HYBRID MONTE CARLO

Simon DUANE [1]
Physics Department, Imperial College, London SW7 2BZ, UK

A.D. KENNEDY
Supercomputer Computations Research Institute [2], Florida State University, Tallahassee, FL 32306-4052, USA

Brian J. PENDLETON and Duncan ROWETH
Physics Department, University of Edinburgh, The King's Buildings, Edinburgh EH9 3JZ, Scotland, UK

Received 8 June 1987

We present a new method for the numerical simulation of lattice field theory A hybrid (molecular dynamics/Langevin) algorithm is used to guide a Monte Carlo simulation. There are no discretization errors even for large step sizes. The method is especially efficient for systems such as quantum chromodynamics which contain fermionic degrees of freedom Detailed results are presented for four-dimensional compact quantum electrodynamics including the dynamical effects of electrons.

Computer simulation of lattice field theory with fermionic degrees of freedom is notoriously difficult. Because of the Grassmann nature of the fermions one cannot use standard methods to perform Monte Carlo calculations. Instead one integrates out the fermion fields leading to an effective action (the logarithm of the fermion determinant) which is highly nonlocal in the remaining bosonic degrees of freedom. This means that local updates require calculations which depend on the state of the whole system. This nonlocality is somewhat reduced by introducing extra bosonic fields coupled through the fermion matrix (pseudofermions) [1], and a "nested" Monte Carlo computation of the change in the effective action is possible. Local updates of the original bosonic fields can now be made at the expense of an entire Monte Carlo calculation on the pseudofermions.

A popular remedy for this problem is to replace the Monte Carlo algorithm by an equation of motion describing the evolution of the system in a new fictitious time variable τ [2–4]. The solution of this equation for asymptotically large times gives the desired probability distribution for each field of the theory. Numerical integration schemes allow one to avoid the problem of non-locality of the effective action by evolving the whole system in parallel through a large number of small steps. The result is that one approximation is replaced by another: instead of an incomplete equilibration during the "inner" pseudofermion Monte Carlo, we have to contend with truncation errors in the numerical integration of the equation of motion. In principle both of these errors can be eliminated by an extrapolation.

It is the purpose of this paper to describe a new algorithm which combines the ease of calculation of an equation of motion method and the absence of truncation error in an exact Monte Carlo. The algorithm is unlike the usual Monte Carlo methods for lattice systems because it involves parallel updates of fields at all lattice sites followed by an accept/reject decision for the whole configuration. It is also unlike any normal discrete integration of a differential equation because there are *no* truncation errors. Roughly speaking, the step size

[1] National Physical Laboratory, Teddington, Middlesex TW11 0LW, UK.
[2] Supported by the US Department of Energy through contract #DE-FC05-85ER250000.

$\delta\tau$ in the standard hybrid stochastic method is chosen as large as possible while keeping the Monte Carlo acceptance rate satisfactorily high.

The fundamental objective of a quantum field theory is to calculate the expectation value of some operator $\Omega(\phi)$, where the field ϕ has dynamics governed by the action $S(\phi)$:

$$\langle\Omega\rangle = \frac{1}{Z}\int [\mathrm{d}\phi]\, \exp[-S(\phi)]\Omega(\phi)\,, \tag{1}$$

with partition function

$$Z = \int [\mathrm{d}\phi]\, \exp[-S(\phi)]\,. \tag{2}$$

The Monte Carlo method computes $\langle\Omega\rangle$ by generating ϕ-field configurations at random with probability $P_S(\phi) = (1/Z)\exp[-S(\phi)]$, and then measuring

$$\bar{\Omega} \equiv \frac{1}{T}\sum_{t=1}^{T} \Omega(\phi_t) \tag{3}$$

on a sequence (ϕ_t) of such configurations. As $T\to\infty$ we find that

$$\bar{\Omega} = \langle\Omega\rangle + \mathrm{O}(1/\sqrt{T})\,. \tag{4}$$

The most useful technique for generating a sequence of configurations with the desired distribution is to construct a Markov process. A Markov process is a stochastic procedure which generates a new configuration ϕ' from its predecessor ϕ with probability $P_{\mathrm{M}}(\phi \mapsto \phi')$. Any Markov process will converge to a unique fixed point distribution P_S provided that it is ergodic and that it satisfies detailed balance:

$$P_S(\phi)P_{\mathrm{M}}(\phi \mapsto \phi') = P_S(\phi')P_{\mathrm{M}}(\phi' \mapsto \phi)\,. \tag{5}$$

