Molecular Simulations of Transmembrane Proteins: VMD & NAMD

Structural Bioinformatics Workshop

Universidad de Talca

University of Illinois
Theoretical and Computational Biophysics Group

Beckman Institute for Advanced Science and Technology

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

(more than 60,000 users worldwide)

John Stone

Jim Phillips
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
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 TclForces and TclBC
  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

• Please give us feedback to improve lectures and tutorials