MOLECULAR DYNAMICS SIMULATIONS OF BIOMOLECULES AT THE BEGINNING OF THE 21st CENTURY

Summary

Computer simulations have become a mature and useful method in studies of molecules of life. As a part of structural bioinformatics carefully planned numerical experiments provide unique data on dynamics and properties of biomolecules. In this article a review of the state of art of molecular dynamics (MD) studies is presented. Current trends involving the steered MD, milestoning and coarse grained MD are described and some examples of MD applications in bio- and nano-technology are presented. The progress in hardware, such as parallel computing and purpose-built processors, is also addressed.