

# Structural Bioinformatics Workshop

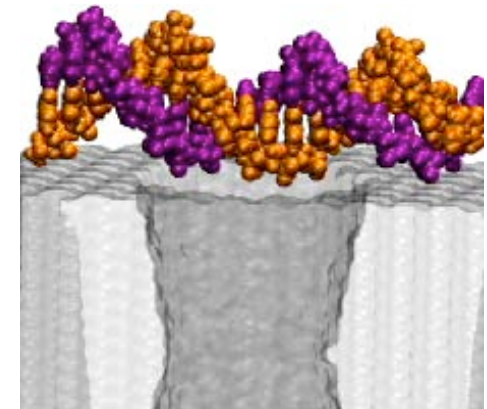
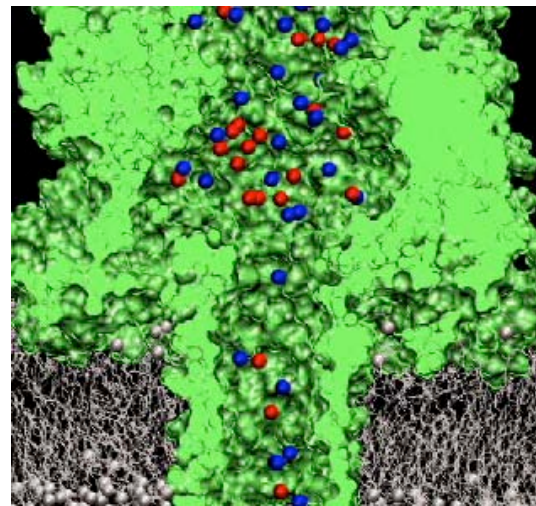
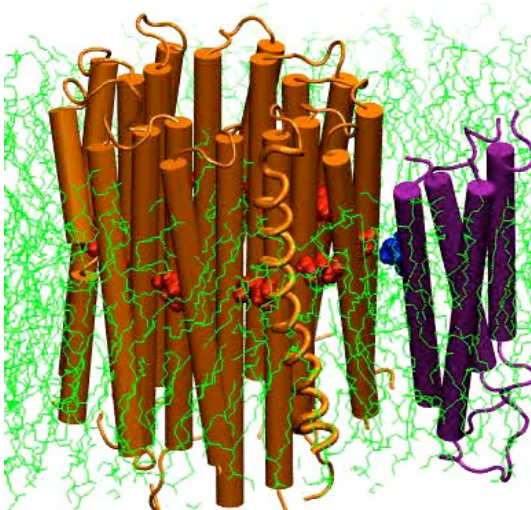


*Universidad de Talca*



*University of Illinois*

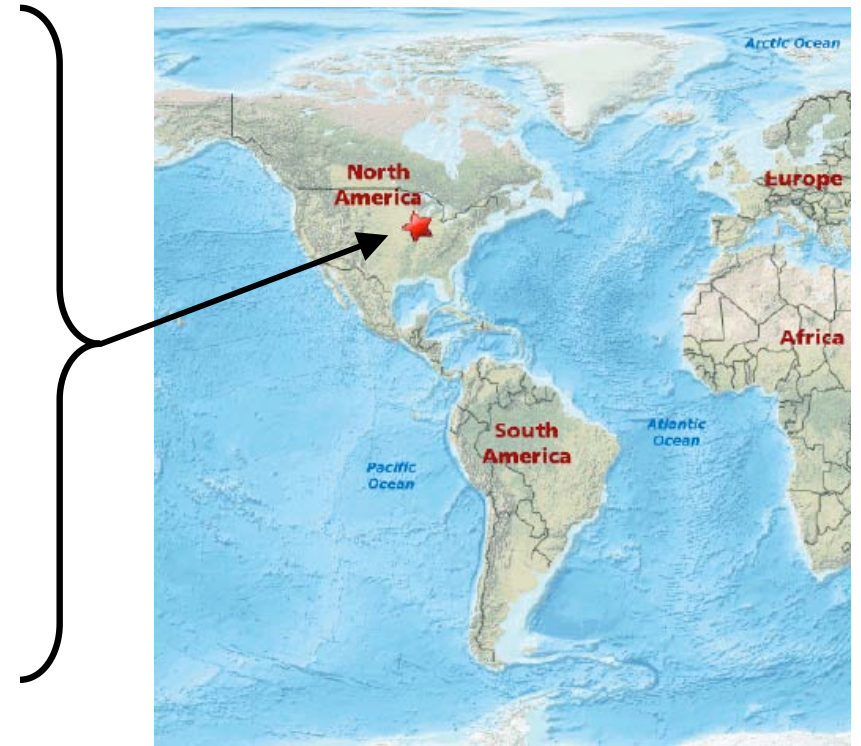
## **Molecular Simulations of Transmembrane Proteins: VMD & NAMD**



# Theoretical and Computational Biophysics Group



Beckman Institute for Advanced  
Science and Technology



Urbana-Champaign and the world



40°N 88°W (5 km from Champaign)

