Reply to Comment on: Reversible multiple time scale molecular dynamics

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This is a response to the preceding comment by Toxvaerd [J. Chem. Phys. **99**, 2277 (1993)]. In the paper *Reversible multiple time scale molecular dynamics*, reversible second order numerical integrators were derived by applying operator expansion techniques (the Trotter expansion)[1] to the Liouville operator formulation of classical mechanics.[2] It was shown that by using appropriate breakups of the full classical propagator, integrators which efficiently handle problems involving disparate masses (light and heavy particles), long range forces and fast vibrational degrees of freedom can be obtained. As introductory examples to the application of the formalism, two simple integrators were derived, the well known velocity Verlet (vv) integrator[3] and the "new" position Verlet (pv) integrator. These integrators were derived from a first principles approach. A less rigorous analysis which does not start from first principles can lead to the result that the integrators are related to the *same* leap-frog algorithm or Stoermer time center formula[4] and thus all differences are a matter of notation. In this response, the relationship between the trajectories of the two algorithms will be determined and the relationship of the integrators to the leap-frog algorithm clarified.

The classical propagator is defined by

$$U(t)=e^{iLt}, \tag{1}$$

where

$$iL=\{\cdots, H\}=\left[\frac{p}{m}\frac{\partial}{\partial x}+F(x)\frac{\partial}{\partial p}\right]. \tag{2}$$

Of course, one cannot in general evaluate the action of the full Liouville operator on the positions and velocities, $(\{x(t)=e^{iLt}x(0),\ v(t)=e^{iLt}v(0)\})$. In order to generate numerical integrators an operator expansion can be applied

$$e^{iLt}=[e^{iL\Delta t}]^P, \tag{3}$$

$$e^{iL\Delta t}=e^{iL_1(\Delta t/2)}e^{iL_2(\Delta t/2)}+O(\Delta t^3), \tag{4}$$

where $iL=iL_1+iL_2$ and $\Delta t=t/P$. Note that time slices smaller than Δt are *not* defined. Velocity Verlet is generated by using $iL_1=F(x)\partial/\partial p$ and $iL_2=(p/m)\partial/\partial x$ and applying the resulting evolution operator

$$\begin{aligned} x(\Delta t)&=x(0)+\Delta t v(0)+\frac{\Delta t^2}{2m}F[x(0)],\\ v(\Delta t)&=v(0)+\frac{\Delta t}{2m}(F[x(0)]+F[x(\Delta t)]). \end{aligned} \tag{5}$$

Position Verlet is generated using the same process but with the definitions iL_1 and iL_2 interchanged

$$\begin{aligned} v(\Delta t)&=v(0)+\frac{\Delta t}{2m}F\left[x(0)+\frac{\Delta t}{2}v(0)\right],\\ x(\Delta t)&=x(0)+\frac{\Delta t}{2}[v(0)+v(\Delta t)]. \end{aligned} \tag{6}$$

The two integrators are derived *directly* from the evolution operator and both the positions and velocities are determined at time, Δt.

The version of the leap-frog algorithm which is *exactly* equivalent to velocity Verlet is given by

$$\begin{aligned} v(t+\Delta t/2)&=v(t-\Delta t/2)+\frac{\Delta t}{m}F[x(t)],\\ x(t+\Delta t)&=x(t)+\Delta t v(t+\Delta t/2), \end{aligned} \tag{7}$$

with

$$v(t)=\tfrac{1}{2}[v(t+\Delta t/2)+v(t-\Delta t/2)] \tag{8}$$

and the initial condition

$$v(-\Delta t/2)=v(0)-\frac{\Delta t}{2m}F[x(0)]. \tag{9}$$

Similarly, the version of the leap-frog algorithm which is *exactly* equivalent to position Verlet is given by

$$\begin{aligned} x(t+\Delta t/2)&=x(t-\Delta t/2)+\Delta t v(t),\\ v(t+\Delta t)&=v(t)+\frac{\Delta t}{m}F[x(t+\Delta t/2)] \end{aligned} \tag{10}$$

with

$$x(t)=\tfrac{1}{2}[x(t+\Delta t/2)+x(t-\Delta t/2)] \tag{11}$$

and the initial condition

$$x(-\Delta t/2)=x(0)-\frac{\Delta t}{2}v(0). \tag{12}$$

It looks like the time origin of the integrators can be shifted by a factor of $\Delta t/2$ and interpolation formulas changed without loss of generality making both position Verlet and velocity Verlet equivalent to the same leap-frog form. Again, however, half-time steps are not formally defined as pointed out in the more careful analysis based on the classical propagator.

