The Five Femtosecond Time Step Barrier*

Robert D. Skeel and Jesús A. Izaguirre

Beckman Institute and Department of Computer Science
University of Illinois at Urbana-Champaign

Abstract. Simulation of the dynamics of biomolecules requires the use of a time step in the range 0.5–1 fs to obtain acceptable accuracy. Nevertheless, the bulk of the CPU time is spent computing interactions, such as those due to long-range electrostatics, which vary hardly at all from one time step to the next. This unnecessary computation is dramatically reduced with the use of multiple time stepping methods, such as the Verlet-I/r-RESPA method, which is based on approximating "slow" forces as widely separated impulses. Indeed, numerical experiments show that time steps of 4 fs are possible for these slow forces but unfortunately also show that a long time step of 5 fs results in a dramatic energy drift. Moreover, this is less pronounced if one uses a yet larger long time step! The cause of the problem can be explained by exact analysis of a simple two degree-of-freedom linear problem, which predicts numerical instability if the time step is just less than half the period of the fastest normal mode. To overcome this, a modification of the impulsive Verlet-I/r-RESPA method is proposed, called the mollified impulse method. The idea is that one modifies the slow part of the potential energy so that it is evaluated at "time averaged" values of the positions, and one uses the gradient of this modified potential for the slow part of the force. Various versions of the algorithm are implemented for water and numerical results are presented.

1 Introduction

Answers to questions in structural biology are often sought by means of long time biomolecular simulations using empirical classical mechanical force fields. Nevertheless, the shortest time scales present in the simulation have limited the integration step to 0.5–1 fs, which is many orders of magnitude smaller than the desired simulation time interval. Fairly recently the introduction of the Verlet-I [8,9]/r-RESPA [23] "impulse" multiple time step (MTS) method has permitted an increase to 4 fs in the length of the longest time step. This article describes this development

* This work was supported in part by NIH Grant P41RR05969 and NSF Grants BIR-9318159 and DMS-9600088.

as well as empirical [4] and analytical [7] evidence indicating that timesteps of 5 fs or greater are not possible with the impulse MTS method (for unconstrained molecular dynamics). Nevertheless, a modification to this method – the "mollified" impulse method [7] – yields stable dynamics for longest timesteps as great as 7 fs.

MTS methods exploit the existence of different time scales arising from the many interactions present in the force field. For expository purposes assume that the potential energy function is expressed as the sum of just two parts $U^{\text{fast}}(x) + U^{\text{slow}}(x)$, where x denotes the collection of all atomic positions. The equations of motion for unconstrained constant NVE dynamics are

$$M\frac{d^2}{dt^2}X = F^{\text{fast}}(X) + F^{\text{slow}}(X) \tag{1}$$

where M is a diagonal matrix of atomic masses, $x = X(t)$ are the atomic trajectories, $F^{\text{fast}} = -U_x^{\text{fast}}$, and $F^{\text{slow}} = -U_x^{\text{slow}}$. The partitioning is chosen so that an appropriate time step Δt for the slow part is significantly larger than an appropriate time step δt for the fast part. To be specific about the length of an appropriate time step, there is a recipe in [17], which suggests that Δt^2 be chosen to be proportional to the reciprocal of the largest eigenvalue of the mass weighted Hessian $M^{-1/2}U_{xx}^{\text{slow}}(x)M^{-1/2}$, and analogously for δt^2.

Although unconstrained dynamics is being considered here, the ideas extend to the case where bond lengths (and bond angles) are constrained. Also, the ideas are applicable to other than constant NVE simulations.

This article is organized as follows: Sect. 2 explains why it seems important to use symplectic integrators, Sect. 3 describes the Verlet-I/r-RESPA impulse MTS method, Sect. 4 presents the 5 femtosecond time step barrier, Sect. 5 introduce a possible solution termed the "mollified" impulse method (MOLLY), and Sect. 6 gives the results of preliminary numerical tests with MOLLY.

2 Importance of Symplectic Integration

It is appropriate to consider first the question of what kind of accuracy is expected from a simulation. In molecular dynamics

(MD) very small perturbations to initial conditions grow exponentially in time until they completely overwhelm the trajectory itself. Hence, it is inappropriate to expect that accurate trajectories be computed for more than a short time interval. Rather it is expected only that the trajectories have the correct statistical properties, which is sensible if, for example, the initial velocities are randomly generated from a Maxwell distribution.

