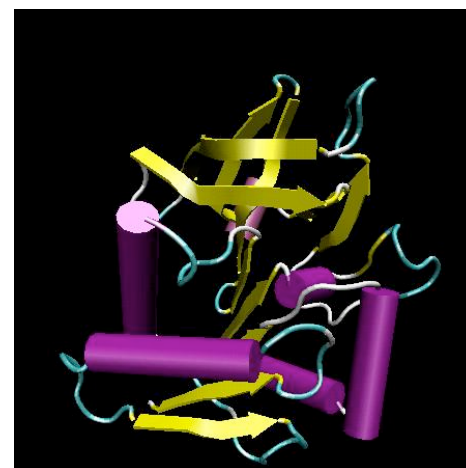
Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

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)

19:00-21:00 Free Session - Model Your Own System (G. Zheng, S. Kumar)

HisH



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

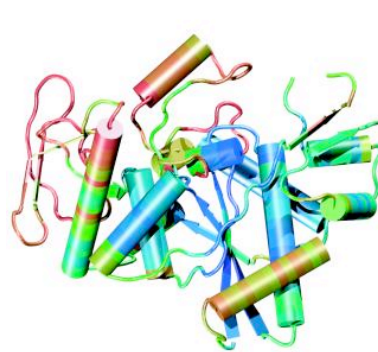
12:30-12:45 Daily Q & A

Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

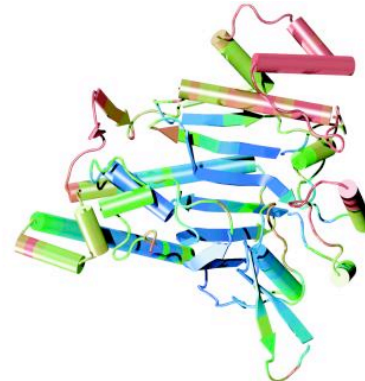
14:30-15:30 Hands-on -- Bioinformatics Introduction on Class II tRNA Synthetases (F. Autenrieth, B. Isralewitz, T. Pogorelov)

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)



Class I Lysyl-tRNA Synthetase



Class II Lysyl-tRNA Synthetase

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

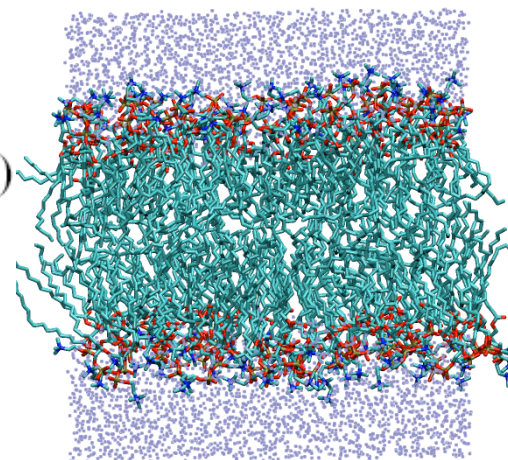
Lunch Break (12:50-13:30 Staff Meeting, 3151 BI)

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)



POPC membrane

Thu, 6/12: *Numerical Algorithms* (T. Schlick, R. Skeel)

09:00-10:00 Force Evaluation, Integrators, and Propagators (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

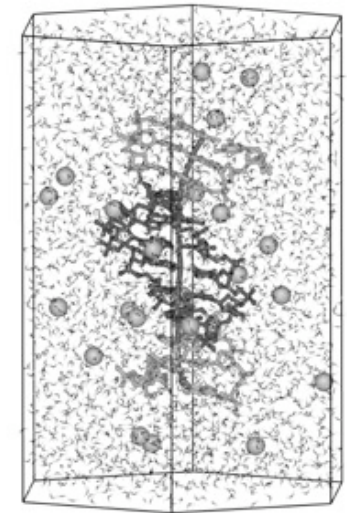
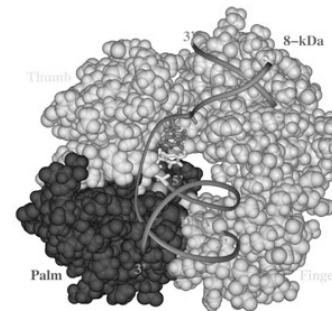
Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

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)

19:30-21:00 Free Session - Model Your Own System (S. Park, M. Bach), Beauty Contest [Beckman Institute Auditorium]



