ON METHODS FOR EFFICIENT AND ACCURATE DESIGN AND SIMULATION OF MULTIBODY SYSTEMS

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ABSTRACT

Molecular modeling has gained increasing importance in recent years. With the development of unprecedented computational power, the research community is edging ever closer to understanding key processes in biomolecular function and behavior. One of the recent and promising development in biomolecular simulations has been a coarse grained articulated multibody approach approximating the biomolecular systems of interest. The methods developed as a part of this research were primarily targeted at coarse grained biomolecular applications although the underlying formulations are directly applicable to the more traditional areas of multibody system analysis such as robotics, biomechanics, complex spacecraft design, MEMS and mechanism design among others. The areas which were studied are:

Intermittent Contact: A complementarity based recursive time-stepping scheme was developed in Featherstone's *Divide-and-Conquer* framework to efficiently model both unilateral and bilateral constraints in the system. It was further demonstrated that the complementarity based contact models can be used with any forward dynamics scheme resulting in a hybrid approach inheriting the properties of the underlying contact model and the associated dynamics schemes. For contact problems in flexible multibody systems involving high frequency vibration, any complementarity based time-steppers require prohibitively small time-steps to retain accuracy. For this class of problems, an iterative scheme was developed which satisfies the complementarity conditions without explicitly imposing them. As such, this scheme does not require discretization of equations of motion to compute the contact force and allows the use of any higher order integration method.

Sensitivity Analysis: A logarithmic complexity recursive method was developed which computes the first order sensitivity information for a flexible multibody system. The equations of motion are differentiated at the body level and the analytical sensitivity information is generated using a hierarchic *Assembly-Disassembly* process. Consequently, the number of differentiations required in this approach is minimal.

Efficient Hybrid DCA: In this work, an efficient hybrid DCA method is designed for the effective use of limited computational infrastructure. This approach uses the Articulated Body Algorithm (ABA) to convert selected subsystems into articulated bodies. The articulated bodies are subsequently used in a DCA framework. This DCA-ABA approach is more efficient than both DCA and ABA in presence of limited parallel infrastructure.

Adaptive Multibody Dynamics: Coarse-grained molecular simulations are particularly well suited to the study of certain biomolecular systems such as RNA because there is strong evidence that large elements of these molecules (e.g. helices) behave effectively as rigid bodies in solution. However, the rigidity of certain molecular elements is highly dependent on the context (molecular environment) of the biomolecule. As a result, a static coarse grain structure could result in inefficient or inaccurate simulation. This work presents an adaptive multibody framework to overcome these modeling challenges in coarse grain molecular systems which cannot be approximated as quasi-static. This approach allows the coarse grain structure to change on-the-fly to obtain the best combination of fidelity and computational speed. Numerical results for a fully adaptive simulation are given for a RNA sequence.