It is convenient to construct the Markov process in two parts. First we choose a new configuration ϕ' with probability $P_{\mathrm{C}}(\phi \mapsto \phi')$ by some as yet unspecified procedure, and then we accept ϕ' with some probability $P_{\mathrm{A}}(\phi \mapsto \phi')$ or reject it and keep the old configuration ϕ instead. One choice of P_{A} which enables detailed balance to be satisfied for any P_{C} is a simple generalization [5] of the Metropolis algorithm [6]

$$P_{\mathrm{A}}(\phi \mapsto \phi') = \min(1, P_S(\phi')P_{\mathrm{C}}(\phi' \mapsto \phi)/P_S(\phi)P_{\mathrm{C}}(\phi \mapsto \phi'))\,. \tag{6}$$

We require a method for choosing candidate configurations which can be computed efficiently and whose reverse probability $P_{\mathrm{C}}(\phi' \mapsto \phi)$ is easy to obtain. Since we are proposing to update all fields ϕ simultaneously we insist that the acceptance rate P_{A} is large and that it does not depend too strongly on the size of our system. Finally, we want to minimize the correlation between successive configurations.

An elegant method for doing this follows the idea of the hybrid molecular dynamics/Langevin algorithm [4,7]. We introduce a new "computer" time parameter τ, and a hamiltonian dynamics to specify the development of the field $\phi(\tau)$ in this time. Introducing a set of conjugate momenta $\pi(\tau)$ we may impose the following hamiltonian by fiat:

$$H'(\phi, \pi) \equiv \tfrac{1}{2}\pi^2 + S'(\phi)\,, \tag{7}$$

where S' is some arbitrary action. This hamiltonian gives the following equations of motion:

$$\dot{\phi} = \delta H'/\delta\pi = \pi\,, \quad \dot{\pi} = -\delta H'/\delta\phi = -\delta S'/\delta\phi\,. \tag{8}$$

As always, the hamiltonian itself is a constant of the motion. A special case of such a hamiltonian is

$$H(\phi, \pi) \equiv \tfrac{1}{2}\pi^2 + S(\phi)\,, \tag{9}$$

where S is the action of eq. (1).

Our procedure for generating a new configuration ϕ' is to select some initial momenta π at random from a gaussian distribution of mean zero and unit variance

$$P_G(\pi) \propto \exp(-\pi^2/2) , \tag{10}$$

and then to let the system evolve deterministically through (ϕ, π)-phase space for a fixed time τ_0 according to Hamilton's equations. If the phase space trajectory $(\phi(\tau), \pi(\tau))$ is a solution of Hamilton's equations (8) then this evolution defines a mapping on phase space by $(\phi, \pi) \equiv (\phi(0), \pi(0)) \mapsto (\phi(\tau_0), \pi(\tau_0))$.

The probability P_H of choosing the candidate phase space "configuration" (ϕ', π') is thus [#1]

$$P_H((\phi, \pi) \mapsto (\phi', \pi')) = \delta[(\phi', \pi') - (\phi(\tau_0), \pi(\tau_0))] . \tag{11}$$

Finally we accept this candidate with probability [#2]

$$P_A((\phi, \pi) \mapsto (\phi', \pi')) = \min(1, \exp(\delta H)) , \tag{12}$$

where $\delta H \equiv H(\phi', \pi') - H(\phi, \pi)$, H being the special hamiltonian of eq. (9).

