LA-SiGMA Molecular Dynamics Course 2012-2013

Instructors:
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Course Listings: (This course is listed differently at each university.)
Louisiana Tech: MSNT 510 3 credit hours
Special Topics in Molecular Sciences; Seq. No. 21863; Time and Days:
LSU:
UNO:

MEETINGS: We will use GOOGLE HANGOUT (bishoptc@gmail.com) to broadcast classes to each other MWF from 1:00pm to 2:00pm

Description (3 hrs)
Molecular Dynamics is an introduction to mastering the art of molecular modeling and dynamics simulations with an emphasis on high performance computing and modeling biomolecular systems. It will be team taught and meet once a week for video lectures. Each student will conduct a molecular simulation project. Students who take this course will learn how to configure a computer cluster (ideally a Little Fe but any two computers and a network switch can be used), install and utilize freely available molecular visualization, analysis and dynamics software tools, construct systems and run simulations on local and remote computing resources. Course work and lectures will essential structural biology and theoretical considerations from basic numerical integration techniques (e.g. Verlet algorithm, Ewald summations) to advanced thermodynamic considerations (e.g. replica exchange and free energy calculations). Projects are designed to explore an important biological application, proper use of an advanced simulation technique, performance characterization (e.g. numeric and performance analysis of gpu vs. traditional cpu).

Objective:
An introduction to mastering the art of molecular molecular modeling and dynamics simulations with an emphasis on high performance computing.
Students who take this course will learn how to:
- assemble and configure a computer cluster (LIttle Fe or similar)
- perform molecular graphics and analysis of static structures
- run molecular dynamics simulations using freely available software
- run simulations on local and remote computing resources
- analyze molecular dynamics trajectories

Requirements:

One or more computers (laptop will do) that can be configured as the user pleases
NOTE: VMD and NAMD will be installed, possibly linux as part of class
Loni account will be required.
You can get a loni account (login) at
https://allocations.loni.org/login_request.php

I have secured an allocation. Please request to join this allocation "**loni_lasigma_md**".. I must approve your addition to this allocation

Computer with VMD and NAMD installed locally (see requirment number 1)
Preferred: Some unix experience, scripting (tcl,shells, other), programming

TOPICS:

1) Hardware Review: have them rebuild the little fe or install/config linux on a machine serves as an introduction to UNIX, usernames,authentication, they shell etc...
2) Install VMD and NAMD (continued unix/OS learning)
3) Molecular Visualization, Graphics and Analysis, an intro to the Protein DataBank
-generic overview of molecular structures:
proteins (amino acids),
DNA(nucleic acids)
membranes/lipids
small organic molecules
5) Static Analysis:
secondary structures (helices, sheets, etc...)
hyrophobicity indices, Ramachandran plot, Electrostatics Calcs, etc..etc..
Poisson Boltzmann calcs & analysis
6) Molecular Dynamics:
-theory: "the art of molecular simulation" from Haile emphasis thermo & stats
-tests to "prove that the MD is working" from an algorithmic point of view
(sims of water or something)
-practice: simple examples from the NAMD (amber/other web sites)
water -> water & ions
bpti everyone's favorite
DNA
membrane
-Advanced techniques...
replica exchange
free energy calcs
thermodynamic integration
steered or activated MD

PROJECTS
Each student will conduct a project with guidance and input from one of the instructors.

0) A simulation of BPTI (the MD equivalent of “hello world”)
1) Bishop: Simulation and Analysis of a Nucleosome or Ensemble of Nucleosomes
2) Bishop: Propagation of an Impulse or Heat Shock thru DNA or Protein
3) Protein Ligand Binding Free Energies of Small Molecules to T4-Lysozyme
4) Rick: Using Replica Exchange to Examine Conformational Changes in the Alanine Polypeptide