The use of a numerical integrator to approximate the exact propagator of a system of ordinary differential equations (ODEs) yields a numerical solution which can be interpreted as the exact solution of a slightly different system of ODEs.[1] If the given system is a Hamiltonian system (as it is for constant-energy MD), then the slightly different system is Hamiltonian if and only if the integrator is symplectic [21]. In particular, this implies that any given energy surface in phase space is changed only slightly by the use of symplectic numerical integration, and it suggests that statistical properties of long-time dynamics are retained.

A transformation in phase space from positions x and momenta p

$$\bar{x} = \xi(x, p), \qquad \bar{p} = \pi(x, p) \tag{2}$$

is said to be *symplectic* if its Jacobian matrix (of partial derivatives) satisfies

$$\begin{bmatrix} \xi_x & \xi_p \\ \pi_x & \pi_p \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \begin{bmatrix} \xi_x & \xi_p \\ \pi_x & \pi_p \end{bmatrix} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}. \tag{3}$$

The exact propagator for a Hamiltonian system for any given time increment Δt is symplectic. As a consequence it possesses the Liouville property of preserving volume in phase space.

Additional evidence favoring the use of symplectic integrators is an observation [18] concerning hybrid Monte Carlo methods: to get the property of detailed balance needed for valid sampling, it is enough to use a numerical integrator which is volume preserving and reversible. As was just mentioned, symplectic integrators preserve volume in phase space.

[1] This statement is not exactly true – the slightly different system of ODEs is defined by an asymptotic expansion in powers of Δt which is generally divergent.

On the basis of these considerations it is suggested that the design of numerical integration techniques might employ the following two hypotheses:

1. desired computables are insensitive to small changes in the Hamiltonian $\frac{1}{2}p^{\mathrm{T}}M^{-1}p + U(x)$, and
2. symplectic numerical integration produces small changes to the Hamiltonian.

3 The Verlet-I/r-RESPA Impulse Method

For MD the reduced system

$$M\frac{d^2}{dt^2}X = F^{\mathrm{fast}}(X) \tag{4}$$

is cheap to integrate compared to the cost of integrating the full system. For example, for the MD program NAMD [19] on an ATM-connected cluster of eight HP 9000-735/125 workstations applied to a system of 36,000 atoms, the CPU time required to compute the "fast" short-range forces is 7 seconds whereas that required for the "slow" long-range forces is 29 seconds. Short-range forces consisted of all forces except electrostatic forces beyond 8 Å. The latter were calculated using a parallel enhanced fast multipole method [15]. An efficient numerical integrator would evaluate F^{slow} sparingly and incorporate its values into an integration of the reduced system in the most advantageous way. The question is how to do this.

A good place to start the discussion is the "impulse method"

$$M\frac{d^2}{dt^2}X = F^{\mathrm{fast}}(X) + \sum_{m=-\infty}^{\infty} \Delta t\ \boldsymbol{\delta}(t - m\Delta t)F^{\mathrm{slow}}(X) \tag{5}$$

proposed by [24], in which the slow force is approximated by a sequence of appropriately weighted impulses. If the reduced system is analytically solvable, then the above approximation to the full system is solvable by inserting jumps into the analytical integration of $(d/dt)X(t)$ at integer multiples of the time step Δt. Let $P = M(d/dt)X$, and suppose values X^{n-1}, P^{n-1}, and

$F^{\mathrm{slow},n-1} = F^{\mathrm{slow}}(X^{n-1})$ are given. Then one step of the impulse method can be expressed as follows:

half a kick

$$P^{n-1+\epsilon} = P^{n-1} + \frac{\Delta t}{2} F^{\mathrm{slow},n-1}. \tag{6}$$

a vibration Propagate X^{n-1}, $P^{n-1+\epsilon}$ by integrating

$$\frac{d}{dt}X = M^{-1}P, \quad \frac{d}{dt}P = F^{\mathrm{fast}}(X) \tag{7}$$

for an interval Δt to get X^n, $P^{n-\epsilon}$.

half a kick

$$F^{\mathrm{slow},n} = F^{\mathrm{slow}}(X^n), \tag{8}$$

$$P^n = P^{n-\epsilon} + \frac{\Delta t}{2} F^{\mathrm{slow},n}. \tag{9}$$

The symbols $P^{n-1+\epsilon}$ and $P^{n-\epsilon}$ represent momenta just after the $(n-1)$st kick, and just before the nth kick, respectively.