The transition probability restricted to the ϕ-field alone is

$$P_M(\phi \mapsto \phi') = \int [d\pi]\, [d\pi']\, P_G(\pi) P_H((\phi, \pi) \mapsto (\phi', \pi')) P_A((\phi, \pi) \mapsto (\phi', \pi')) , \tag{13}$$

and we wish to show that this satisfies the detailed balance condition (5) exactly. For this to be the case we require the dynamics to be reversible

$$P_H((\phi, \pi) \mapsto (\phi', \pi')) = P_H((\phi', -\pi') \mapsto (\phi, -\pi)) , \tag{14}$$

which is certainly the case for the hamiltonian dynamics introduced previously. From the identity

$$\begin{aligned} &\exp[-H(\phi, \pi)] \min(1, \exp(-\delta H)) = \min(\exp[-H(\phi, \pi)], \exp[-H(\phi', \pi')]) \\ &\quad = \exp[-H(\phi', \pi')] \min(\exp(\delta H), 1) , \end{aligned} \tag{15}$$

and observing that $P_S(\phi) P_G(\pi) \propto \exp[H(\phi, \pi)]$ and H is invariant under $\pi \mapsto -\pi$ we obtain

$$\begin{aligned} &P_S(\phi) P_G(\pi) P_A((\phi, \pi) \mapsto (\phi', \pi')) = P_S(\phi') P_G(\pi') P_A((\phi', \pi') \mapsto (\phi, \pi)) \\ &\quad = P_S(\phi') P_G(-\pi') P_A((\phi', -\pi') \mapsto (\phi, -\pi)) . \end{aligned} \tag{16}$$

Multiplying this equation by P_H, integrating over π and π' and using the reversibility condition (14) we find

$$\begin{aligned} &\int [d\pi]\, [d\pi']\, P_S(\phi) P_G(\pi) P_H((\phi, \pi) \mapsto (\phi', \pi')) P_A((\phi, \pi) \mapsto (\phi', \pi')) \\ &\quad = \int [d\pi]\, [d\pi']\, P_S(\phi') P_G(-\pi') P_H((\phi', -\pi') \mapsto (\phi, -\pi)) P_A((\phi', -\pi') \mapsto (\phi, -\pi)) , \end{aligned} \tag{17}$$

which yields the detailed balance equation (5) from (13) and the invariance of the measure $[d\pi]\, [d\pi'] = [d(-\pi)] \times [d(-\pi')]$.

In the case where we take $H' = H$ the dynamics conserves energy, that is $\delta H = 0$, so the acceptance rate $P_A = 1$: This limit is just the usual hybrid algorithm. However we have proved a more general result, that our algorithm will generate ϕ-field configurations with the correct distribution for *any* δH.

In practice we can only approximately integrate the equations of motion taking some discrete sequence of steps of duration $\delta\tau$. A simple scheme for the numerical integration of the equations of motion which ensures

[#1] This probability distribution is a δ-function because the dynamics we have introduced is completely deterministic. This is not necessary: as long as P_H is reversible (eq. (14)) our algorithm is still valid.

[#2] This is a slight generalization of the definition (6), as P_A depends on the conjugate momenta π as well as the ϕ-field itself.

exact reversibility (14) and generates an area-preserving map on phase space for any value of $\delta\tau$ is the *leapfrog* algorithm. An initial half-step

$$\pi(\delta\tau/2)=\pi(0)-[\delta S(0)/\delta\phi]\delta\tau/2 \tag{18}$$

is followed by $n=\tau_0/\delta\tau$ steps in ϕ and $n-1$ steps in π of the form

$$\phi(\tau+\delta\tau)=\phi(\tau)+\pi(\tau+\delta\tau/2)\cdot\delta\tau\,,\quad \pi(\tau+\delta\tau/2)=\pi(\tau-\delta\tau/2)-[\delta S(\tau)/\delta\phi]\cdot\delta\tau\,, \tag{19, 20}$$

and a final half-step

$$\pi(\tau_0)=\pi(\tau_0-\delta\tau/2)-[\delta S(\tau_0)/\delta\phi]\cdot\delta\tau/2\,. \tag{21}$$

The half-steps differ from the exact integration of Hamilton's equations by errors of order $\delta\tau^2$, whereas the intermediate steps have errors of order $\delta\tau^3$.

