Backward error analysis of multiscale symplectic integrators and propagators.

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Abstract

Symplectic integrators are used in molecular dynamics simulations for their to excellent long term behavior, due to the existence of the associated shadow Hamiltonian. Improvements in the efficiency of simulations can be obtained by the introduction of multiple timestep methods such as Verlet-I/r-RESPA, but these schemes generally require switches to separate the forces efficiently. The authors derive the shadow Hamiltonian for this method, using backward error analysis, and show its dependence on the smoothness of these switches.

1 Introduction

In this paper we consider both the backward error analysis for Verlet-I/r-RESPA and the effect of the addition of switching functions to split the potential energy. It had been previously noted [1] that the lack of smoothness in a C^1 continuous piecewise potential had a "deleterious effect on the conservation of interpolated shadow Hamiltonians". We expand upon this result and extend it to switched potentials and the backward error analysis of the Verlet-I/r-RESPA integrator.

2 Shadow Hamiltonian for the Verlet-I integrator

Given that a shadow Hamiltonian (for which the numerical results are the exact solution), $\hat{H}$, exists it can be calculated using either the truncated or interpolated methods. The truncated method, which can be found in [2], is

$$\hat{H} = H + \delta t \hat{H}^{(1)} + \delta t^2 \hat{H}^{(2)} + \cdots, \tag{1}$$

where H is the original Hamiltonian and $\hat{H}^{(i)}$ are the additional terms of the modified Hamiltonian which are calculated by the backward error analysis [3] for timestep δt. In general the series does not converge for non-linear systems and is truncated at some point. The Verlet-I multiple timestep method, for a total time-step of $r\delta t$ where r is the ratio between the fast and slow steps, has the 4^{th} order truncated shadow Hamiltonian

$$\begin{aligned}\hat{H}_{[4T]} &= H + \frac{\delta t^2}{24}\Big[2\left(\mathbf{U}_f'\right)^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{U}_f' - r^2\left(\mathbf{U}_s'\right)^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{U}_s' - 2r^2\left(\mathbf{U}_f'\right)^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{U}_s' \\ &\quad - \mathbf{p}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{U}_f''\,\mathbf{M}^{-1}\mathbf{p} + 2r^2\mathbf{p}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{U}_s''\,\mathbf{M}^{-1}\mathbf{p}\Big] + \mathcal{O}(\delta t^4),\end{aligned}$$

where $\mathbf{q}$ are the positions, $\mathbf{p}$ the momenta and $\mathbf{M}$ the matrix of body masses. Potential energies $U_s(\mathbf{q})$ gives rise to the 'slow' forces, with derivative $\mathbf{U}'_s$ and Hessian $\mathbf{U}''_s$, and $U_f(\mathbf{q})$ to the 'fast' forces, with derivative $\mathbf{U}'_f$ and Hessian $\mathbf{U}''_f$. The original Hamiltonian being $H = \frac{1}{2}\mathbf{p}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{p} + U_s + U_f$. We can see from this result that the continuity of the potential energy terms U_s and U_f, and hence the existence of derivatives, will provide an upper bound to the order of the shadow Hamiltonian.

In [4] an alternative scheme was proposed whereby a homogeneous extension of the original Hamiltonian, $\tilde{H}$, is considered. Given the extended homogeneous Hamiltonian system

$$\dot{y}_h(t) \;=\; \tilde{J}\tilde{H}_{y_h}\left(y_h(t)\right),$$

for some $\tilde{J}$ and extended phase-space variables y_h. We can then define

$$A_{i,j} \;=\; \frac{\nabla^i y_h(t)^{\mathrm{T}}\tilde{J}\nabla^j y_h(t)}{2\delta t},$$

here the backward difference operator, for some function $\omega(t)$, is defined as $\nabla^0\omega(t) = \omega(t)$, $\nabla^k\omega(t) = \nabla^{k-1}\omega(t) - \nabla^{k-1}\omega(t-h)$. It is then possible to derive k^{th} order approximations for $\hat{H}$ in terms of the $A_{i,j}$ using Newton's interpolation. We then have, for example, $\hat{H}_{[4]} = A_{1,0} - \frac{1}{2}A_{2,0} + \frac{2}{3}A_{2,1}$, where $\hat{H}_{[k]}$ is the k^{th} order approximation of $\hat{H}$.