The application in [24] is to celestial mechanics, in which the reduced problem for U^{fast} consists of the Keplerian motion of planets around the sun and in which the U^{slow} impulses account for interplanetary interactions. Application to MD is explored in [14]. It is not easy to find a reduced problem that can be integrated analytically however. The choice $U^{\mathrm{fast}} \equiv 0$ is always possible and this yields the simple but effective leapfrog/Störmer/Verlet method, whose use according to [22] dates back to at least 1793 [5]. This connection should allay fears concerning the quality of an approximation using Dirac delta functions.

The need to integrate the fast forces analytically can be avoided by approximating it by a sequence of suitably weighted impulses but more closely spaced in time than the slow force impulses:

$$M\frac{d^2}{dt^2}X = \sum_{m=-\infty}^{\infty} \delta t\, \boldsymbol{\delta}(t-m\delta t) F^{\mathrm{fast}}(X) + \sum_{n=-\infty}^{\infty} \Delta t\, \boldsymbol{\delta}(t-n\Delta t) F^{\mathrm{slow}}(X). \tag{10}$$

The idea is illustrated by Fig. 1. These equations constitute a readily understandable and concise representation of the widely

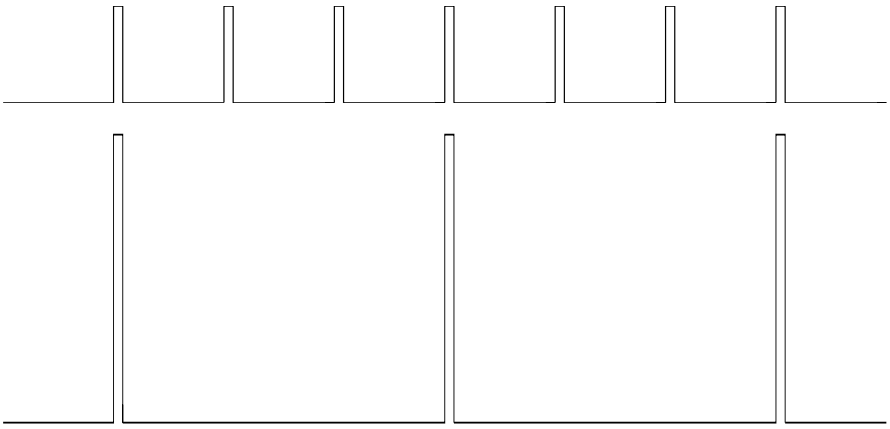

Fig. 1. Schematic for the impulse multiple time stepping method.

used Verlet-I/r-RESPA impulse MTS method. The method was described first in [8,9] but tested first in [23]. This latter reference describes the method in terms of an operator splitting and proposes the splitting of nonbonded interactions using switching functions. The symplecticness of this method is first noted in [3]. Of course, the idea generalizes to more than two different time steps. Also, it is most practical to choose time steps with ratios that are integers.

4 Time Step Barriers

Based on accuracy considerations alone, it seems that time steps of the order $\Delta t = 16\,\text{fs}$ should be possible for the slowest forces for MD [6]. Contrast this with the 0.5–1 fs value needed for the fastest forces.

Nevertheless, it was recognized already in the first paper on the impulse method [9] that resonance might be expected if the timestep Δt is approximately equal to the period of the fastest normal mode, which is 9 or 10 fs for biomolecules with flexible bonds to hydrogen. (Flexible bonds to hydrogen give modes with the highest frequency because bond stretching interactions have the largest force constants and hydrogen atoms have the smallest

mass.) This resonance can be most readily explained if one assumes δt is infinitesimal and neglects the dependence of the slow force on X. Then, the impulse MTS method simplifies to

$$M\frac{d^2}{dt^2}X = F^{\text{fast}}(X) + \sum_n \Delta t\ \boldsymbol{\delta}(t - n\Delta t)F^{\text{slow}}, \qquad (11)$$

which is a system of ODEs with a periodic forcing function. If the frequency of the forcing function coincides with a natural frequency of the unforced system, then resonance produces an oscillation in the trajectory whose amplitude increases with time. This artifact of the impulse MTS method was first demonstrated, for simple problems, in [3]. A more recent analytical study [7] shows that the trajectory error in the impulse method is proportional to Δt rather than Δt^2 if F^{fast} is fast enough to produce resonance.

