8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

STABILITY OF ASYNCHRONOUS VARIATIONAL INTEGRATORS

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Key Words: *Stability of Time Integrators, Variational Integrators, Symplectic Integrators, Multistep Methods.*

ABSTRACT

Symplectic integrators are widely used in molecular dynamics simulations of many-body systems (such as proteins and crystals) as well as in some computational solid mechanics problems. One distinguishing feature of these integrators is their long-time energy conservation which is a highly desirable trait for dynamical simulations. A framework for deriving symplectic integrators involves the application of the discrete version of Hamilton's variational principle. First an appropriate discretization of the action integral, called the action sum, is made. Then the variational integrators are constructed by requiring that the discrete trajectory is a stationary point of this action sum. Any variational integrator is symplectic and vice versa.

Asynchronous variational integrators (AVI) are a class of variational integrators characterized by their allowance for the choice of different time steps for different potential energy contributions in a mechanical system. These integrators have much in common with other multiple time-stepping schemes used in computational mechanics such as subcycling and element-by-element methods. However a critical difference is that the aforementioned methods are not symplectic. In molecular dynamics r-RESPA is a commonly used multistep algorithm and it can be shown that r-RESPA is a specific instance of AVI. The main distinction between AVI and some of the other multiple time-stepping schemes such as r-RESPA is the flexibility in the choice of time steps. For example r-RESPA requires all pairs of time steps to be in integer relation. This restriction is relaxed with AVI so that arbitrary time step combinations may be selected. In solid mechanics this extra flexibility allows for choosing a set of time steps that varies smoothly across a finite element mesh. For molecular dynamics more general potential decompositions may be considered where each potential has a characteristic time and length scale.

Previous studies have shown that r-RESPA exhibits resonance instabilities in molecular dynamics applications. The existence of these instabilities limits the size of the time steps that can be taken. On the

other hand resonances do not impose the same restrictions in computational mechanics. Stability analyses for subcycling methods have detailed many intriguing aspects about these algorithms. From these observations it was postulated that resonance instabilities are not observed in solid mechanics simulations because the set of resonant time steps is a small subset of all possible time step combinations. As a result in practice it is very unlikely that a random set of time steps chosen according to appropriate stability guidelines, e.g. the CFL criterion, will exhibit resonant behavior. Although this analysis applies to non-symplectic subcycling methods we will show that this proposition is also true for AVI.

In this work the stability analysis of multiple time-stepping schemes is extended to AVI with rational time step ratios and the results of this study comprise the first main contribution. Consider a single degree-of-freedom harmonic oscillator whose potential energy is decomposed into two components, a stiff and soft part. For the described system a complete linear stability analysis of AVI can be done for rational time step ratios. From the instability criterion obtained from this analysis, we conjecture that the set of resonant time steps is dense and that arbitrarily small unstable time steps exist. In a systematic numerical investigation, this conjecture was verified. Note that these resonances are extremely weak and of no practical importance (typically millions of time step or more are needed to observe a significant error growth). This conjecture is consistent with known results regarding symplectic integrators such as their long time energy conservation.

AVI produces resonance instabilities when weak long-range forces are integrated with a large time step near an integer multiple of the half-period of a natural mode of the system. This instability appears as an exponential growth in the amplitude of the excited mode. The strength and width (interval of unstable time steps) of the resonances vary with the stiffness of the long-range forces. Softer long-range forces will lead to slower amplitude growth in the excited mode and a narrower interval of resonant time steps thereby reducing the probability of encountering these instabilities in practice.

The second key contribution is the investigation of resonance instabilities in molecular dynamics and the lack thereof in solid mechanics. An elucidation of this dichotomy is given using the AVI stability analysis for the harmonic oscillator. In molecular dynamics the dense distribution of natural frequencies in the structure makes it highly likely that any moderately large time step taken for the integration of the long-range forces will be in resonance with at least one of the natural modes. For finite element discretizations in solid mechanics, the element stiffnesses typically vary smoothly across the mesh. It can be shown that the amplitude of stiff modes decays exponentially over soft regions. This implies that the coupling of the soft elements to the stiff modes is extremely weak. Therefore the intervals of resonant time-steps for the soft elements are very narrow and as a result are rarely observed in solid mechanics simulations.

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