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Force Gradient Integrators

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We present initial results of the use of Force Gradient integrators for lattice field theories. These promise to give significant performance improvements, especially for light fermions and large lattices. Our results show that this is indeed the case, indicating a speed-up of more than a factor of two, which is expected to increase as the integration step size becomes smaller for larger lattices and smaller fermion masses.

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1. Introduction

Our goal is to construct more accurate molecular dynamics integrators for use in Hybrid Monte Carlo (HMC) computations for lattice quantum field theories. In particular we shall consider symmetric symplectic integrators whose errors are of higher order in the integration step size than those of the leapfrog (also known as the Störmer or Verlet) method. These integrators improve the scaling behaviour $\delta H = k \cdot \delta\tau^n$ from $n = 2$ to $n = 4$, which reduces the cost for large enough volume and small enough fermion masses for which $\delta\tau \to 0$. Previous methods for constructing higher-order integrators [1, 2] were thwarted by large values for the coefficient k; the new idea considered here is to compute second derivatives "analytically" rather than "numerically" [3, 4].

2. Symplectic Integrators

As described in [5, 6, 7] we may define a Hamiltonian system for a gauge field by introducing the symplectic fundamental 2-form $\omega \equiv -d(p^i \theta_i)$ with θ_i being the frame of left-invariant Maurer-Cartan forms; this ensures that the Hamiltonian dynamics is gauge invariant. For every 0-form F on phase space this defines a Hamiltonian vector field $\hat{F}$ satisfying $dF = i_{\hat{F}}\omega$, and the Hamiltonian evolution for the system corresponds to an integral curve of the Hamiltonian vector field $\hat{H}$ for the Hamiltonian function H. We can find a closed-form integral curve of $\hat{F}$, that is evaluate $e^{\hat{F}\tau}$ explicitly, if F depends only on the "positions" (fields) q or momenta p. This is particularly useful when the Hamiltonian is of the form $H(q,p) = S(q) + T(p)$ as then we can integrate the Hamiltonian vector fields $\hat{S}$ and $\hat{T}$ exactly.

3. Shadow Hamiltonians and Force Gradient Integrators

We recall the Baker–Campbell–Hausdorff (BCH) formula, which states that if A and B belong to any (in general non-commutative) associative algebra then $e^A e^B = e^{A+B+\delta}$ where δ is in the free Lie algebra generated by A and B. Furthermore it gives an explicit expansion for δ, and correspondingly for the symmetric product

$$\ln\left(e^{A/2} e^B e^{A/2}\right) = A + B - \frac{1}{24}\Big([A,[A,B]] + 2\,[B,[A,B]]\Big) + \cdots.$$

Using the Jacobi identity one may show that the commutator of two Hamiltonian vector fields is itself a Hamiltonian vector field, $[\hat{S},\hat{T}] = \widehat{\{S,T\}}$, where $\{S,T\} = -\omega(\hat{S},\hat{T})$ is the Poisson bracket of the two 0-forms S and T. We therefore find that any integrator constructed from a sequence of symplectic steps exactly conserves a shadow Hamiltonian $\tilde{H}$ obtained from the BCH formula by replacing commutators with Poisson brackets.

As a very simple example consider the PQPQP integrator

$$\left(e^{\alpha\hat{S}\delta\tau} e^{\frac{1}{2}\hat{T}\delta\tau} e^{(1-2\alpha)\hat{S}\delta\tau} e^{\frac{1}{2}\hat{T}\delta\tau} e^{\alpha\hat{S}\delta\tau}\right)^{\tau/\delta\tau}$$

whose shadow Hamiltonian is

$$\tilde{H} = H + \left(\frac{6\alpha^2 - 6\alpha + 1}{12}\{S,\{S,T\}\} + \frac{1-6\alpha}{24}\{T,\{S,T\}\}\right)\delta\tau^2 + \mathscr{O}(\delta\tau^4).$$