More surprisingly, there is also a problem for time steps Δt just smaller than *half* the period of the fastest normal mode, which is approximately 5 fs. There is in [4] a revealing experiment for the Verlet-I/r-RESPA impulse MTS method. In a 1000-fs simulation on a 36000-atom water–protein–DNA system it was found that $\Delta t = 4$ fs produces very little energy drift, that $\Delta t = 5$ fs yields dramatic energy growth, and that $\Delta t = 6$ fs gives only half as much energy growth as $\Delta t = 5$ fs. In all cases the small time step δt was 1 fs. This experiment suggests a *stability* problem associated with timesteps Δt approximately equal to half the period of the fastest normal mode. As a check a power spectrum was computed for 20 ps of a 180 K simulation of a 20 Å diameter sphere of the flexible TIP3P water used in that simulation. This is shown by Fig. 2. Peaks are discernible at frequencies corresponding to periods of 9.3 and 12.1 fs, evidently the periods of the two normal modes for the stretching of the O–H bonds.

An upper limit of 4 fs on the longest time step is also the experience of other researchers. For example, Fig. 2 in [10] shows that energy conservation is good for long time steps in the range 0.5 to 4 fs but dramatically worsens for a 5 fs time step. See also [12,13] for evidence of a time step barrier at half the period of the fastest normal mode.

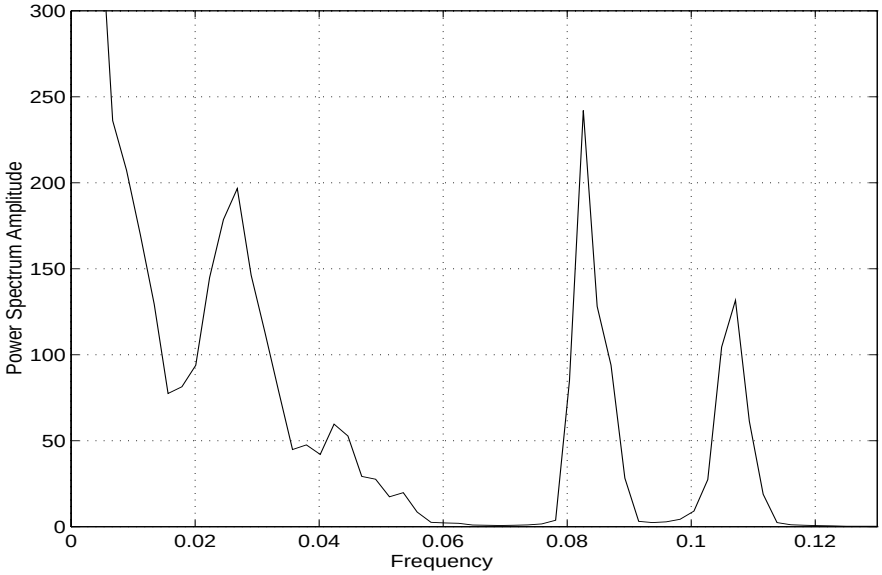

Fig. 2. Power spectrum of water dynamics with frequency in units of fs^{-1}.

An instability of the impulse MTS method for Δt slightly less than half the period of a normal mode is confirmed by an analytical study of a linear model problem [7]. For another analysis, see [2]. A special case of this model problem, which gives a more transparent description of the phenomenon, is as follows: Consider a two-degree-of-freedom system with Hamiltonian $\frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \frac{1}{2}\omega_1^2 x_1^2 + \frac{1}{4}(x_2 - x_1)^2$ This models a system of two springs connecting two balls of unit mass where one spring of stiffness ω_1^2 connects an immovable object to the first ball and a second spring of stiffness $\frac{1}{2}$ connects the balls together. The x_1, x_2 are displacements from equilibrium. The instability for the impulse MTS method is studied by choosing a timestep Δt for the second spring (the term $\frac{1}{4}(x_2 - x_1)^2$ in the Hamiltonian) and an infinitesimal timestep for the first spring (which in effect is method (5)). Analysis shows that the dynamics depends on only the two parameters $\gamma = \omega_1 \Delta t$ and Δt. Instability occurs for certain combinations of γ and Δt. This is shown by Fig. 3, where the region above the curve constitutes the region of instability. In