Dynamical fermions may be included just as in the hybrid or molecular dynamics approaches. The Grassmann fields ψ and $\bar{\psi}$ are replaced by bosonic fields χ^* and χ with non-local interactions:

$$P_S(\phi)=\frac{1}{Z}\int[\mathrm{d}\bar{\psi}]\,[\mathrm{d}\psi]\exp[-S(\phi)-\bar{\psi}\mathscr{M}\psi]=\frac{1}{Z'}\det(\mathscr{M})\exp[-S(\phi)]$$

$$=\frac{1}{Z''}\int[\mathrm{d}\chi^*]\,[\mathrm{d}\chi]\exp[-S(\phi)-\chi^*(\mathscr{M}^\dagger\mathscr{M})^{-1}\chi]\,. \tag{22}$$

The quadratic form $\mathscr{M}^\dagger\mathscr{M}$ is used to ensure convergence of the bosonic gaussian integrals. The form of the fermion kernel $\mathscr{M}$ for the case of interest allows us to keep χ fields on even lattice sites only, thus avoiding the apparent doubling above.

The hamiltonian and equations of motion become

$$H(\phi,\pi)=\tfrac{1}{2}\pi^2+S(\phi)+\chi^*(\mathscr{M}^\dagger\mathscr{M})^{-1}\chi\,, \tag{23}$$

$$\dot{\phi}=\pi\,,\quad \dot{\pi}=-\delta S/\delta\phi+\chi^*(\mathscr{M}^\dagger\mathscr{M})^{-1}[\mathscr{M}^\dagger\delta\mathscr{M}/\delta\phi+(\delta\mathscr{M}^\dagger/\delta\phi)\mathscr{M}](\mathscr{M}^\dagger\mathscr{M})^{-1}\chi\,. \tag{24}$$

The χ field is held fixed during the molecular dynamics steps and is updated by an exact heatbath, $\chi=\mathscr{M}\eta$ for gaussian noise η, in between [8]. The generalization of the leapfrog algorithm to include fermions is trivial. A single conjugate gradient inversion is required for each molecular dynamics step.

This completes our description of the basic technique by which we propose to bring together the conventional hybrid scheme and Monte Carlo methods. Whether or not this idea works in practice can only be answered by numerical experiment.

We have tested the algorithm on compact quantum electrodynamics, a lattice gauge theory model of interacting photons and electrons. We used the standard Wilson action for the gauge field and the staggered fermion formulation for the electrons. The hamiltonian is

$$H=\frac{1}{2}\sum_{x\mu}\pi_\mu^2(x)+S(U,\bar{\psi},\psi)\,, \tag{25}$$

where the action S is

$$S(U,\bar{\psi},\psi)=\beta\sum_{\substack{x\nu\mu\\ \nu>\mu}}[1-\mathrm{Re}\,U_{\mu\nu}(x)]+\sum_{xy}\bar{\psi}(x)(-\mathbb{D}^2+m^2)^{-1}\psi(y)\,. \tag{26}$$

The phases $U_{\mu\nu}(x)$ are the usual products of link variables around the elementary plaquettes of the lattice. The equations of motion can be derived from (25) in the standard way [9].

Our initial tests were performed on the pure gauge theory without fermions. In fig. 1 we show the average

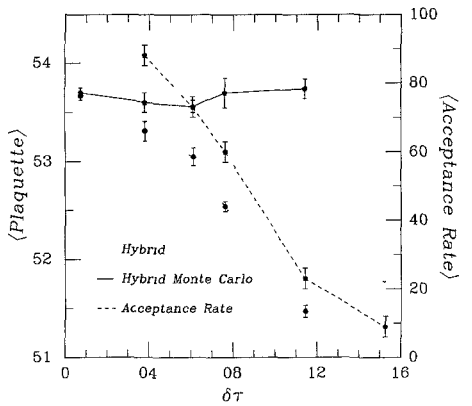

Fig 1. The average plaquette as a function of the integration step size $\delta\tau$ for quenched QED on an 8^4 lattice with coupling constant $\beta = 0.97$. For the hybrid Monte Carlo results the acceptance rates are shown as well.

