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A PARALLEL DIVIDE-AND-CONQUER ALGORITHM FOR FINDING MINIMUM ENERGY TRAJECTORIES

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ABSTRACT

In the present paper, an extension to the Featherstone's divide-and-conquer algorithm (DCA) [1] is developed to model constrained multibody systems, by splitting the integration time using the finite-temperature string (FTS) method proposed by E. Vanden-Eijnden [2]. This is a very stable and effective way of identifying optimal trajectories between system states. The system trajectory is discretized in a string of time-frames, where each frame describes an admissible conformation. The local propensity and dynamics in each frame configuration space neighbourhood is evaluated in parallel using the DCA.

Keywords: multibody system, generalized divide-and-conquer algorithm; energy landscape.

INTRODUCTION

Molecular dynamics (MD) simulations have become a popular tool for simulating a variety of complex systems [3]. With the advent of massively parallel computer resources, one now routinely sees applications of MD to systems as large as several million atoms, which is almost the size of most nano-materials [4]. However, it is not yet possible to reach laboratory time-scales of milliseconds and beyond with MD simulations. The diversity of time scales are devastating the direct dynamic simulation. The dynamic of this systems is characterized by sequences of rare events [5], long waits periods around stable conformations followed by sudden jumps from one state to another produced by external phenomena like impact or thermal fluctuations. These changes are assumed to occur on a time scale that is much larger than the micro-time scale in the system dynamics. Due to the essentially sequential nature of time, parallel computers have been of limited use in solving this so-called time-scale problem. Instead, over the years a large range of approaches have been proposed for accessing time-scales that are well beyond the reach of the fastest computers [6].

RESULTS AND CONCLUSIONS

Each conformation is subjected to propensity forces and thermal fluctuations and its dynamic is used to sampling the energy landscape [7]. Here the divide and conquer formulation, is similar to that presented in [8] and [9], using penalty and augmented Lagrangian approach for constraint imposition and absolute coordinates for the system state description. The FTS method is used to stabilise the string structure and identify the isocommitter surfaces in each frame configuration space neighbourhood, where the most probable conformations are concentrated [8]. In this scheme generalized constraint forces are considered in the equations

of motion to enforce the system algebraic constraints and to enforce the kinematic constraints imposed by the FTS method to define the effective transition tube inside which the trajectories must stay. For the FTS implementation, we followed [7], where the process is decomposed in smoothing mean string phase, a re-parametrization phase and reinitialization. Here the smoothing phase is used to avoid numeric instability on the gradients used for the DCA implementation. The re-parametrization is done by polynomial interpolation and used on the string structure preservation, by normalizing the total trajectory time-step arc-length.

This methodology is tested in finding minimum-energy trajectories between different conformations of a simple protein, 1HJE ALPHA-CONOTOXIN SI. For that the macro molecule is modelled as an open-chain multibody system, with strong local propensity [10], where the conformational transitions is dominated by changes in soft torsional angles and its potential energy is generated from the CHARMM22 force field. Our code was integrated in the Lammps project [4], using part of the POEMS fix source code [11], and used for our test example in a GPU cluster of several nodes with APACHE MESOS and DC/OS on Amazon AWS.

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