Speeding up HMC with better integrators

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We discuss how dynamical fermion computations may be made yet cheaper by using symplectic integrators that conserve energy much more accurately without decreasing the integration step size. We first explain why symplectic integrators exactly conserve a "shadow" Hamiltonian close to the desired one, and how this Hamiltonian may be computed in terms of Poisson brackets. We then discuss how classical mechanics may be implemented on Lie groups and derive the form of the Poisson brackets and force terms for some interesting integrators such as those making use of second derivatives of the action (Hessian or force gradient integrators). We hope that these will be seen to greatly improve energy conservation for only a small additional cost and that their use will significantly reduce the cost of dynamical fermion computations.

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1. Symplectic Integrators

We are interested in finding the classical trajectory in phase space of a system described by the Hamiltonian $H(q,p) = T(p) + S(q) = \frac{1}{2}p^2 + S(q)$. The idea of a *symplectic integrator* is to write the time evolution operator as

$$\exp\left(\tau\frac{d}{dt}\right) = \exp\left(\tau\left\{\frac{dp}{dt}\frac{\partial}{\partial p} + \frac{dq}{dt}\frac{\partial}{\partial q}\right\}\right) \equiv e^{\tau\hat{H}}$$

where the *vector field*

$$\hat{H} = -\frac{\partial H}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H}{\partial p}\frac{\partial}{\partial q} = -S'(q)\frac{\partial}{\partial p} + T'(p)\frac{\partial}{\partial q} \equiv \hat{S} + \hat{T}.$$

Since the kinetic energy T is a function only of p and the potential energy S is a function only of q it follows that the action of $e^{\tau\hat{S}} : f(q,p) \mapsto f(q, p - \tau S'(q))$ and $e^{\tau\hat{T}} : f(q,p) \mapsto f(q + \tau T'(p), p)$ are just translations of the appropriate variable.

We now make use of the Baker–Campbell–Hausdorff (BCH) formula, which tells us that the product of exponentials in any associative algebra can be written as $\ln(e^{A/2}e^B e^{A/2}) - (A+B) = \frac{1}{24}\left\{[A,[A,B]] - 2[B,[A,B]]\right\} + \cdots$ where all the terms on the right hand side are constructed out of commutators of A and B with known coefficients. We find that for a simple PQP symmetric integrator with step size $\delta\tau$ the evolution operator for a trajectory of length τ may be written as

$$\begin{aligned}
U_{\text{PQP}}(\delta\tau)^{\tau/\delta\tau} &= \left(e^{\frac{1}{2}\delta\tau\hat{S}}e^{\delta\tau\hat{T}}e^{\frac{1}{2}\delta\tau\hat{S}}\right)^{\tau/\delta\tau} \\
&= \left(\exp\left[(\hat{T}+\hat{S})\delta\tau - \frac{1}{24}\left([\hat{S},[\hat{S},\hat{T}]] + 2[\hat{T},[\hat{S},\hat{T}]]\right)\delta\tau^3 + \mathcal{O}(\delta\tau^5)\right]\right)^{\tau/\delta\tau} \\
&= \exp\left[\tau\left(\hat{T}+\hat{S} - \frac{1}{24}\left([\hat{S},[\hat{S},\hat{T}]] + 2[\hat{T},[\hat{S},\hat{T}]]\right)\delta\tau^2 + \mathcal{O}(\delta\tau^4)\right)\right].
\end{aligned}$$

2. Shadow Hamiltonians

For every symplectic integrator there is a *shadow Hamiltonian* $\tilde{H}$ that is exactly conserved; this may be obtained by replacing the commutators $[\hat{S},\hat{T}]$ in the BCH expansion with the *Poisson bracket* $\{S,T\} \equiv \frac{\partial S}{\partial p}\frac{\partial T}{\partial q} - \frac{\partial S}{\partial q}\frac{\partial T}{\partial p}$ [1]. For example our PQP integrator above exactly conserves the shadow Hamiltonian $\tilde{H} \equiv T + S - \frac{1}{24}\left(\{S,\{S,T\}\} + 2\{T,\{S,T\}\}\right)\delta\tau^2 + \cdots$.

We now make the simple observation that any symplectic integrator is constructed from the same Poisson brackets, and that these Poisson brackets are extensive quantities. We therefore propose to measure the average values of the Poisson brackets and then optimize the integrator (by adjusting the step sizes, order of the integration scheme, integrator parameters, number of pseudofermion fields, etc. [2, 3]) offline so as to minimize the cost. This is possible because the acceptance rate and instabilities are completely determined by $\delta H = \tilde{H} - H$.

