Simulating molecular dynamics through intelligent software agents

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Abstract

Molecular dynamics (MD) is a form of computer simulation wherein atoms and molecules are allowed to interact for a period of time governed by known laws of physics, thus giving an overview of the motion of the atoms. In most of the cases the number of particles involved in a simulation is large enough, therefore hindering the analytical computation of the properties of the system in question. MD circumvents this problem by employing numerical approaches. Utilizing theories and concepts from mathematics, physics and chemistry and employing algorithms from computer science and information theory, MD is a clear case of a multidisciplinary method.

At the core of any MD simulation lies the potential function (or force field), which describes the terms of interaction between the particles of the simulation. This function may be defined at many levels of physical accuracy, ranging from quantum mechanics (QM), which provides the finest level of detail but is extremely complex, to molecular mechanics (MM) and reduced representations. The latter is one of the fastest approaches, nevertheless it is not very accurate and requires extensive parameterization. There are also intermediate tecniques, such as hybrid QM/MM, which attempt to treat a small target region using quantum mechanics and the rest of the system utilizing classical mechanics.

In this paper a new framework for MD simulations is presented, which utilizes software agents as particle representations and an empirical potential function as the means of interaction. A software agent, in computer science, is a piece of software that acts on behalf of a user or other program. Such "action on behalf of" implies the ability to decide when (and if) action is appropriate. The main concept is that agents are not strictly invoked for a task, but activate themselves according to stimuli. As a part of a multi-agent system (MAS), agents can co-operate towards a single goal by communicating and sharing information with each other.

Every agent in the MAS corresponds to a single particle and at each cycle of the MD simulation the agent probes its environment for candidate agent-particles with which an interaction is possible. The interaction is performed through agent communication, utilizing an empirical potential function for the calculation of the forces applied. However, the agent also continually monitors the overall status of the simulated system. In case that the function's result leads to an undesirable or improbable situation in the overall system, the agent has the authority and the ability to override the potential function with a milder interaction.

The proposed framework has been applied on protein structural data (PDB[1] files), using an implicit solvent environment and a timestep of 5 femtoseconds (5×10^{-15} sec). Goal of the simulation is to study the emergent behaviours and trends in the movement of the agent-particles of the protein complex. This information can be then used to construct an abstract model of the rules that govern the motion of the particles.

[1]http://www.rcsb.org/pdb/