1 Single precision Molecular Dynamics.

Single precision calculation offers considerable computational efficiency compared to double precision, but the effect of the loss of precision is difficult to determine.

Use of symplectic integrators gives rise to the idea of the Shadow Hamiltonian, backward error analysis finds a Hamiltonian which is arbitrarily close to a quantity which is exactly preserved by the numerical method. Shadow Hamiltonian methods are extremely sensitive to errors in dynamics and has been used successfully to determine the stability limits of integrators (linear and non-linear) and accuracy of force fields, particularly in relation to the continuity of cutoffs and their complements. Clearly the methods can only be used for symplectic integrators but when used as an analysis tool for force fields the results are pertinent to non-Hamiltonian methods.

In this report I have used Shadow Hamiltonian techniques to analyze the effects of reducing the arithmetic precision from double to single for our molecular dynamics code 'Protomol'. In line with the comments I received the 'extensive' variables, which are summed over the whole model (i.e. energies), retained double precision, as did the code for calculating the Shadow Hamiltonian.

1.1 Interpolated methods for the Shadow Hamiltonian

Calculating the Shadow Hamiltonians analytically, even to 4^{th} order, is difficult and specific to both the method of integration and the forces employed in the model. The backward error analysis has to be completed for the chosen integrator and will involve terms in the Hessian, and higher derivatives, of the model forces depending on the required order of calculation. In [2] an alternative scheme was proposed whereby a homogeneous extension of the original Hamiltonian, with the addition of a new position variable α and its conjugate momentum β, is considered. Given an extended Hamiltonian $\bar{H}_h(y)$, where h is the time-step and y represents the augmented variables, which is homogeneous of order 2 then it can be shown,

$$\begin{aligned} \bar{H}_h(y_h(t)) &= \frac{1}{2}\dot{y}_h(t)^T \bar{J} y_h(t), \qquad (1) \\ \bar{J} &= \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \end{aligned}$$

using this the Shadow Hamiltonian can be calculated by forming and approximation for $y_h(t)$ from the numerical solutions of the extended Hamiltonian system.

The basis of this method comes from studying quadratic Hamiltonian systems. For example, given a quadratic Hamiltonian

$$H = \frac{\mathbf{p^T} M^{-1} \mathbf{p}}{2} + \frac{\mathbf{q^T} \Omega^{-1} \mathbf{q}}{2},$$

where M^{-1} is the diagonal matrix of inverse masses $1/m_i$ and Ω is the diagonal matrix of squared frequencies w_i^2. The equations of motion are then

$$\begin{aligned} \dot{\mathbf{q}} &= M^{-1}\mathbf{p}, \qquad (2) \\ \dot{\mathbf{p}} &= -\Omega \mathbf{q}. \qquad (3) \end{aligned}$$

Substituting (2) and (3) into the RHS of (1) gives

$$\frac{1}{2}[M^{-1}\mathbf{p}, -\Omega\mathbf{q}] \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} = \frac{\mathbf{p^T} M^{-1} \mathbf{p}}{2} + \frac{\mathbf{q^T} \Omega^{-1} \mathbf{q}}{2},$$

as required. Clearly the quadratic Hamiltonian is homogeneous of order 2, but the method holds for all Hamiltonians which are homogeneous of order 2.

The implemented method used Newton's Divided Difference Interpolation for the approximation of $y_h(t)$ and used centered differences to calculate $\bar{H}_h(y)$. An efficient method of storing the difference equations was devised in [1] based on backward differences.

The equations of motion for the extended Hamiltonian will be as follows. Given $y = [q^T, \alpha, p^T, \beta]^T$ and $\bar{H}(q, \alpha, p, \beta) = \alpha^2 H(\alpha^{-1}q, \alpha^{-1}p)$ then the augmented equations of motion will be

$$\begin{aligned} \dot{q} &= \alpha H_p(\alpha^{-1}q, \alpha^{-1}p), \quad \dot{p} = -\alpha H_q(\alpha^{-1}q, \alpha^{-1}p), \\ \dot{\alpha} &= 0, \quad \dot{\beta} = q^T H_q(\alpha^{-1}q, \alpha^{-1}p) + p^T H_p(\alpha^{-1}q, \alpha^{-1}p) - 2\alpha H(\alpha^{-1}q, \alpha^{-1}p). \end{aligned}$$

Using initial condition $\alpha(0) = 1$ s.t. $\alpha(t) = 1$, $\forall t$ and for an underlying system $H(q,p) = \frac{1}{2}p^T M^{-1} p + U(q)$ with extended Hamiltonian $\bar{H}(q, \alpha, p, \beta) = \frac{1}{2}p^T M^{-1} p + \alpha^2 U(\alpha^{-1}q)$ the equations of motion simplify to

$$\dot{q} = M^{-1}p, \quad \dot{p} = -U_q(q), \quad \dot{\beta} = q^T U_q(q) - 2U(q).$$