As a very simple example consider the minimum norm PQPQP integrator

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

	Flat Manifold	General
Symplectic 2-form	$dp \wedge dq$	$\omega : d\omega = 0$
Hamiltonian vector field	$\hat{H} = \frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p}$	$dH = i_{\hat{H}}\omega$
Equations of motion	$\dot{q} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial q}$	$\frac{d}{dt}\big|_\sigma = \hat{H}$
Poisson bracket	$\{A,B\} = \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} - \frac{\partial A}{\partial q}\frac{\partial B}{\partial p}$	$\{A,B\} = -\omega(\hat{A},\hat{B})$

Table 1: Comparison of quantities in flat space and on a general manifold [1].

whose shadow Hamiltonian is

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

With only one degree of freedom α we cannot completely eliminate the coefficient of the $O(\delta\tau^2)$ contribution, however, we may optimize this integrator by setting the parameter $\alpha = \frac{1}{2} + \frac{1}{4}\frac{\langle\{T,\{S,T\}\}\rangle}{\langle\{S,\{S,T\}\}\rangle}$. There have been alternative optimization strategies proposed: minimizing the L_2 norm of coefficients assuming $|\{S,\{S,T\}\}| = |\{T,\{S,T\}\}|$ [4], and setting the coefficient of one of the two Poisson brackets to zero by choosing $\alpha = \frac{1}{2}(1 - \frac{1}{\sqrt{3}})$ or $\frac{1}{6}$. However, these strategies clearly break down when optimizing higher order minimum norm integrators, i.e., for $O(\delta\tau^4)$ integrators there are 6 Poisson bracket contributions that must be considered (see Table 3).

3. Hessian Integrators

We now make another simple observation: consider again the PQPQP integrator, where we set $\alpha = \frac{1}{6}$ so that the $\{T,\{S,T\}\}$ contribution is eliminated. The remaining leading order Poisson bracket $\{S,\{S,T\}\}$ depends only on q, which means that we can evaluate the integrator step $e^{\{\widehat{S,\{S,T\}}\}\delta\tau^3}$ explicitly (it is again just a shift of p). The force for this integrator step involves second derivatives of the action, and therefore they are called Hessian or force gradient integrators [5, 6]. By putting such an integration step into a multistep integrator we can eliminate all the leading $\mathcal{O}(\delta\tau^2)$ terms in δH. The advantage of such an integrator over that of Campostini [7, 8] is that the coefficients of the next order terms are approximately two orders of magnitude smaller (see Table 3). We want to stress that although eliminating the leading term must be best asymptotically as $\delta\tau \to 0$ it might well not be the optimal solution in practice; the optimal solution may be obtained by minimizing δH as discussed in §2.

4. Beyond Scalar Field Theory

We now have to construct the Poisson brackets and Hessian integrators for gauge fields, where the field variables are constrained to live on a group manifold. To do this we need to use some differential geometry. Table 1 summarizes the difference between the formulation on flat space that we have discussed up to this point and that on general manifolds.

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In order to construct a Hamiltonian system on a manifold we need not only a Hamiltonian function but also a fundamental closed 2-form ω. On a Lie group manifold this is most easily found using the globally defined *Maurer–Cartan* forms $\{\theta^i\}$ that are dual to the generators and satisfy the relation $d\theta^i = -\frac{1}{2}c^i_{jk}\theta^j \wedge \theta^k$, where c^i_{jk} are the structure constants of the group. We choose to define $\omega \equiv -d\sum_i \theta^i p^i = \sum_i(\theta^i \wedge dp^i - p^i d\theta^i) = \sum_i(\theta^i \wedge dp^i + \frac{1}{2}p^i c^i_{jk}\theta^j \wedge \theta^k)$. Using this fundamental 2-form we can define a Hamiltonian vector field $\hat{A}$ corresponding to any 0-form A through the relation $dA = i_{\hat{A}}\omega$, and in the natural coordinates $(e_i, \frac{d}{dp^i})$ on the contangent bundle this gives

$$\hat{A} = \sum_i \left(\frac{\partial A}{\partial p^i}e_i + \left[\sum_{jk} c^k_{ji}p^k \frac{\partial A}{\partial p^j} - e_i(A) \right] \frac{\partial}{\partial p^i} \right). \tag{4.1}$$

The classical trajectories $\sigma_t = (Q_t, P_t)$ are then the integral curves of this vector field, $\dot{\sigma}_t = \hat{A}(\sigma_t)$.