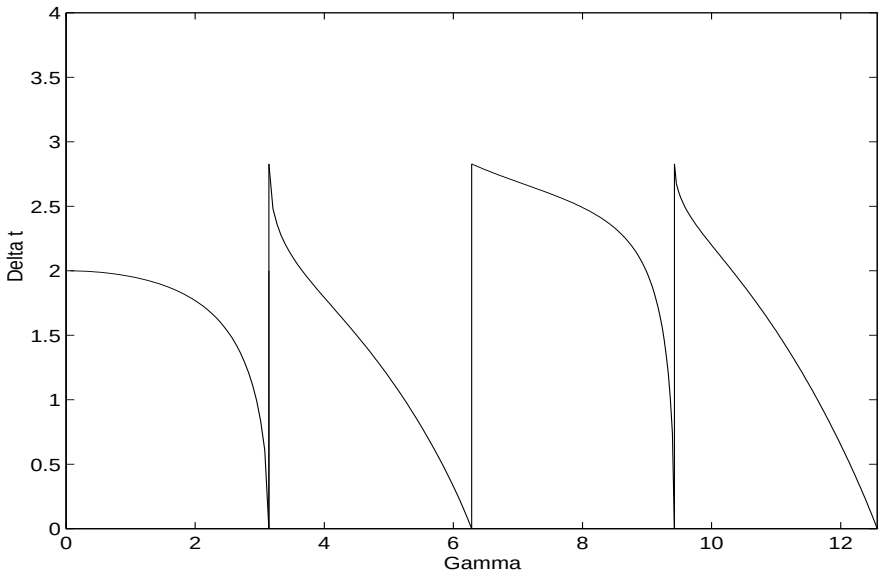

Fig. 3. Stability boundary for impulse method applied to the 2-spring problem. Gamma is $\omega_1 \Delta t$ and Delta t is Δt.

this diagram, a change in Δt with ω_1 held fixed corresponds to a move in the radial direction. Details concerning the construction of this diagram are given in Appendix A.

It is to be expected that this barrier on the long time step would be shifted upward if the highest frequencies were eliminated. These frequencies can be removed with only modest loss of accuracy by constraining selected bond lengths and bond angles. The resulting constrained system of ODEs can be numerically integrated by the popular SHAKE [20] extension of the leapfrog/Verlet method. Although SHAKE is not symplectic, there is a cosmetic modification to it known as RATTLE [1] which is symplectic [16].

The method presented in the next section is an attempt to overcome the barrier due to the highest frequencies whatever their origin. Although it has been implemented and tested for unconstrained dynamics only, there is no fundamental reason why it

cannot be applied to overcome the less restrictive time step barrier arising in constrained dynamics.

5 The Mollified Impulse Method

In an effort to counteract the accuracy reduction of the impulse method in a resonance situation, a modification to the impulse method is proposed in [7]. There, the term $U^{\text{slow}}(x)$ is replaced by $U^{\text{slow}}(\mathcal{A}(x))$, where $\mathcal{A}(x)$ represents a time averaging of positions x due to motion producible by the fast forces F^{fast} in the neighborhood of x. The purpose of this change to the potential [2] is to change the slow forces from $F^{\text{slow}}(x)$ to $\mathcal{A}_x(x)^{\mathrm{T}} F^{\text{slow}}(\mathcal{A}(x))$. Modifying the potential instead of the force ensures that the force is conservative and that the integrator is symplectic. Therefore, this generalization of the impulse method preserves symplecticness and at the same time improves the impulse method's accuracy and stability, as explained below.

The original motivation [7] for using $\mathcal{A}_x(x)^{\mathrm{T}} F^{\text{slow}}(\mathcal{A}(x))$ was to compensate for the inaccuracies arising from evaluating $F^{\text{slow}}(x)$ at point values of $x = X(t)$ sampled at large time increments Δt. Changing the point of evaluation of F^{slow} from x to $\mathcal{A}(x)$ brings about some *accuracy* gains, because $F^{\text{slow}}(\mathcal{A}(x))$ is a better description of the quickly varying $F^{\text{slow}}(X(t))$ than values of F^{slow} at step points. A more important benefit, however, is gained by multiplying the force $F^{\text{slow}}(\mathcal{A}(x))$ by the matrix $\mathcal{A}_x(x)^{\mathrm{T}}$. The latter also tremendously benefits the *stability* of the integrator by filtering out those components of the slow force that would excite components of the fast force susceptible to resonance. The F^{slow} impulse is *mollified*.