Position Verlet and velocity Verlet generate *different* trajectories whose relationship is nontrivial. A numerical

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TABLE I. The first five steps of a trajectory generated by the velocity Verlet and position Verlet integrators for a harmonic oscillator with Hamiltonian $H=(v^2+x^2)/2$ starting with initial conditions $x(0)=1.0$ and $v(0)=0.5$.

	Velocity Verlet		Position Verlet	
Step	$x(t)$	$v(t)$	$x(t)$	$v(t)$
1	1.004 950 047	0.489 975 2438	1.004 949 927	0.489 975 0054
2	1.009 799 480	0.479 901 4926	1.009 799 242	0.479 901 0158
3	1.014 548 063	0.469 779 7596	1.014 547 706	0.469 779 0146
4	1.019 195 080	0.459 611 0582	1.019 194 603	0.459 610 0450
5	1.023 740 292	0.449 396 3718	1.023 739 576	0.449 395 1201

example is provided in Table I in which the phase space points $x(t)$, $v(t)$ along single trajectories generated using the two integrators and the same initial conditions are tabulated ($H=[v^2+x^2]/2$). In addition, a general relationship between the two trajectories can be obtained. Let $A=\Delta t F(x)\partial/\partial p$ and $B=\Delta t(p/m)\partial/\partial x$. The evolution operators for the two integrators and their inverses are

$$U_{vv}(P)=[e^{A/2}e^{B}e^{A/2}]^{P}=e^{-A/2}[e^{A}e^{B}]^{P}e^{A/2}, \tag{13}$$

$$U_{vv}^{-1}(P)=e^{-A/2}[e^{-B}e^{-A}]^{P}e^{A/2} \tag{14}$$

and

$$U_{pv}(P)=[e^{B/2}e^{A}e^{B/2}]^{P}=e^{B/2}[e^{A}e^{B}]^{P}e^{-B/2}, \tag{15}$$

$$U_{pv}^{-1}(P)=e^{B/2}[e^{-B}e^{-A}]^{P}e^{-B/2}. \tag{16}$$

Therefore,

$$U_{vv}(P)=e^{-A/2}e^{-B/2}U_{pv}(P)e^{B/2}e^{A/2}, \tag{17}$$

$$U_{pv}(P)=e^{B/2}e^{A/2}U_{vv}(P)e^{-A/2}e^{-B/2}. \tag{18}$$

This demonstrates that simply using two sets of related initial conditions for the two methods will *not* lead to the same trajectories. However, it is also clear that the trajectories mirror each other, that is, despite being different, they do not diverge as a function of time, $P\Delta t$. This occurs because the forces are evaluated at the same phase space points in the two integrators as pointed out in the Toxvaerd comment.

In conclusion, it has unambiguously been shown, both formally and numerically, that velocity Verlet and position Verlet generate different trajectories. These differences result in the equivalence of velocity Verlet to the standard leap-frog algorithm and the equivalence of position Verlet to the time-displaced leap-frog algorithm, Eq. (10). It has also been shown that the trajectories of the two methods mirror each other and do not diverge in time. We did not explicitly point this out in our original paper but present it now in response to the comment. The simpler analysis in Toxvaerd's comment does not correctly define the relationship between the trajectories and Toxvaerd incorrectly implies that these trajectories are identical.

[1] H. F. Trotter, Proc. Am. Math Soc. **10**, 545 (1959).
[2] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, MA, 1980).
[3] W. C. Swope, H. C. Andersen, P. H. Berens, and K. R. Wilson, J. Chem. Phys. **76**, 637 (1982).
[4] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Oxford University, Oxford, England, 1989).