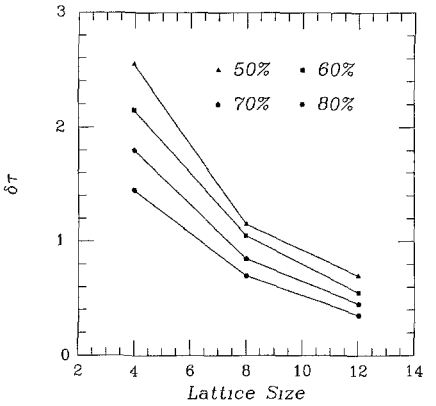

Fig 2 Curves of constant acceptance rate are shown as a function of the integration step size $\delta\tau$ on the lattices of size 4^4, 8^4 and 12^4 in quenched QED at a coupling of $\beta = 0.97$.

plaquette on an 8^4 lattice as a function of step size $\delta\tau$ for both the standard hybrid algorithm and for the new hybrid Monte Carlo algorithm. Also shown is the acceptance rate for each step size. The results agree with previous high statistics data [10]. Optimization of τ_0, or equivalently of the number of molecular dynamics steps between each acceptance test, can be performed just the as for the standard hybrid algorithm. The equilibration time measured in units of τ is similar in both cases. The optimal step size for the new algorithm on this lattice with coupling $\beta = 0.97$ is roughly 0.1. The effective step size ($a\delta\tau$ where a is the acceptance rate) is then 0.06, several times larger than the maximum "safe" hybrid step size of 0.01 or 0.02. In addition, the new algorithm does not require that we extrapolate our results to $\delta\tau = 0$.

In order to study how the efficiency of the algorithm scales with lattice volume we have performed simulations on lattices of size 4^4, 8^4 and 12^4. Fig. 2 shows how the step size must be scaled to keep a constant acceptance rate as the lattice size is changed. The data is consistent with $\delta\tau \propto 1/L$ for a constant acceptance rate, where L is the linear size of the lattice. It is also consistent with the acceptance rate being proportional to $\exp(-L^2\delta\tau^2)$, which we might expect from some simple arguments.

In fig. 3 we show the dependence of the plaquette and the chiral condensate $\langle\bar{\psi}\psi\rangle$ on the step size for the full theory with fermions. Although the fermionic effects are quite large, the step size dependence of the results is similar to that for the pure gauge theory. A detailed description of our results for several values of the mass will be published elsewhere [11].

In the hybrid Monte Carlo method the hamiltonian serves two distinct roles. Firstly the *acceptance* hamiltonian H defines the equilibrium distribution, entering the expression for the acceptance probability (12), and secondly the *guidance* hamiltonian H' appears in the equations of motion (9). There is nothing in the hybrid Monte Carlo algorithm which requires these two hamiltonians to be equal, and the generalization $H \neq H'$ introduces some scope for optimization of the acceptance rate.

It has been observed [3,12] that in some cases the effects of discretization errors in the integration of the Langevin or molecular dynamics equations of motion are equivalent to performing an exact computation for a theory with an unknown action S'', which differs from the desired action S by some renormalizations. If we adjust the parameters in the guidance hamiltonian [#3] there should be an optimal $H' \neq H$ for which the equivalent action S'' for the discretized dynamics approaches the desired action S appearing in the acceptance hamiltonian H. For this guidance hamiltonian the acceptance rate will be a maximum.

[#3] We may also introduce new parameters as coefficients of irrelevant operators