An example of a time averaging function $\mathcal{A}(x)$ is the formula termed *LongAverage* in [7]:

$$\mathcal{A}(x) = \frac{1}{\Delta t} \int_0^{\Delta t} \tilde{X}(t) dt \tag{12}$$

[2] This is not inconsistent with the problem being solved, because in the limit as $\Delta t \to 0$, one would have $\mathcal{A}(x) = x$.

where $\tilde{X}(t)$ solves an *auxiliary* problem

$$M\frac{d^2}{dt^2}\tilde{X} = F^{\text{fast}}(\tilde{X}), \quad \tilde{X}(0) = x, \quad \frac{d}{dt}\tilde{X}(0) = 0. \tag{13}$$

The derivation of the mollified impulse method in [7] suggests that the same integrator be used for the auxiliary problem as that used for integrating the *reduced primary* problem $M(d^2/dt^2)X = F^{\text{fast}}(X)$ between impulses. Of course, $\mathcal{A}_x(x)^{\text{T}}$ is also needed. For the partitionings $U^{\text{fast}} + U^{\text{slow}}$ typically used in MD, this would lead unfortunately to a matrix $\mathcal{A}_x(x)^{\text{T}}$ with a great many nonzeros. However, it is probably important to take into account only the fastest components of U^{fast} [7]. Hence, it would seem sufficient to use only the fastest forces $F^{\text{fastest}}(x)$ in the time averaging calculation.

Suppose values X^{n-1}, P^{n-1}, and $F^{\text{slow},n-1} = F^{\text{slow}}(X^{n-1})$ are given. One step of the efficient version of MOLLY just described can be expressed as follows:

half a mollified kick

$$P^{n-1+\epsilon} = P^{n-1} + \frac{\Delta t}{2}F^{\text{slow},n-1}. \tag{14}$$

a vibration Propagate X^{n-1}, $P^{n-1+\epsilon}$ by integrating

$$\frac{d}{dt}X = M^{-1}P, \quad \frac{d}{dt}P = F^{\text{fast}}(X) \tag{15}$$

for an interval Δt to get X^n, $P^{n-\epsilon}$.

a time averaging Calculate a temporary vector of time-averaged positions $\bar{X}^n = \mathcal{A}(X^n)$ and a Jacobian matrix $J^n = \mathcal{A}_x(X^n)^{\text{T}}$. The time averaging function $\mathcal{A}(x)$ uses only $F^{\text{fastest}}(x)$.

half a mollified kick

$$F^{\text{slow},n} = J^n F^{\text{slow}}(\bar{X}^n), \tag{16}$$

$$P^n = P^{n-\epsilon} + \frac{\Delta t}{2}F^{\text{slow},n}. \tag{17}$$

The symbols $P^{n-1+\epsilon}$ and $P^{n-\epsilon}$ represent momenta just after the $(n-1)$st kick, and just before the nth kick, respectively. Note that $\bar{X}^n$ is used only for the purpose of evaluating F^{slow}; it does not replace the value of X^n.

The calculation of $\mathcal{A}(x)$ and $\mathcal{A}_x(x)$ can be done in a systematic manner. First the calculation of $\mathcal{A}(x)$ is coded, and then this is differentiated with respect to each of the components of x to yield code for $\mathcal{A}_x(x)$. An example of this procedure for the leapfrog method is given in Appendix B.

Different time averagings are, of course, possible. Various time averagings can be defined by

$$\mathcal{A}(x) = \frac{1}{\Delta t} \int_0^\infty \phi\left(\frac{t}{\Delta t}\right) \tilde{X}(t) dt \tag{18}$$

where $\phi(s)$ is a weight function. Some interesting choices are

LongAverage

$$\phi(s) = \begin{cases} 1, & |s| < 1, \\ \frac{1}{2}, & |s| = 1, \\ 0, & |s| > 1. \end{cases} \tag{19}$$

LongLinearAverage

$$\phi(s) = \begin{cases} 1 - \frac{1}{2}s, & 0 \le s \le 2, \\ 0, & s \ge 2. \end{cases} \tag{20}$$

LongQuadraticAverage

$$\phi(s) = \begin{cases} \frac{1}{4}(3 - s^2), & 0 \le s \le 1, \\ \frac{1}{8}(3 - s)^2, & 1 \le s \le 3, \\ 0, & s \ge 3. \end{cases} \tag{21}$$

If the fastest forces F^{fastest} consist only of bond stretching and angle bending, then it is possible to define a time averaging $\mathcal{A}$ as

a projection onto the equilibrium value of the bond lengths and bond angles. This technique appears to have better stabilizing properties. Further details are to be provided elsewhere [11]. Here this time averaging is called *Equilibrium*.

