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Multiple-shooting methods for boundary-value approaches to molecular dynamics simulation

ABSTRACT

Biomolecules can transition from one conformation to another. Molecular transitioning between different conformations is an important component of many normal biological processes. It also can have an detrimental in some cases. All-atom molecular dynamics simulation (AAMDS) using an empirical force field can be an informative way to study molecular transitioning. This type of simulation can be defined mathematically as an initial value problem (IVP) for ordinary differential equations. IVP-based AAMDS can be applied to study local motions near a stable conformation of a molecule, but it also can used a tool for the study of transitioning between different conformations ([Kim2003], [Zag2001]). A boundary value problem (BVP) can be defined for molecular transitioning when beginning and ending structures are known. A multiple-shooting approach for BVP-based AAMDS is introduced and applied to the study of protein folding. A force field has been developed in MATLAB using an empirical energy function based on MOIL9/AMBER99 form and parameterization. Algorithms for generating initial guesses based on elastic network interpolation ([Kim2002]) are outlined. Results from simulation of conformational transitions of alanine dipeptide are presented. The convergence behavior of the algorithm is demonstrated. The feasibility of the approach for larger systems is investigated and approaches that may address some of the computational challenges are considered.