Visualization of Molecular Simulations

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During the last decades molecular computer simulations have become an indispensable instrument in studies of matter. Computer simulations are now routinely used for interpretation of experimental data, for visualization of molecular structures and motion, for explanation and understanding processes and phenomena on the molecular level. A highly attractive feature of molecular simulations is the possibility to use it as a virtual microscope to follow the three-dimensional motion of molecules in great details.

We are currently unifying our parallel scalable molecular dynamics package MDynaMix [1] with a graphical interface and 3D engine from the program referenced in [2]. The aim of this project is to create an integrated environment in which each step of molecular modeling is done in an interactive manner with immediate visualization of the performed actions using the 3D graphics. We start from building up of molecular models; either from scratch or by adding of previously prepared molecular fragments such as amino acids of proteins. Such features as editing of molecules by changing bond and angles parameters can be done, as well as building a crystal or adding a solvent. The next step is prescribing the force field parameters and setting up parameters for molecular dynamics. During a molecular dynamics run the current state of the system is instantly updated on the screen. The molecular dynamics is carried out in an interactive manner, so that it can be stopped at any moment, and continued afterwards after correction of some parameters. Finally, a real-time analysis of the results can be also done, showing for example graphs of energy or density time dependence.

The software (except the MDynaMix code) is written in C++ with the use of Qt library and can be run under Windows or Linux OS. In a longer perspective, more editing capabilities to the program will be added and possibility to running molecular dynamics on remote (super) computer will be introduced. We are also planning to implement several features from our previous projects such as VIMS [3] as well as an early sonification project where frequencies of vibrational and librational motion are made to audible signals. Sonification will be developed later to a “poor man’s haptics” to be used together with interactive graphics in modeling of close-range interactions and docking.

References

1. A.P.Lyubartsev, A.Laaksonen, *MDynaMix - a scalable portable paralle MD simulation package for arbitrary molecular mixtures"* Computer Physics Communications, 128, 565 (2000)

2. Y.V. Kravatsky and A.M. Nikitin. *Efficient methods for adequate graphical presenting molecules and molecular complexes.* The Third International Conference on Bioinformatics of Genome Regulation and Structure (BGRS'2002). Novosibirsk, 2002.

3. K.-M. Jää-Aro, J. Ihren, F. Zetterling and A. Laaksonen, *Visual Interactive Molecular Simulation*, in “Grand Challenges in Computer Simulations” (A. Tentner, Ed.), SCS, (1999).