

# Verlet-I/r-RESPA is Limited by Non-Linear Instability

QUN MA, JESUS IZAGUIRRE, AND ROBERT SKEEL

Department of Computer Science and Engineering

University of Notre Dame

Notre Dame, IN 46556, USA

qma1@cse.nd.edu

izaguirr@cse.nd.edu

skeel@cs.uiuc.edu

## Abstract

We show that in molecular dynamics (MD) when constant-energy (NVE) simulations of Newton's equations of motion are attempted using the multiple time stepping (MTS) integrator Impulse, there are nonlinear instabilities when the longest step size is a third or possibly a fourth of the period(s) of the fastest motion(s) in the system. This is demonstrated both through a thorough set of computer experiments and through the analysis of a nonlinear model problem. The numerical experiments include not only the un-constrained dynamics simulation of a droplet of flexible water and a flexible protein, but also the constrained dynamics simulation of a solvated protein, representing a range of simulation protocols commonly in use by bio-molecular modelers. The observed and predicted instabilities match exactly. Previous work has identified and explained a linear instability for Impulse at around half the period of the fastest motion. Mandziuk and Schlick discovered nonlinear resonances in single time stepping MD integrators, but unstable nonlinear resonances for MTS integrators are reported here for the first time. This paper also offers an explanation on the instability of MTS constrained molecular dynamics simulations of explicitly solvated proteins.