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Perspective

Brief Note on Applications of Molecular Dynamics Simulation

Stella Meiri*

Department of Materials Science and Engineering, University of North Texas, Denton TX, USA

INTRODUCTION

Molecular Dynamics (MD) is a computer simulation method for studying atoms and molecules' physical motions. The atoms and molecules are allowed to interact for a set amount of time, providing a perspective of the system's dynamic "evolution". The trajectories of atoms and molecules are determined in the most common version by numerically solving Newton's equations of motion for a system of interacting particles, with forces between the particles and their potential energies calculated using interatomic potentials or molecular mechanics force fields. Chemical physics, biophysics, and materials science are some of the fields where the method is applied.

Because molecular systems often contain a large number of particles, determining their properties analytically is impossible; MD simulation solves this challenge by use numerical approaches. On the other hand, long MD simulations are mathematically ill-conditioned, resulting in cumulative numerical integration errors that can be reduced but not eliminated totally by choosing proper algorithms and parameters [1].

The evolution of one molecular dynamics simulation can be utilized to establish macroscopic thermodynamic properties of a system that obeys the erotic hypothesis: the time averages of an erotic system correspond to micro canonical ensemble averages. MD has been dubbed statistical mechanics by numbers and Laplace's vision of Newtonian mechanics for its ability to anticipate the future by animating nature's forces and providing atomic-scale insight into molecular motion.

DESCRIPTION

Applications

Understanding allosteric: The majority of protein regulation is explained by conformational changes. Since the dawn of protein biochemistry, the idea of allosteric, which converts conformational dynamics into functional implications, has been studied. Allosteric involves conformation alterations ranging from minor rearrangements to large quaternary shifts, as accounted by the Monod model. The conformational shifts involved in allosteric transitions are generally thought to be straightforward in terms of collective movements [2]. As a result, molecular simulations may be a natural tool to recognize allosteric.

Molecular docking and drug design: Docking methods, whether small molecule or protein docking, are one of the most practical applications of the principle of molecular recognition. Understanding how a ligand, such as a substrate or a regulator, binds to its macromolecular equivalent is critical to understanding function and is the foundation of structurally driven drug design. By its very nature, the recognition process is dynamic [3]. Molecules are flexible entities, and the recognition process necessitates structural rearrangements. This shape change is an integral aspect of the binding process, both structurally and energetically.

Refining structure predictions: One of the earliest difficulties in structural bioinformatics has been structure prediction. Molecular Dynamics (MD) has been widely utilized for ab initio protein structure prediction [4], with the goal of simulating protein folding from the ground up, although this is not the preferred technique for obtaining a theoretical model of protein structure. Template-based modeling, on the other hand, is the most efficient method. One or more 3D protein structures with a fair degree of similarity to the protein of interest are used as templates in template based modeling. Regardless of the modeling algorithm employed, the end result is a model with a new amino acid sequence and a structure based on the templates used.

CONCLUSION

Molecular Dynamics (MD) has developed temporal frames that are starting to resemble biological processes. Conformational changes and ligand binding can now be effectively modeled when routine simulations approach the microsecond scale. The advancement of computational equipment, particularly the use of GPUs, as well as advances in the optimization of MD algorithms, including coarse grained MD algorithms, have enabled us to move from the analysis of single structures, which is the foundation of molecular modeling as we know it, to the analysis of conformational ensembles. Conformational ensembles provide a much better depiction of real macromolecules since they account for flexibility and dynamic

Correspondence to: Stella Meiri, Department of Materials Science and Engineering, University of North Texas, Denton TX, USA; E-mail: stella-meiri@unt.edu

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features (including all thermodynamic information) and make experimental results easier to match.

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