3 Switching

Switches are required to split the force between short and long ranges so that a multiple time-step integrator can be used. In order to retain the Hamiltonian the switch must be applied to the energy. Commonly used switches for Lennard-Jones and Coulombic forces have C^1 continuity (NAMD and ProtoMol) which yield a vector field which is C^0. The following scheme, which can provide switches of arbitrary smoothness, was used for testing

$$Y^n(a_{ij}) \;=\; \begin{cases} 1 & \text{if } a_{ij} \le r_o, \\ \sum_{k=0}^{2n+1} \gamma_k \left(\frac{a_{ij}-r_c}{r_o-r_c}\right)^k & \text{if } r_o \le a_{ij} < r_c, \\ 0 & \text{if } a_{ij} > r_c. \end{cases}$$

Here r_o is the switch-on value and r_c the cutoff. The coefficients γ_k for a switch which is C^n can be determined from the conditions, in addition to $Y^n(r_o) = 1$, $Y^n(r_c) = 0$, that all derivatives up to d^nY^n/da_{ij}^n must be zero when equated at r_c and r_o. The coefficients for switches C^2, C^3, C^4 and C^6 are shown in Tab. 1.

n	coefficients γ_i										
	3	4	5	6	7	8	9	10	11	12	13
2	10	-15	6								
3	0	35	-84	70	-20						
4	0	0	126	-420	540	-315	70				
6	0	0	0	0	1716	-9009	20020	-24024	16380	-6006	924

Table 1: Coefficients for a C^n switches. Note $\gamma_1 = \gamma_2 = 0$ for all switches C^2 and above.

4 Experiments

To illustrate the effect of the switches on approximating the shadow Hamiltonian a model of 216 water molecules using periodic boundary conditions (PBC) was used with the Verlet-I integrator utilizing a step ratio $r = 3$. The results can be seen in Fig. 1 for a 12^{th} order interpolated shadow Hamiltonian, it is clear that the the order of the calculated shadow Hamiltonian is dependent on the continuity of the switch.

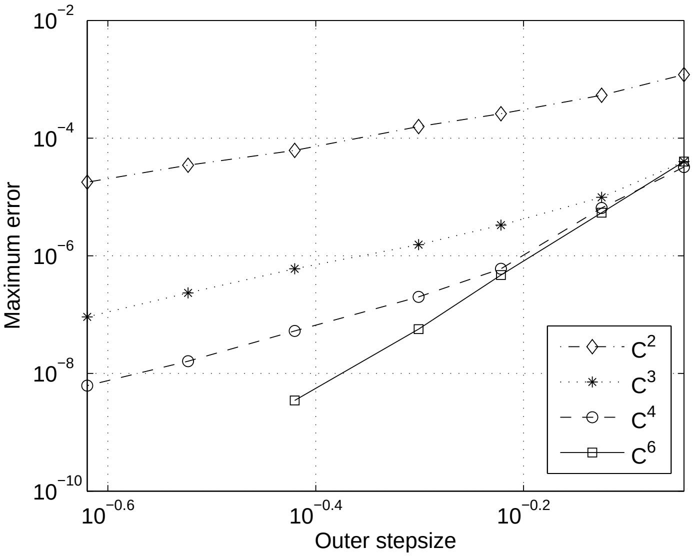

Figure 1: $\hat{H}_{[12]}$ interpolated Shadow Hamiltonian for the Verlet-I method, 216 water molecules with PBC model, for C^2, C^3, C^4 and C^6 switches.

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