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

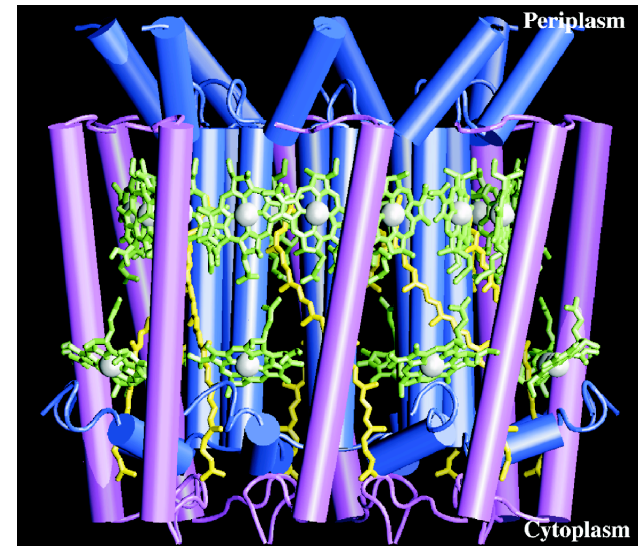
12:00-12:15 Daily Q & A

12:15-12:45 Concluding Remarks

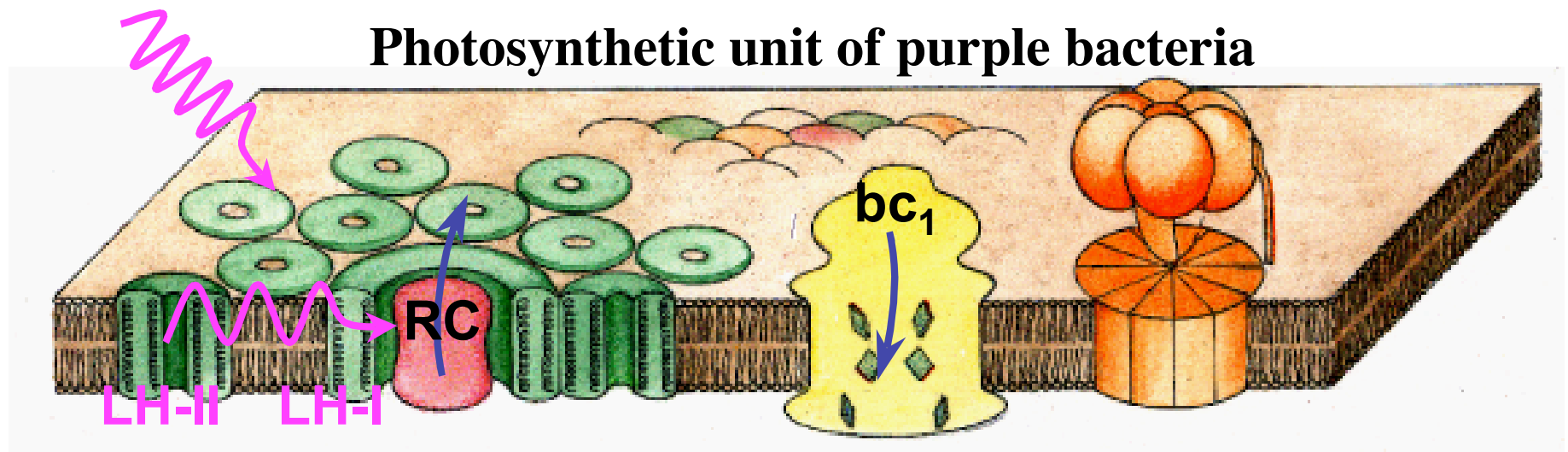
Lunch Break (12:45-13:30 Staff Meeting, 3151 BI)

14:30-15:30 Hands-on -- Excitation Transfer (M. Sener, C. Kanchanawarin)

15:45-17:00 Hands-on -- Electron Transfer (M. Sener, C. Kanchanawarin)



Photosynthetic unit of purple bacteria



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 provide tutorials for you**
- **The optimal course is that you help each other**

- **Beauty contest: opportunity to model your system**
- **Sign up for Saturday trip to Chicago**

- **Please give us feedback to improve tutorials**
- **Please give us feedback to encourage more schools**

**Let's enjoy
two great
weeks of
learning and
friendship**