# Theoretical and Computational Biophysics Group

Aleksei Aksimentiev (**Physics**)

Zan Schulten (**Chemistry**)



Klaus Schulten (**Physics**)

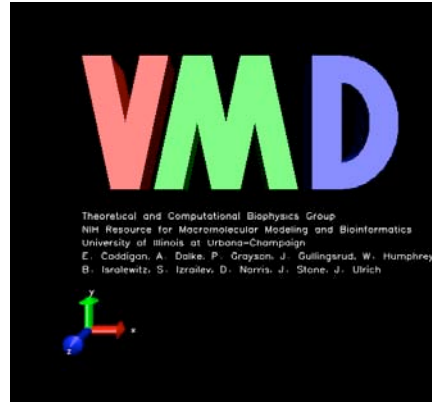


Sanjay Kale (**Computer Science**)

Emad Tajkhorshid (**Pharmacology**)

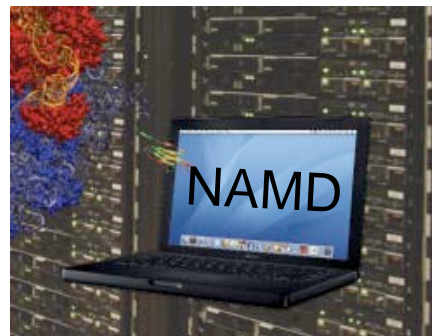
# Theoretical and Computational Biophysics Group

## Home of **VMD** and **NAMD**



John Stone

(more than 60,000 users worldwide)