5. Putting It All Together

Recalling that $H = S + T$ we can compute the Hamiltonian vector fields corresponding to S and T using equation (4.1), and from these we can evaluate the lowest-order Poisson bracket

$$\{S,T\} = -\omega(\hat{S},\hat{T}) = -(\theta^i \wedge dp^i + \tfrac{1}{2}p^i c^i_{jk}\theta^j \wedge \theta^k)(\hat{S},\hat{T}) = -p^i e_i(S) = -\operatorname{Re}\operatorname{Tr}\left(\frac{\partial S}{\partial U}PU \right),$$

and the Hamiltonian vector field corresponding to it,

$$\widehat{\{S,T\}} = \sum_i \left(\frac{\partial \{S,T\}}{\partial p^i}e_i + \left[\sum_{jk} c^k_{ji}p^k \frac{\partial \{S,T\}}{\partial p^j} - e_i(\{S,T\}) \right] \frac{\partial}{\partial p^i} \right)$$

$$= -e_i(S)e_i + \left[-c^k_{ji}p^k e_j(S) + p^j e_i e_j(S) \right] \frac{\partial}{\partial p^i}.$$

From this we can derive expressions for the third- and fifth-order Poisson brackets that are needed for symmetric symplectic integrators, and these are listed in Table 2. Similarly, we can then evaluate the corresponding Hamiltonian vector fields for any Poisson brackets we wish to include in the integration (e.g., $\widehat{\{S,\{S,T\}\}}$ for force gradient integrators).

The explicit form of the shadow Hamiltonian for a variety of integrators is show in Table 3.

6. Conclusions

Our work in this area is still very preliminary, so far we have concentrated on developing these ideas. Future work shall focus on implementing and testing the performance of these integrators for dynamical fermion calculations. We expect that modest gains in performance can be expected through directly measuring the leading order Poisson brackets to optimize the minimum norm family of integrators. However, we hope that very significant performance improvements can be obtained from force gradient integrators.

Acknowledgments

$\{S,\{S,T\}\}$	$e_i(S)e_i(S)$
$\{T,\{S,T\}\}$	$-p^i p^k e_i e_j(S)$
$\{S,\{S,\{S,\{S,T\}\}\}\}$	0
$\{\{S,T\},\{S,\{S,T\}\}\}$	$-2e_i(S)e_j(S)e_i e_j(S)$
$\{\{S,T\},\{T,\{S,T\}\}\}$	$3c^i_{jk}p^i p^\ell e_j(S)[e_k e_\ell(S)+e_\ell e_k(S)]$ $+p^i p^j \Big[e_k(S)e_k e_i e_j(S)-[e_k e_i(S)+e_i e_k(S)]e_k e_j(S)\Big]$
$\{T,\{S,\{S,\{S,T\}\}\}\}$	0
$\{T,\{T,\{S,\{S,T\}\}\}\}$	$2p^i p^j[e_i e_j e_k(S)e_k(S)+e_i e_k(S)e_j e_k(S)]$
$\{T,\{T,\{T,\{S,T\}\}\}\}$	$-p^i p^j p^k p^\ell e_i e_j e_k e_\ell(S)$

Table 2: Poisson brackets required for symmetric symplectic integrators.

