Institute of Information and Communication Technologies – BAS

Seminar
„Parallel Algorithms and Scientific Computations"

On 21 April 2015 in room 218 at the Institute of Information and Communication Technologies, BAS, Acad. G. Bonchev St., Block 25 A, **Elena Lilkova, Assistant, IICT-BAS,** will give a presentation on the following topic:

Molecular Dynamics Simulations – Basic Concepts and Methods

Abstract

Molecular Dynamics simulations (MD) are a very powerful tool in modern molecular modeling, and enables one to follow and understand structure and dynamics with extreme detail – on scales where motion of individual atoms can be tracked, by calculating the time dependent behavior of a molecular system. The method of MD is a valuable bridge between experiment and theory and has been routinely used to the study the structure, thermodynamics and transport properties of condensed phase systems, including neat alkanes, molecular and ionic liquids, liquid metals, the many phases of water, the solvation and binding of small molecules, as well as biological macromolecules and their complexes.
An introduction in the theoretical concepts and methods of MD will be presented, including semi-empirical potentials, integrators, maintaining different thermodynamic ensembles, etc.