Visualization of molecular simulations

Alexei Nikitin, Alexander Lyubartsev, Aatto Laaksonen

Div. Physical Chemistry, Stockholm University, 10691, Stockholm

Molecular dynamics: solution of Newtonian equations of motion in the molecular system

For each atom at each time:

\[ v_i(t+1/2\Delta t) = v_i(t-1/2\Delta t) + F_i(x_j(t))/m_i \Delta t \]

\[ x_i(t+\Delta t) = x_i(t) + v_i(t+1/2\Delta t) \Delta t \]

1998: MdynaMix - parallel scalable molecular dynamics for arbitrary molecular mixtures

http://www.fos.su.se/physical/sasha/md_prog.html
Current project: Interactive Visualisation

includes:

• initial preparing of molecular structures
• parameter (force field) association
• real-time visualization
• real-time analysis of result
• interactive: correction of simulation during the run

All these feature are implemented in MDX project

OS: Windows & Linux
Snapshots from the program:
Building system from available structures
Building arbitrary molecular structures
Building proteins
Geometry editing
Building a periodic system
Control of molecular dynamics run
Monitoring physical quantities