

A comparison of integration formulas for Molecular Dynamics simulation

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Explicit integrators have found common use in Molecular Dynamics (MD) simulations because they are easy to implement and work well under many conditions. However, in other classical mechanics applications that require the numerical solution of the equations of motion for complex systems, explicit methods have encountered major difficulties. In these cases, the state of the art relies on implicit methods, which are stable under large time steps and therefore can be used to decrease the number of integration steps necessary for a simulation. This in turn results in an overall reduction of CPU time that opens the door to an increase in the dimension of the problem that can be considered. The premise of this work is that numerical methods that are suitable for efficient simulation of mechanical systems will lead to significant gains when used in MD. The goal of the proposed work is to investigate this assumption and as such (a) proposes a set of two benchmark problems used to validate new numerical solution techniques, and (b) presents simulation results obtained with several classes of implicit integrators (Implicit Runge-Kutta, HHT, BDF) and compares their performance against current explicit MD integrators when used in conjunction with the proposed benchmark problems.

Molecular Dynamics is an extremely powerful tool that is based on a rather simple idea. Newton's second law says that the force on an object is equal to its mass times its acceleration. If the force on the particle is known as a function of space and time then the trajectory of the particle can be computed by integrating Newton's equations of motion. Classical Molecular Dynamics assumes that molecules can be treated as if they were under the influence of classical forces. This assumption works remarkably well for many situations and computer simulations based on this idea have already found many applications. In addition to yielding microscale dynamical information, the methods of statistical mechanics can be applied to derive macroscale properties of interest.

Implicit methods are stable under large time steps and therefore can be used to decrease the number of integration steps, resulting in an overall reduction of CPU time. Although Molecular Dynamics has already been applied to many problems on short time and length scales, many interesting phenomena, such as biochemical reactions, currently reside on the border or outside of what is feasible to simulate. In order to explore these areas, new more efficient numerical methods must be developed and tested.

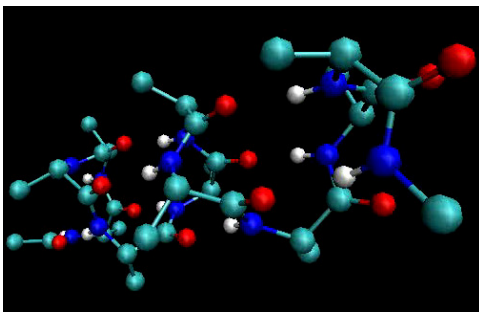


Fig. 1. Alanine Dipeptide

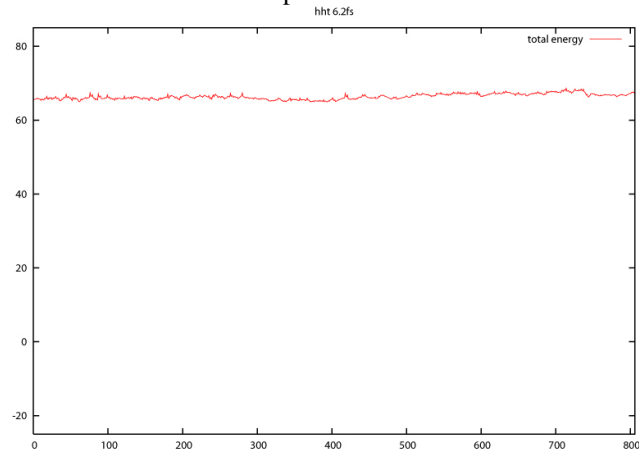


Fig. 2. Energy Conservation: HHT Integrator

Figures 1 and 2 show an alanine dipeptide molecule and respectively its total energy for 800 time steps taken using the HHT integrator at a step-size of 6.2 fs, which is about three times larger than the largest step size that a Verlet type formula can use. Reaching step-sizes of 15 or 20 fs while continuing to preserve the total energy has proved to be an elusive task so far due to difficulties in Newton convergence, an issue that is currently under investigation and the paper will report on.