Instabilities in Molecular Dynamics Integrators used in Hybrid Monte Carlo Simulations

B. Joó UKQCD Collaboration

We discuss an instability in the leapfrog integration algorithm, widely used in current Hybrid Monte Carlo (HMC) simulations of lattice QCD. We demonstrate the instability in the simple harmonic oscillator (SHO) system where it is manifest. We demonstrate the instability in HMC simulations of lattice QCD with dynamical Wilson-Clover fermions and discuss implications for future simulations of lattice QCD.

1. INTRODUCTION

The subject of instabilities in molecular dynamics (MD) integrators is not new. Studies of the phenomenon for the case of lattice QCD have been reported in [1,2]. In [1] the lattices used were small (4^4 sites). The onset of instabilities was investigated as a function of the integration step size (δτ) for heavy and light quark masses. For both masses studied the instabilities set in at some critical step size. The critical value of δτ was smaller for the lighter mass than for the heavier one. However, in both cases δτ was still so large that the energy change (δH) from the step size induced errors along an MD trajectory was sufficiently great to make simulations impractical in the unstable region of parameter space anyway.

Our study [2] using larger lattices and quark masses that are relatively light (by current standards) encountered instabilities at step sizes that are small enough to be relevant for large scale simulations. Our motivation to summarise these results is to highlight the impact these instabilities may have on future simulations using MD integrators as components, in particular HMC.

This article is organised as follows. In section 2 we demonstrate the instability in the simple harmonic oscillator (SHO) system. At this point we will restate the hypothesis of [1] to explain the onset of the instability. We present our main results in section 3 and show that they are completely consistent with this hypothesis. Finally in section 4 we will draw our conclusions.

2. SHO RESULT AND HYPOTHESIS

In the case of the SHO system a leapfrog update can be written as:

\[
\begin{bmatrix}
q(t + δτ) \\
p(t + δτ)
\end{bmatrix} = \begin{bmatrix}
1 - \frac{1}{2}(ωδτ)^2 & \frac{ωδτ}{2} \\
-\frac{ωδτ}{2} & 1 - \frac{ωδτ}{2}
\end{bmatrix} \begin{bmatrix}
q(t) \\
p(t)
\end{bmatrix}
\]

(1)

where \(q, p\) are the coordinates and conjugate momenta, \(t\) is MD time and \(ω\) is the angular frequency.

The eigenvalues of the matrix in (1) are

\[
λ_± = e^{\pm i \cos^{-1}(1-\frac{1}{2}(ωδτ)^2)}
\]

(2)

When \(ωδτ < 2\) the inverse cosine in (2) is real, the eigenvalues are complex, and the phase space trajectories describe ellipses. However, when \(ωδτ > 2\), the inverse cosine becomes imaginary, and one eigenvalue is greater than one. At this point the phase space trajectories become hyperbolic, and the energy change along a trajectory grows exponentially.

The hypothesis of [1] is that the short distance modes of an asymptotically free quantum field theory behave like a collection of loosely coupled SHO modes. It is then anticipated that the MD integration of lattice QCD will go unstable when the highest frequency mode goes unstable.

We note that in the SHO example \(ω\) plays the role of the MD force \(F\). Hence we surmise that for QCD the instability will occur when the combination \(Fδτ\) reaches a critical value. Furthermore, we expect that the fermionic contribution to the force will increase in some manner with the inverse quark mass. This suggests that as the quark masses are decreased, the \(Fδτ\) term will reach its
critical value for smaller values of $\delta \tau$. This indeed is exactly what is reported in [1] and [2].

3. NUMERICAL RESULTS

Our numerical computations were carried out using 10 lattice configurations from a UKQCD lattice computation [3]. The lattices were picked evenly spaced from a larger ensemble. The lattice volume was $16^3 \times 32$ sites, and the physical parameters for the ensemble were $\beta = 5.2$ for the gauge coupling, $\kappa = 0.1355$ for the hopping parameter and $c_{SW} = 2.0171$ for the $O(a)$–improvement coefficient [4,5]. These parameters correspond to a regime where the ratio of the pseudoscalar to vector masses is $m_\pi/m_\rho \approx 0.6$ [3,6].

