Visual Computing Forum

Molecular dynamics simulations for biomolecules: principles and examples

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Abstract

Molecular Dynamics (MD) simulations are widely used to model biomolecules in conditions that mimic the ones of in vitro experiments. The raw result of a MD simulation is a trajectory file containing the position of each atom in the molecule at every time step of the simulation, similar to a movie representing how the biomolecule is wiggling and giggling along simulation time. MD simulations are sometimes referred to as a 'computational microscope' because they allow the investigation of biomolecules dynamics at the atomic level of detail, something that is virtually impossible with the experimental methods currently available.

I will introduce the basic assumptions and principles behind MD simulations for biomolecules; molecular mechanics force fields, equations of motion and their integration, treatment of long-range interactions, etc... Further I will present the practicalities of running MD simulations and the different steps from system setup to trajectory post-processing.