Integrator	Update steps	Shadow Hamiltonian
PQP	$e^{\frac{1}{2}\delta\tau\hat{S}}\, e^{\delta\tau\hat{T}}\, e^{\frac{1}{2}\delta\tau\hat{S}}$	$T+S-\frac{\delta\tau^2}{24}\Big(\{S,\{S,T\}\}+2\{T,\{S,T\}\}\Big)+\mathscr{O}(\delta\tau^4)$
QPQ	$e^{\frac{1}{2}\delta\tau\hat{T}}\, e^{\delta\tau\hat{S}}\, e^{\frac{1}{2}\delta\tau\hat{T}}$	$T+S+\frac{\delta\tau^2}{24}\Big(2\{S,\{S,T\}\}+\{T,\{S,T\}\}\Big)+\mathscr{O}(\delta\tau^4)$
PQPQP $\alpha=\frac{1}{6}$ [4, 8, 9]	$e^{\frac{1}{6}\delta\tau\hat{S}}\, e^{\frac{1}{2}\delta\tau\hat{T}}$ $\times\, e^{\frac{2}{3}\delta\tau\hat{S}}$ $\times\, e^{\frac{1}{2}\delta\tau\hat{T}}\, e^{\frac{1}{6}\delta\tau\hat{S}}$	$T+S+\frac{\delta\tau^2}{72}\{S,\{S,T\}\}+\mathscr{O}(\delta\tau^4)$
PQPQP $\alpha=\frac{1}{2}\left(1-\frac{1}{\sqrt{3}}\right)$ [4, 8, 9]	$e^{\frac{3-\sqrt{3}}{6}\delta\tau\hat{S}}\, e^{\frac{1}{2}\delta\tau\hat{T}}$ $\times\, e^{\frac{1}{\sqrt{3}}\delta\tau\hat{S}}$ $\times\, e^{\frac{1}{2}\delta\tau\hat{T}}\, e^{\frac{3-\sqrt{3}}{6}\delta\tau\hat{S}}$	$T+S+\frac{\sqrt{3}-2}{24}\delta\tau^2\{T,\{S,T\}\}+\mathscr{O}(\delta\tau^4)$
Campostrini PQPQPQP [1, 2]	$e^{\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{12}\delta\tau\hat{T}}$ $\times\, e^{\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{6}\delta\tau\hat{S}}$ $\times\, e^{\frac{-\sqrt[3]{4}-2\sqrt[3]{2}+2}{12}\delta\tau\hat{T}}$ $\times\, e^{-\frac{\sqrt[3]{4}+2\sqrt[3]{2}+1}{3}\delta\tau\hat{S}}$ $\times\, e^{\frac{-\sqrt[3]{4}-2\sqrt[3]{2}+2}{12}\delta\tau\hat{T}}$ $\times\, e^{\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{6}\delta\tau\hat{S}}$ $\times\, e^{\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{12}\delta\tau\hat{T}}$	$T+S$ $+\frac{\delta\tau^4}{34560}\left(\begin{array}{c} -\left(40\sqrt[3]{4}+40\sqrt[3]{2}+48\right)\{S,\{S,\{S,\{S,T\}\}\}\} \\ +\left(180\sqrt[3]{4}+240\sqrt[3]{2}+312\right)\{\{S,T\},\{S,\{S,T\}\}\} \\ +\left(60\sqrt[3]{4}+80\sqrt[3]{2}+104\right)\{\{S,T\},\{T,\{S,T\}\}\} \\ +\left(-20\sqrt[3]{4}+8\right)\{T,\{S,\{S,\{S,T\}\}\}\} \\ +\left(20\sqrt[3]{2}+32\right)\{T,\{T,\{S,\{S,T\}\}\}\} \\ +\left(5\sqrt[3]{2}+8\right)\{T,\{T,\{T,\{S,T\}\}\}\} \end{array}\right)$ $+\mathscr{O}(\delta\tau^6)$
Force Gradient PQPQP	$e^{\frac{1}{6}\delta\tau\hat{S}}\, e^{\frac{1}{2}\delta\tau\hat{T}}$ $\times\, e^{\frac{48\delta\tau S-\delta\tau^3\,\widehat{\{S,\{S,T\}\}}}{72}}$ $\times\, e^{\frac{1}{2}\delta\tau\hat{T}}\, e^{\frac{1}{6}\delta\tau\hat{S}}$	$T+S$ $-\frac{\delta\tau^4}{155520}\left(\begin{array}{c} 41\{S,\{S,\{S,\{S,T\}\}\}\} \\ +36\{\{S,T\},\{S,\{S,T\}\}\} \\ +72\{\{S,T\},\{T,\{S,T\}\}\} \\ +84\{T,\{S,\{S,\{S,T\}\}\}\} \\ +126\{T,\{T,\{S,\{S,T\}\}\}\} \\ +54\{T,\{T,\{T,\{S,T\}\}\}\} \end{array}\right)+\mathscr{O}(\delta\tau^6)$

Table 1: A selection of integrators with their exactly conserved shadow Hamiltonians.