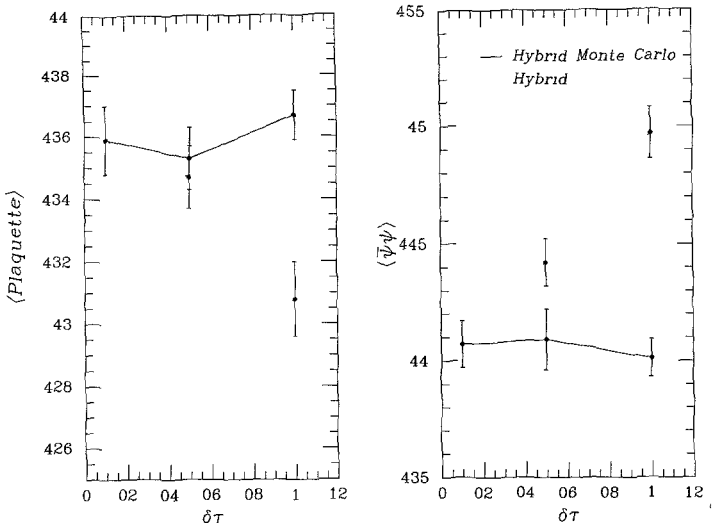

Fig. 3 The dependence of the plaquette and the chiral condensate $\langle\bar{\psi}\psi\rangle$ on the step size $\delta\tau$ for QED including dynamical electrons of mass 0.25 in lattice units The lattice size is 8^4 and $\beta=0\,8$

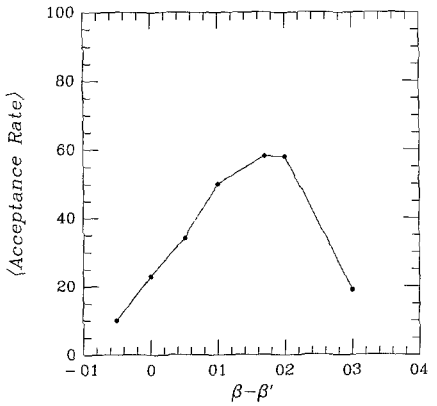

Fig 4. The acceptance rate as a function of $\beta-\beta'$ for "quenched" QED on an 8^4 lattice with $\beta=0.97$ and $\delta\tau=0\,15$.

In fig. 4 we show the acceptance rate as a function of $\beta-\beta'$ for "quenched" QED on an 8^4 lattice, where β is the coupling constant in H and β' the coupling constant in H'. As expected from the preceding argument the acceptance rate shows a peak for $\beta\neq\beta'$, and there is a noticeable improvement in the acceptance rate over that obtained with $H=H'$.

The method is easily generalized to the case of quantum chromodynamics with dynamical quark fields, and this is currently under investigation.

Our programs were written in Occam and run on the Meiko Computing Surface at Edinburgh. The current program uses 16 Transputers in a binary hypercube arrangement. The Edinburgh Computing Surface is supported by the United Kingdom Department of Trade and Industry and by the Computer Board. The work of BJP was supported by an SERC Advanced Fellowship. DR was supported by the UK SERC and by Inmos UK, Ltd. ADK would like to acknowledge the support of the US DOE and DFG. We wish to thank R.D. Kenway for useful discussions.

References

[1] F Fucito, E. Marinari, G. Parisi and C. Rebbi, Nucl. Phys. B 180 [FS2] (1981) 369
[2] J. Polonyi and H.W. Wyld, Phys. Rev. Lett. 51 (1983) 2257.
[3] G.G. Batrouni, G R. Katz, A S. Kronfeld, G P. Lepage, B. Svetitsky and K.G Wilson, Phys Rev. D 32 (1985) 2735.
[4] S. Duane, Nucl. Phys. B 257 [FS14] (1985) 652.
[5] R.T. Scalettar, D.J. Scalapino and R.L Sugar, Phys. Rev B 34 (1986) 7911
[6] N A. Metropolis, M.N Rosenbluth, A.H. Rosenbluth, E. Teller and J. Teller, J. Chem. Phys. 21 (1953) 1087.
[7] S. Duane and J.B Kogut, Nucl. Phys. B 275 (1986) 398.
[8] S. Gottlieb, W. Liu, D. Toussaint, R L. Renken and R.L. Sugar, Phys. Rev. D 35 (1987) 2531.
[9] S. Duane, R.D Kenway, B.J Pendleton and D. Roweth, Phys. Lett B 176 (1986) 143.
[10] C B Lang, Phys. Rev Lett. 57 (1986) 1828.
[11] S Duane, A.D. Kennedy, B J. Pendleton and D Roweth, in preparation.
[12] J. Zinn-Justin, Nucl Phys. B 275 (1986) 135.