6 Numerical Tests for MOLLY

The mollified impulse method was implemented in NAMD and tested on a 20 Å diameter sphere of flexible TIP3P water at 370 K. The switching function in [10] was used with a transition distance of 4 Å to 6.5 Å to separate the slow long-range electrostatic interactions from the remaining forces. The cutoff was chosen to be short to ensure that slow forces are of significant magnitude. Experiments such at those in [4] suggest that flexible water models are particularly sensitive to destabilizing artifacts in numerical integrators.

Shown in Fig. 4 are plots of total pseudoenergy vs. simulation time for two time averaging methods mentioned in this article, plus the *Equilibrium* and impulse method. The pseudoenergy is the true total energy with $U^{\text{slow}}(x)$ replaced by $U^{\text{slow}}(\mathcal{A}(x))$. This is the quantity which the integrator is trying to conserve, so it is a more sensitive indicator than the true energy of instability. In all cases the long time step Δt is 8 fs and the short time step δt is 1 fs. Only the *Equilibrium* version of MOLLY does not lead to energy increase in this experiment. The *LongQuadraticAverage* version gives a slight energy increase while the *LongAverage* gives a large energy increase. Ranking of the two time averagings is in direct relation to the extensiveness of their time averaging and is consistent with the stability analysis of [7]. Notice the dramatic rise in energy for the impulse method.

The *Equilibrium* version was tested also on a 40 Å diameter sphere of water with a switching function transition distance of 8 Å to 13 Å. There was in this case a slight rise in energy when Δt was 8 fs.

Fig. 5 shows that all three time averaging methods succeed for a long timestep Δt of 5 fs.

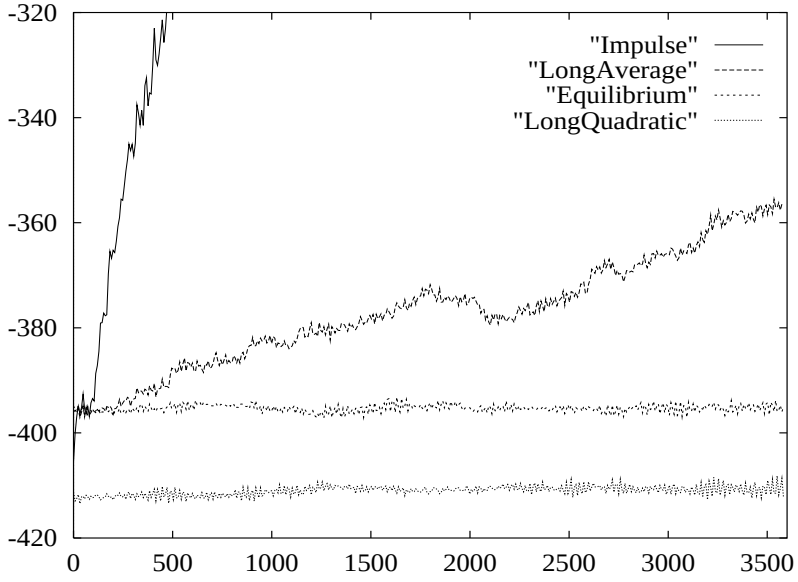

Fig. 4. Total pseudoenergy (in kcal/mol) vs. simulation time (in fs) for time averaging, *Equilibrium*, and impulse methods. (Δt for all methods equals 8 fs.)