As the Poisson bracket $\{S,\{S,T\}\}$ does not depend on momentum we can integrate the Hamiltonian vector field $\widehat{\{S,\{S,T\}\}}$ exactly, and this "second derivative" corresponds to the *Force Gradient* just as the Hamiltonian vector field $\hat{S}$ corresponds to the "force". The explicit form of the shadow Hamiltonian for a variety of integrators is shown in Table 1, the simplest Force Gradient integrator is given in the last entry.

4. Computing the Force Gradient

As shown in our previous proceedings [5, 6] Poisson brackets for gauge theories may be written in terms of momenta p_i and linear differential operators e_i that provide gauge-covariant generalizations of the vector fields $\partial/\partial q^i$; in particular we have $\{S,\{S,T\}\} = e^i(S)e_i(S)$. The "equations

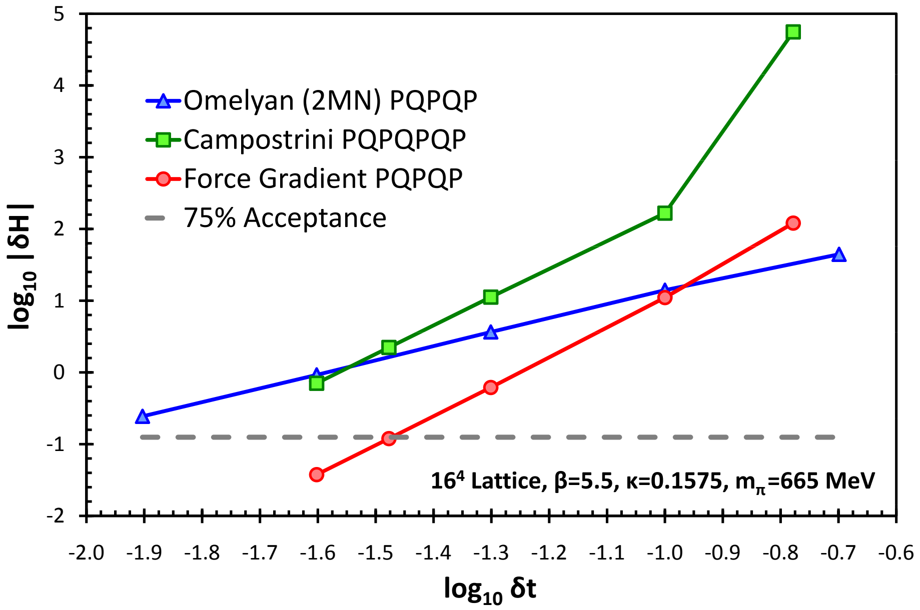

Figure 1: Change δH in the Hamiltonian over an entire trajectory as a function of the integration step size $\delta\tau$. The dashed line indicates the value of δH which corresponds to a 75% HMC acceptance rate.

of motion" for the $\{S,\widehat{\{S,T\}}\}$ vector field are $\dot{P} = \{S,\widehat{\{S,T\}}\}P \equiv -G$ where $P \equiv p_i T^i$, and we may use the relation $e_i(U) = -T_i U$, where T_i are the adjoint generators of the gauge group, to show that the Force Gradient vector field is the "second derivative" $G = e^j(S)e_j e_i(S)T^i$.

If we consider a generic pseudofermion action $S = \phi^\dagger \mathscr{M}^{-1}(U)\phi$ where ϕ is a pseudofermion field, U the gauge field, and $\mathscr{M}$ any hermitian fermion kernel, then

$$e_i(S) = -\phi^\dagger \mathscr{M}^{-1} e_i(\mathscr{M})\mathscr{M}^{-1}\phi = -X^\dagger e_i(\mathscr{M})X$$

where $X \equiv \mathscr{M}^{-1}\phi$. The Force Gradient can be computed by applying the linear differential operator $\mathscr{F} \equiv e^j(S)e_j$ to the above equation; by the Leibnitz rule

$$-G = -\mathscr{F}\big(e_i(S)\big) = \mathscr{F}(X^\dagger)e_i(\mathscr{M})X + X^\dagger \mathscr{F}\big(e_i(\mathscr{M})\big)X + X^\dagger e_i(\mathscr{M})\mathscr{F}(X);$$

defining $Y \equiv \mathscr{F}(X) = -\mathscr{M}^{-1}\mathscr{F}(\mathscr{M})X$, we obtain

$$-G = Y^\dagger e_i(\mathscr{M})X + X^\dagger \mathscr{F}\big(e_i(\mathscr{M})\big)X + X^\dagger e_i(\mathscr{M})Y.$$

Note that the cost of computing the Force Gradient in an HMC integrator is the inversion required to compute Y in addition to the usual inversion needed to compute X.