Jim Phillips

# THE TEAM



Marcos

David

Alek

# Day 1

- Overview (now)
- Introduction to VMD & NAMD

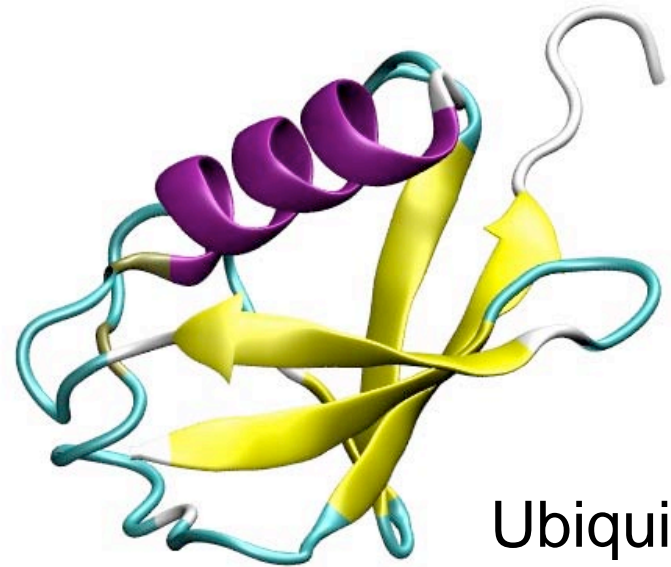
11:20 to 13:00

“Hands-on” lab VMD

14:00 to 17:00

“Hands on” lab NAMD

18:00 to 21:00



Ubiquitin



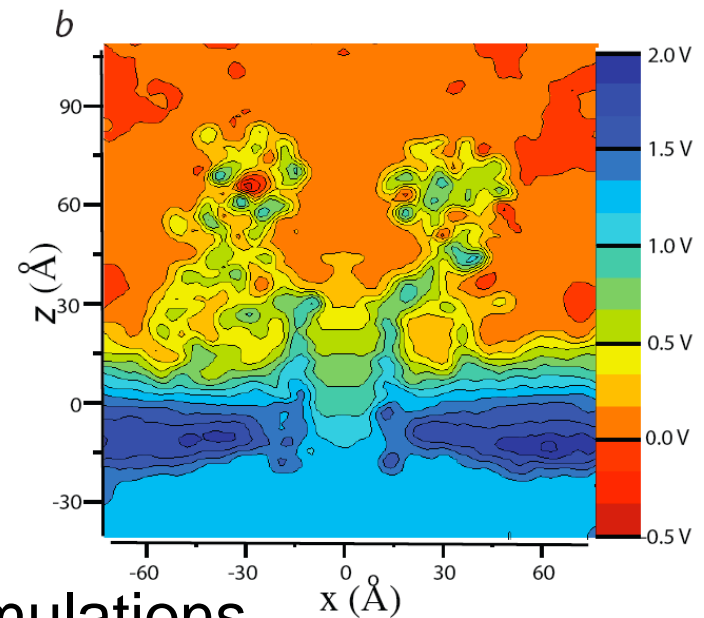
# Day 2

- Simulation of membrane proteins

Lecture: 9:00-10:00

“Hands-on” lab

10:00-13:00



- Analysis of membrane channel simulations

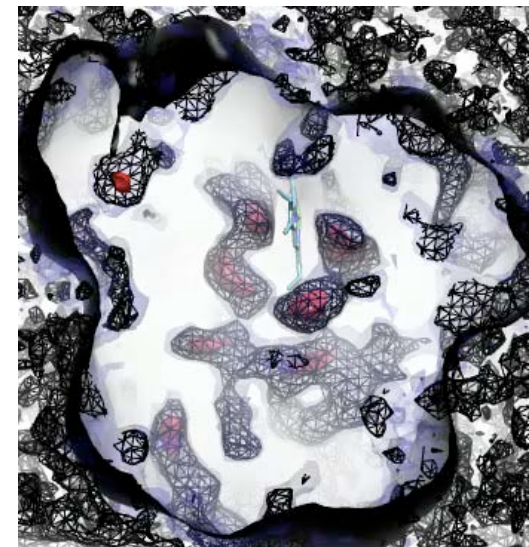
Lecture: 14:00-15:00

“Hands-on” lab:

15:00-18:00

- “Hands-on” lab: Images and Movies

18:00-20:00



# Day 3

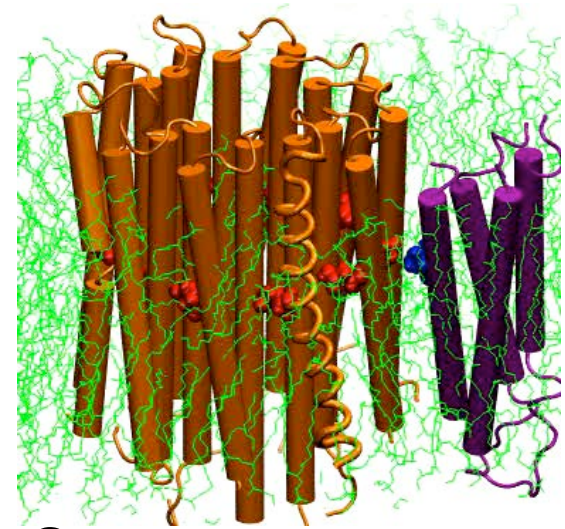
- Introduction to TcIForces and TcIBC

Lecture:

9:00-10:00

“Hands-on” lab:

10:00-13:00



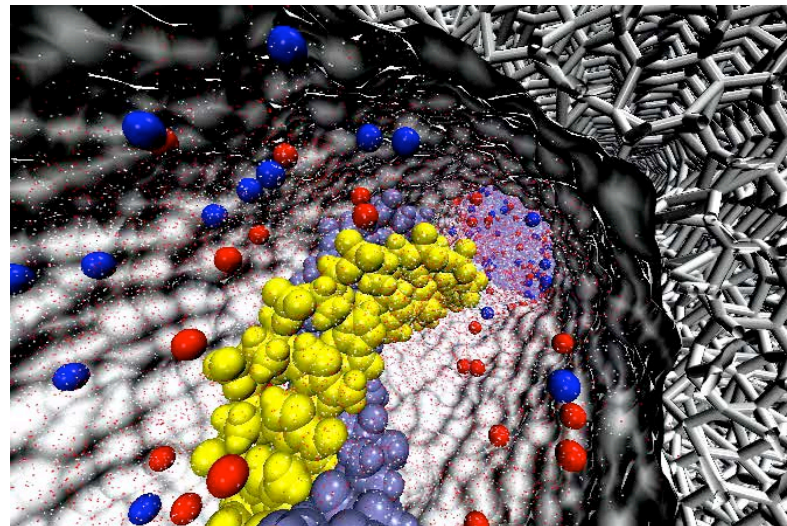
- Simulations of Biomolecular/Inorganic Systems

Lecture:

14:00-15:00

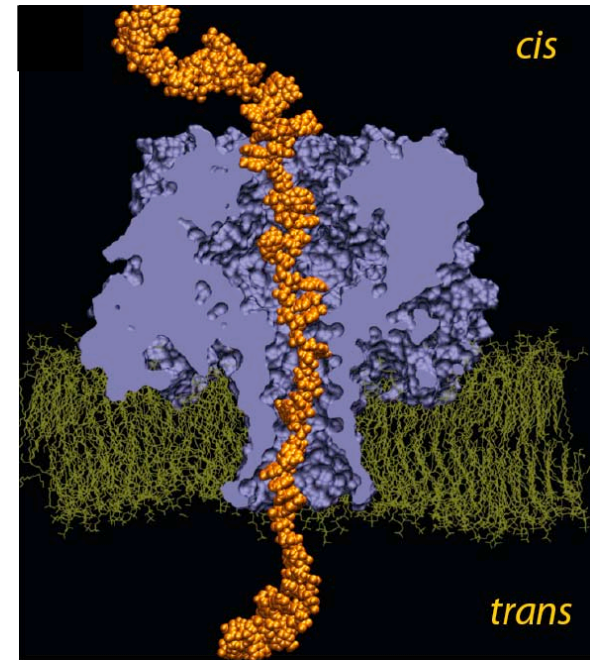
“Hands-on” lab:

15:00-18:00





# General Remarks



- **The course 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**
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- **Please give us feedback to improve lectures and tutorials**