We evolved the configurations for unit length MD trajectories using a variety of step sizes at a variety of $\kappa$ values. Along each trajectory we computed $\delta H$ as well as the 2-norms and $\infty$ norm of the gauge and fermionic contributions to the MD force ($||F_g||_2, ||F_f||_2, ||F_g||_\infty, \text{and } ||F_f||_\infty$) averaged over all the time steps along the trajectory.

In figure 1 we show the results of fitting the fermionic force norms (averaged over configurations) to the fit ansatz:

$$||F|| = C (am)^\alpha$$

in order to check that the forces increase in some inverse manner with the quark mass. To calculate $am$ we used the formula

$$am = \frac{1}{2} \left( \frac{1}{\kappa} - \frac{1}{\kappa_{crit}} \right)$$

where $\kappa_{crit}$ is the critical value of $\kappa$ corresponding to the massless limit of the pion. In our fits we have left $\kappa_{crit}$ as a free parameter, however to determine $am$ for the axes of figure 1 we used the value $\kappa_{crit} = 0.13633$, determined from spectroscopy on the ensemble [6].

One can see from figure 1 that the values of $\alpha$ are negative for both the 2-norm and the $\infty$-norm indicating that the forces do indeed grow inversely with $am$. The fits for $\kappa_{crit}$ are consistent with the spectroscopic determinations indicating that the forces will diverge as $am \to 0$.

In figure 2 we plot the variation of the force norms and $\delta H$ against the step size $\delta \tau$ at a fixed value of $\kappa = 0.1355$ for a single configuration. It can be seen that at a value of about $\delta \tau = 0.0105$, the fermionic forces start increasing and that $\delta H$ increases exponentially indicating the onset of the instability. The gauge contributions to the force norms seem to show no change in behaviour.

![Figure 1. $||F||_2$ and $||F||_\infty$ vs $am$.](image1)

![Figure 2. 2-norms (bottom), $\infty$-norms (middle) and corresponding values of $\delta H$ (top) vs $\delta \tau$.](image2)
of a corresponding set of loosely coupled SHOs whereas the 2–norm of the force can be likened to the behaviour of the corresponding bulk modes. Hence this result is consistent with the earlier hypothesis, that the highest frequency modes drive the system unstable.

In figure 3 we show the behaviour of $\|F_f\|_\infty$, $\|F_g\|_\infty$ and $\delta H$ against the hopping parameter $\kappa$ for $\delta \tau = 0.01$ and $\delta \tau = 0.012$. When $\delta \tau = 0.01$ the system is completely stable for all values of $\kappa$ (for this single configuration); however, for $\delta \tau = 0.012$ the fermionic force norm rises sharply for $\kappa = 0.1355$ accompanied by a large increase in $\delta H$ signalling the onset of the instability. This again is consistent with our earlier hypothesis that instabilities set in when the $F \delta \tau$ term reaches a critical value.

4. CONCLUSIONS AND DISCUSSION

We have exhibited the onset of an instability in the leapfrog MD integration scheme, used in HMC simulations and inexact simulation algorithms. The instability is manifest in the leapfrog scheme for a simple SHO system. We have also presented numerical evidence demonstrating that the instability is present also in lattice QCD systems. We have shown that our data is consistent with the hypothesis that the instability occurs when the $F \delta \tau$ term in the leapfrog equations reaches some critical value, and that the fermionic contribution to the force increases with decreasing quark mass. We have shown that as quark masses become lighter the instability sets in at smaller values of $\delta \tau$. Furthermore, for simulations with light dynamical quarks the instability sets in at values of $\delta \tau$ that are small enough to be relevant to large scale numerical simulations.

We anticipate that the major stumbling block for simulations with lighter quark masses will not come from “exceptional” configurations, where the value of $\kappa$ may become supercritical for some configurations, but rather from the onset of the instability which we expect to set in before $\kappa$ can become supercritical.

The instability problem is exponentially bad, but can be controlled easily by reducing $\delta \tau$. We are concerned for simulations with inexact algorithms, where the instability may be hard to detect as there is no $\delta H$ to monitor, and full finite step size extrapolations are seldom made.

Finally we wish to mention that neither the use of higher order integration schemes nor the use of double precision arithmetic are expected to alleviate the instability problem.

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