1.2 Backward difference implementation.

The backward difference operator, for some function $\omega(t)$, is defined as

$$\begin{aligned} \nabla^0 \omega(t) &= \omega(t), \\ \nabla^k \omega(t) &= \nabla^{k-1}\omega(t) - \nabla^{k-1}\omega(t-h). \end{aligned}$$

We can then define

$$A_{i,j} = \frac{\nabla^i y_h(t) \bar{J} \nabla^j y_h(t)}{2h},$$

and it is then possible to derive k^{th} order approximations for $\bar{H}_h(y)$ in terms of the $A_{i,j}$ using Newton's interpolation as described in [2, 1]. We then have, for example,

$$\begin{aligned} H_{[4]} &= A_{1,0} - \frac{1}{2}A_{2,0} + \frac{2}{3}A_{2,1}, \\ H_{[8]} &= A_{1,0} - \frac{3}{2}A_{2,0} + \frac{16}{7}A_{2,1} + \frac{13}{21}A_{3,0} - \frac{32}{21}A_{3,1} + \frac{36}{35}A_{3,2} - \frac{5}{8}A_{4,0} \\ &\quad + \frac{22}{105}A_{4,1} - \frac{9}{5}A_{4,2} + \frac{4}{35}A_{4,3}, \end{aligned}$$

where $H_{[k]}$ is the k^{th} order approximation of $\bar{H}_h$.

1.3 Verlet/Leapfrog implementation.

This scheme was implemented in Protomol as follows.

The leapfrog method with the additional β variable becomes

$$\begin{aligned} p^{n+\frac{1}{2}} &= p^n - \frac{h}{2}U_q(q^n), \\ \beta^{n+\frac{1}{2}} &= \beta^n + \frac{h}{2}\left((q^n)^T U_q(q^n) - 2U(q^n)\right), \end{aligned}$$

$$
\begin{aligned}
q^{n+1} &= q^n + hM^{-1}p^{n+\frac{1}{2}}, \\
p^{n+1} &= p^{n+\frac{1}{2}} - \frac{h}{2}U_q(q^{n+1}), \\
\beta^{n+1} &= \beta^{n+\frac{1}{2}} + \frac{h}{2}\left((q^{n+1})^T U_q(q^{n+1}) - 2U(q^{n+1})\right).
\end{aligned}
$$

2 Results.

Separate tests were carried out to determine the effect of (2.1) storing the position and momenta as single precision, where the force calculations are double precision, and (2.2) single precision calculation/storage. The model consist of a box of 384 water molecules with periodic boundary conditions and is included in the tar archive referred to in section 3.

2.1 Single precision storage.

The code was modified to store the positions and momenta as single precision. From Figure 1 we can see that the results are almost identical, indicating that storing the data in single precision format does not significantly perturb the simulation results.

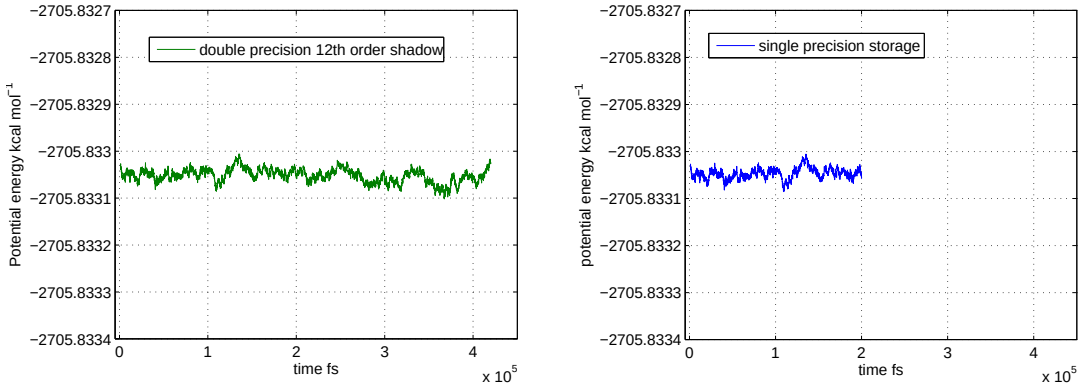

Figure 1: Comparison between the 12^{th} order Shadow Hamiltonians for single and double precision storage of position and momenta for Protomol.

2.2 Single precision Molecular dynamics.

The code was further modified to perform all calculations to single precision store with the exception of variables which are summed over the whole model, i.e. energies, and the code for calculating the Shadow Hamiltonian. From Figure 2 the 'drift' is almost 10000 greater, indicating that the collisions are not resolved correctly for single precision and a hybrid precision scheme may be required.

In this case the drift is sufficiently large over the relatively short trajectory to be visible in the Hamiltonian itself as seen in Figure 3.