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Integrator	Update steps	Shadow Hamiltonian
PQP	$e^{\frac{1}{2}\delta\tau\hat{S}}\,e^{\delta\tau\hat{T}}\,e^{\frac{1}{2}\delta\tau\hat{S}}$	$T+S-\frac{\delta\tau^2}{24}\left(\{S,\{S,T\}\}+2\{T,\{S,T\}\}\right)$
QPQ	$e^{\frac{1}{2}\delta\tau\hat{T}}\,e^{\delta\tau\hat{S}}\,e^{\frac{1}{2}\delta\tau\hat{T}}$	$T+S+\frac{\delta\tau^2}{24}\left(2\{S,\{S,T\}\}+\{T,\{S,T\}\}\right)$
PQPQP $\alpha=\frac{1}{6}$ [6, 4, 3]	$e^{\frac{1}{6}\delta\tau\hat{S}}\,e^{\frac{1}{2}\delta\tau\hat{T}}$ $\times\,e^{\frac{2}{3}\delta\tau\hat{S}}$ $\times\,e^{\frac{1}{2}\delta\tau\hat{T}}\,e^{\frac{1}{6}\delta\tau\hat{S}}$	$T+S+\frac{\delta\tau^2}{72}\{S,\{S,T\}\}$
PQPQP $\alpha=\frac{1}{2}(1-\frac{1}{\sqrt{3}})$ [6, 4, 3]	$e^{\frac{3-\sqrt{3}}{6}\delta\tau\hat{S}}\,e^{\frac{1}{2}\delta\tau\hat{T}}$ $\times\,e^{\frac{1}{\sqrt{3}}\delta\tau\hat{S}}$ $\times\,e^{\frac{1}{2}\delta\tau\hat{T}}\,e^{\frac{3-\sqrt{3}}{6}\delta\tau\hat{S}}$	$T+S+\frac{\sqrt{3}-2}{24}\delta\tau^2\{T,\{S,T\}\}$
Campostrini [7, 8]	$\exp\left(\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{12}\delta\tau\hat{T}\right)$ $\times\,\exp\left(\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{6}\delta\tau\hat{S}\right)$ $\times\,\exp\left(\frac{-\sqrt[3]{4}-2\sqrt[3]{2}+2}{12}\delta\tau\hat{T}\right)$ $\times\,\exp\left(-\frac{\sqrt[3]{4}+2\sqrt[3]{2}+1}{3}\delta\tau\hat{S}\right)$ $\times\,\exp\left(\frac{-\sqrt[3]{4}-2\sqrt[3]{2}+2}{12}\delta\tau\hat{T}\right)$ $\times\,\exp\left(\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{6}\delta\tau\hat{S}\right)$ $\times\,\exp\left(\frac{\sqrt[3]{4}+2\sqrt[3]{2}+4}{12}\delta\tau\hat{T}\right)$	$T+S$ $+\frac{\delta\tau^4}{34560}\left(\begin{array}{l}-\left(40\sqrt[3]{4}+40\sqrt[3]{2}+48\right)\{S,\{S,\{S,\{S,T\}\}\}\}\\+\left(180\sqrt[3]{4}+240\sqrt[3]{2}+312\right)\{\{S,T\},\{S,\{S,T\}\}\}\\+\left(60\sqrt[3]{4}+80\sqrt[3]{2}+104\right)\{\{S,T\},\{T,\{S,T\}\}\}\\+\left(-20\sqrt[3]{4}+8\right)\{T,\{S,\{S,\{S,T\}\}\}\}\\+\left(20\sqrt[3]{2}+32\right)\{T,\{T,\{S,\{S,T\}\}\}\}\\+\left(5\sqrt[3]{2}+8\right)\{T,\{T,\{T,\{S,T\}\}\}\}\end{array}\right)$
Force Gradient #1 [5, 6]	$e^{\frac{1}{6}\delta\tau\hat{T}}\,e^{\frac{3}{8}\delta\tau\hat{S}}\,e^{\frac{1}{3}\delta\tau\hat{T}}$ $\times\,e^{\frac{48\delta\tau S-\delta\tau^3\widehat{\{S,\{S,T\}\}}}{192}}$ $\times\,e^{\frac{1}{3}\delta\tau\hat{T}}\,e^{\frac{3}{8}\delta\tau\hat{S}}\,e^{\frac{1}{6}\delta\tau\hat{T}}$	$T+S$ $+\frac{\delta\tau^4}{6635520}\left(\begin{array}{l}2259\,\{S,\{S,\{S,\{S,T\}\}\}\}\\+3024\,\{\{S,T\},\{S,\{S,T\}\}\}\\+768\,\{\{S,T\},\{T,\{S,T\}\}\}\\+5616\,\{T,\{S,\{S,\{S,T\}\}\}\}\\+4224\,\{T,\{T,\{S,\{S,T\}\}\}\}\\+896\,\{T,\{T,\{T,\{S,T\}\}\}\}\end{array}\right)$
Force Gradient #2	$e^{\frac{6}{\delta\tau}\hat{S}}\,e^{\frac{2}{\delta\tau}\hat{T}}$ $\times\,e^{\frac{48\delta\tau S-\delta\tau^3\widehat{\{S,\{S,T\}\}}}{72}}$ $\times\,e^{\frac{2}{\delta\tau}\hat{T}}\,e^{\frac{6}{\delta\tau}\hat{S}}$	$T+S$ $-\frac{\delta\tau^4}{155520}\left(\begin{array}{l}41\,\{S,\{S,\{S,\{S,T\}\}\}\}\\+36\,\{\{S,T\},\{S,\{S,T\}\}\}\\+72\,\{\{S,T\},\{T,\{S,T\}\}\}\\+84\,\{T,\{S,\{S,\{S,T\}\}\}\}\\+126\,\{T,\{T,\{S,\{S,T\}\}\}\}\\+54\,\{T,\{T,\{T,\{S,T\}\}\}\}\end{array}\right)$

Table 3: A collection of integrators with the leading terms in their exactly conserved shadow Hamiltonians.