5. Results

We have implemented this PQPQP Force Gradient integrator for lattice QCD with dynamical Wilson fermions, and we present our initial results for a 16^4 lattice at $\beta = 5.5$ and $\kappa = 0.1575$, which corresponds to a pion mass of $m_\pi = 665$ MeV. We used the usual even-odd preconditioning, which does not introduce any significant complications into our formalism.

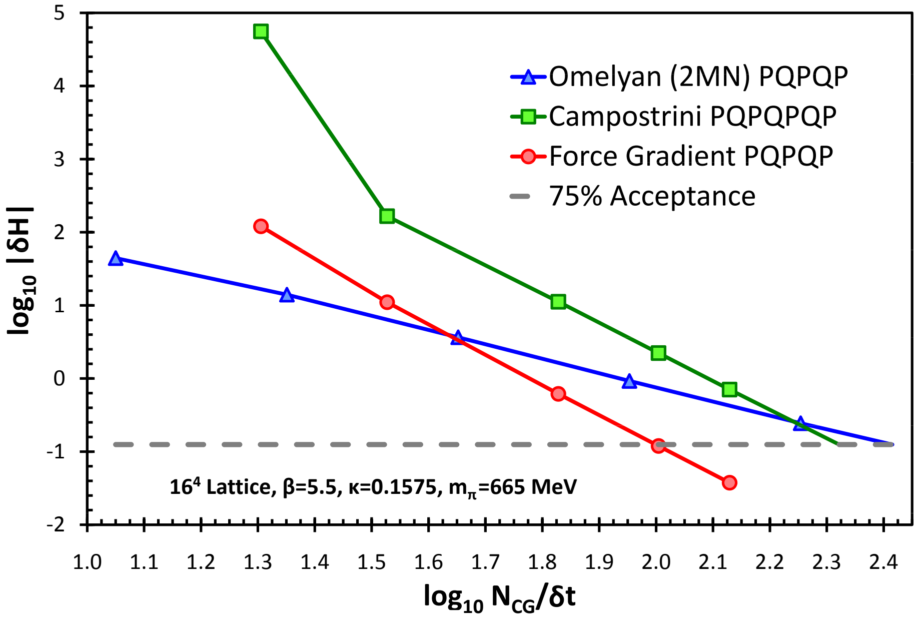

Figure 2: Change δH in the Hamiltonian over an entire trajectory as a function of an estimate of the computational cost. The dashed line again indicates the value of δH corresponding to a 75% HMC acceptance rate.

In Figure 1 we show the change δH in the Hamiltonian over an entire trajectory as a function of the integration step size $\delta\tau$ on a log-log plot. To guide the eye we have also drawn a line to indicate the value of δH which corresponds to a 75% HMC acceptance rate. The slopes of the lines correspond to the expected order of the integrators, and the Force Gradient integrator is more than order of magnitude more accurate than the Campostrini integrator at any step size, indicating that the coefficient k discussed in the introduction is indeed much smaller.

In Figure 2 we replot the same data as a function of an estimate of the cost, namely the number of CG solutions divided by the step size. The Omelyan integrator requires two inversions of the Wilson–Dirac operator per step, one[1] for each $\hat{S}$ (P) integration step, whereas the Campostrini and Force Gradient integrators require three inversions (one for each $\hat{S}$ and $\widehat{\{S,\{S,T\}\}}$). From the intercepts with the dashed line (75% acceptance) we find that the Force Gradient integrator is a factor of 2.6 cheaper than the Omelyan integrator, which was up to now the preferred choice of integrator.

6. Conclusions

Our Force Gradient integrator is cheaper by more than a factor of two even for small lattices with fairly heavy quarks, and the benefit increases as the integration step size becomes smaller. We expect that the integrators will be improved by tuning using measured average values of Poisson brackets, as described in [6]. We also note that our formalism for computing Force Gradient integrators is compatible with all common actions, smearing, and so forth.

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[1] As initial and final “half steps” can be combined we count each as half an inversion.

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