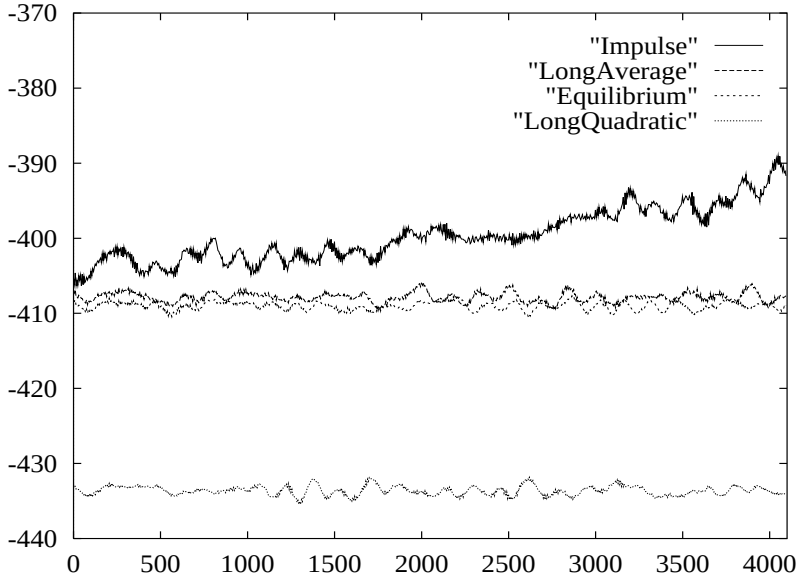

Fig. 5. Total pseudoenergy (in kcal/mol) vs. simulation time (in fs) for time averaging, *Equilibrium*, and impulse methods. (Δt for all methods equals 5 fs.)

Acknowledgment

We are grateful to Dorina Kosztin for reviewing a draft of the manuscript.

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Appendix A Stability Conditions for the Impulse Method

Here are given details indicating how Fig. 3 was obtained from the analytical study in [7]. The problem considered there is a system with Hamiltonian $\frac{1}{2}p_1^2+\frac{1}{2}p_2^2+\frac{1}{2}\omega_1^2x_1^2+\frac{1}{4}(x_2-x_1)^2+\frac{1}{2}\omega_2^2x_2^2$, which models a system of *three* springs connecting two balls of unit mass where the third spring is of stiffness ω_2^2 and connects the second ball to an immovable object. Instability is studied by choosing a timestep Δt for the second spring and an infinitesimal timestep for the other two springs. Presented here is the special case $\omega_2 = 0$, which, of course, simplifies the stability conditions given in [7]. These simplified stability conditions depend on the two parameters $\gamma = \omega_1\Delta t$ and Δt. Instability occurs when

$$\left(\frac{\Delta t}{2}\right)^2 > 2(1+\cos\gamma)(1+\cos\gamma+2\gamma^{-1}\sin\gamma)^{-1}$$
$$\text{for } 0 \le \gamma < \pi \text{ or } 2\pi \le \gamma < 3\pi \text{ or } \ldots$$

and

$$\left(\frac{\Delta t}{2}\right)^2 > (1-\cos\gamma)(1+|\gamma^{-1}\sin\gamma|^{1/2})^{-2}$$
$$\text{for } \pi \le \gamma < 2\pi \text{ or } 3\pi \le \gamma < 4\pi \text{ or } \ldots ,$$

which is shown in Fig. 3 with the region above the curve constituting the region of instability.

Appendix B Calculation of the Jacobian Matrix of an Averaging Function

As an example suppose that the leapfrog method with time step δt is coded for the calculation of $\mathcal{A}(x)$. This is then differentiated to obtain $\mathcal{A}_x(x)$. The result is the following code for calculating $\mathcal{A}(x)$ and $\mathcal{A}_x(x)$: Initialization is given by

$$\begin{array}{ll} X := x, & X_x := I, \\ P := 0, & P_x = 0, \\ B := 0, & B_x = 0, \end{array} \tag{22}$$

and step by step integration by

$$\begin{array}{ll} P := P + \frac{1}{2}\delta t F^{\text{fastest}}(X), & P_x := P_x + \frac{1}{2}\delta t F_x^{\text{fastest}}(X)X_x, \\ B := B + \frac{1}{2}\delta t X, & B_x := B_x + \frac{1}{2}\delta t X_x, \\ X := X + \delta t M^{-1} P, & X_x := X_x + \delta t M^{-1} P_x, \\ B := B + \frac{1}{2}\delta t X, & B_x := B_x + \frac{1}{2}\delta t X_x, \\ P := P + \frac{1}{2}\delta t F^{\text{fastest}}(X), & P_x := P_x + \frac{1}{2}\delta t F_x^{\text{fastest}}(X)X_x. \end{array} \tag{23}$$

The value $(1/\Delta t)B$ is used for $\mathcal{A}(x)$ and $(1/\Delta t)B_x$ for $\mathcal{A}_x(x)$.