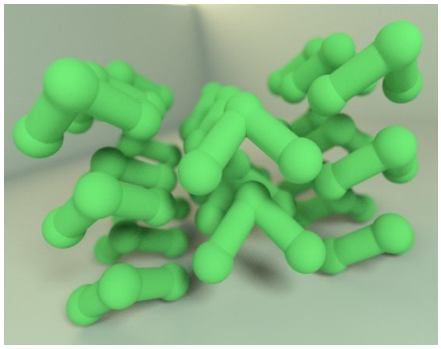
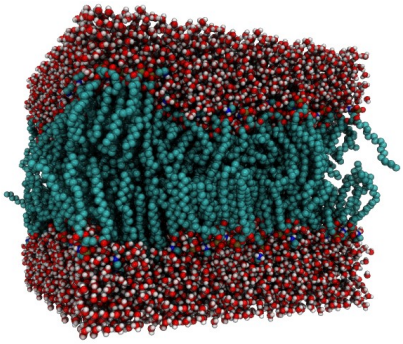
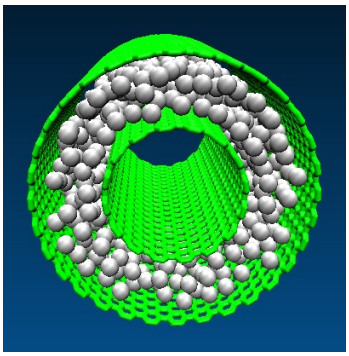
Topical Meeting on Molecular Dynamics

May 26, 2014

Purpose: Molecular dynamics (MD) is increasingly used by researchers in many branches of physics, chemistry and biology. The aim of this workshop is to bring researchers in Denmark and southern Sweden who are users and/or developers of molecular dynamics together to discuss current research in the region, discuss issues of general and current interest, including: hardware/software/algorithms, applications, challenges and opportunities for collaboration.

Venue:
Royal Danish Academy of Sciences and Letters
(Videnskabernes Selskab)
H.C. Andersens Boulevard 35
DK-1553 København V
http://www.royalacademy.dk

This workshop is organized and sponsored by the Center for Viscous Liquid Dynamics ("Glass and Time", http://glas.ruc.dk) at the Dept. Of Sciences, Roskilde University. Our research interests are primarily in the area of liquid state dynamics, particularly in the viscous regime close to the glass transition, but we are increasingly interested in other applications of MD. Since 2008 we have invested heavily in graphical processing unit (GPU) computation and have developed our own GPU-based MD code RUMD (http://rumd.org).

Danmarks Grundforskningsfond
Danish National Research Foundation

Program

The allocated time for a talk is either 20 or 30 minutes, but please allow 5 minutes for discussion. A signal will be given by the chair five minutes before the discussion should begin.

10.30-11.00: Registration
11.00-11.05: Jeppe Dyre (RUC): Welcome
11.05-11.35: Thomas Schrøder (RUC): *Studying viscous liquids by a GPU based MD code (RUMD.org)*
11.35-11.55: Kresten Lindorff-Larsen (KU): *Accuracy and precision in molecular dynamics simulations of proteins*
11.55-12.15: Jesper Schmidt Hansen (RUC): *Molecular dynamics simulations of confined fluids*
12.15-12.35: Jacco van de Streek (KU): *Molecular Dynamics with Tailor-Made Force Fields for Pharmaceutical Materials Science*

12.35:13.10: Lunch (35 minutes; upstairs)

13.10-13.40: Birgit Schiøtt (AU): *Modelling Membrane Proteins*
13.40-14.00: Henriette Elisabeth Autzen (AU): *Multiscale dynamics of a bacterial P-type ATPase in its native membrane*
14.00-14.20: Sheeba Jem Irudayam (AU): *Simulation of Amyloid Fibrils and binding of Imaging Agents*
14.20-14.50: Himanshu Khandelia (SDU): *Simulations of Ion Pumps with Virtual Sites and a 5 fs time step*

14.50-15.20: Coffee (30 minutes; upstairs)

15.20-15.50: Per Linse (LU): *Virus self-assembly induced by polyions*
15.50-16.10: Katrine Kirkeby Skeby (AU): *Capturing Membrane Binding of an Amyloid Peptide Using a Highly Mobile Membrane Model*
16.10-16.30: Carsten Svaneborg (SDU): *Using MD simulations to study viscoelastic properties of rubber materials*
16.30-17.00: Jens Walther (DTU): *Molecular and Continuum Simulations of Flow in Membranes*

17.00-17.30: Coffee (30 minutes; upstairs)

17.30-18.00: Mark Hagen: *An overview of the Data management and Software Centre at the ESS*
18.00-18.20: Heloisa N. Bordallo (KU): *Molecular Dynamics Simulations: Getting the most of Inelastic Neutron Scattering data*
18.20-18.40: Sofie Jakobsen (AU): *Dynamical Effects of Multipoles in MD Simulations*
18.40-19.00: Ulf Pedersen (RUC): *Computing the rate along a reaction coordinate with a bias potential*

19:15- : Dinner (NIMB, Tivoli)