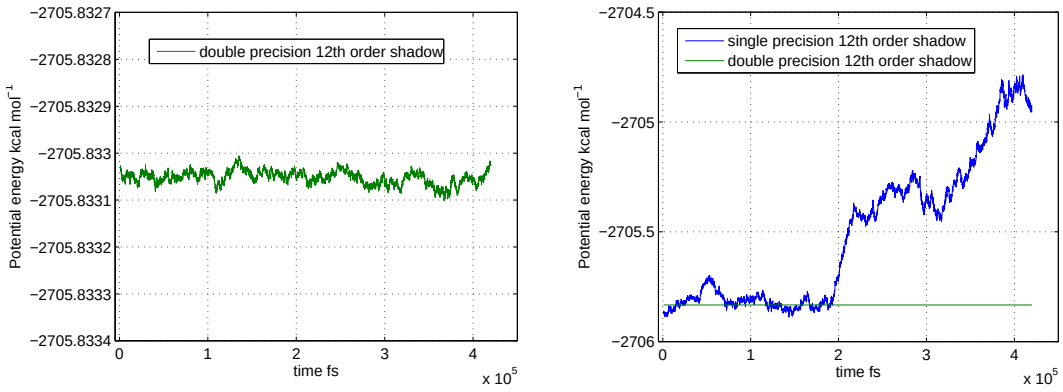

Figure 2: Comparison between the 12^{th} order Shadow Hamiltonians for single and double precision calculations in Protomol. Note the x-axis scale change between plots.

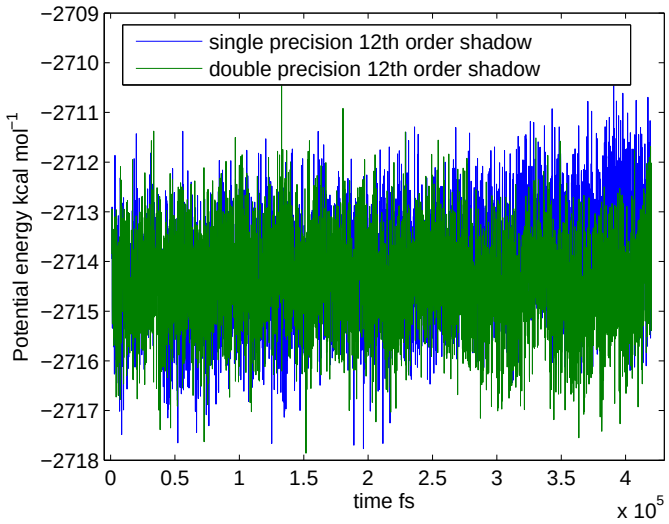

Figure 3: Comparison between the Hamiltonians for single and double precision calculations in Protomol.

To further isolate the problem the simulation was run without the Columbic forces, so that only local forces remain, and using the 24^{th} order Shadow Hamiltonian. The results are similar, with variations several orders of magnitude greater for single precision, as seen in Figure 4.

3 Code.

Protomol is an open-source molecular dynamics package and can be found at http://protomol.sourceforge.net, the single precision version used for this report can be obtained at http://www.chris.sweet.name/pmolsingle.tar. The code for the Interpolated Shadow Hamiltonian is in /framework/integrators/ModifierShadow.h/cpp and the update for the additional degree of freedom in /framework/integrators/Integrator.h/cpp.

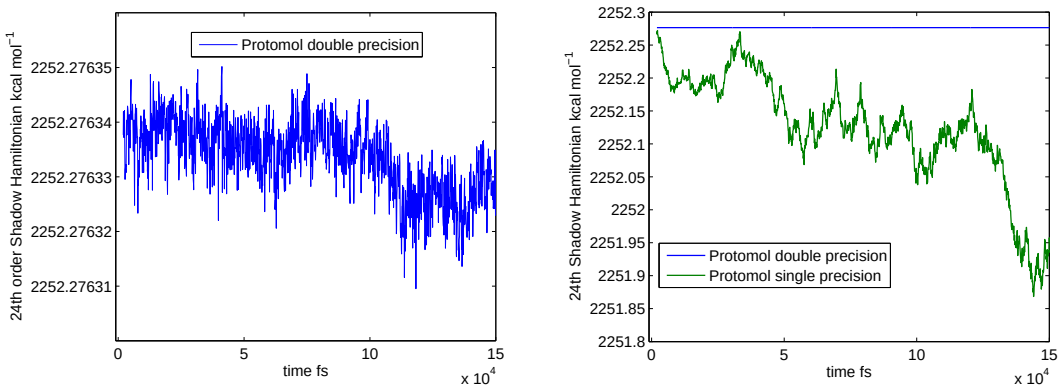

Figure 4: Comparison between the 24th order Shadow Hamiltonians for single and double precision calculations in Protomol. In this simulation the Columbic forces have been removed.

References

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[2] R. D. Skeel, D. J. Hardy, Practical construction of modified Hamiltonians
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C.R. Sweet 03/12/2008.