Metropolis and Langevin time

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We show that a linear relation between Metropolis and Langevin time in computer simulations observed by Meakin *et al.* for spinodal decomposition is also true for lattice gauge theories.

Some time ago Meakin, Metiu, Petschek, and Scalapino[1] observed that there was a linear relationship between the evolution of a lattice model of spinodal decomposition in two dimensions under Monte Carlo dynamics and the evolution of the same system under Langevin dynamics for suitably small values of the Monte Carlo hit size. They pointed out that, although their explicit numerical results were for this model alone, the analysis was quite general and should apply to other systems. Martin, Otto, and Flower[2] made use of the claimed generality of the relation between the hit size h and the Langevin time step $\delta\tau$,

$$h^2 \propto \delta\tau \ , \tag{1}$$

to derive an estimate for the systematic errors of the pseudofermion method for simulating lattice QCD. They observed that the Monte Carlo evolution of the pseudofermion action

$$S = S_{\text{gauge}} - \ln\det(\not{D} + m) \ , \tag{2}$$

under a change in a link variable $U \to U + \delta U$ became the Langevin process in the limit $\delta U \to 0$, with $\delta U \sim \sqrt{\delta\tau}$ assuming the validity of (1). They then used a result they had derived for the systematic errors of the Langevin approach to show that the errors due to linearization were of the order of $\delta U^2 \xi_\pi^2$, where ξ_π was the lattice correlation length. In view of the utility of Eq. (1) we thought it worthwhile to verify that it did, in fact, hold true in the regimes of interest in lattice gauge theory. We carried out numerical investigations of the equilibration of the plaquette energy in two-dimensional Abelian gauge theory and four-dimensional non-Abelian gauge theory (both without fermions), and compared the results with predictions.

We shall consider first the derivation of Eq. (1) for an Abelian lattice gauge theory, such as QED. The action is taken to be the standard Wilson action[3]

$$S = \beta \sum_{\square} (1 - \cos U_{\square}) \ , \tag{3}$$

where $\square$ denotes a plaquette (and $U_{\square}$ denotes the product of link variables around a plaquette). The Langevin equation used to evolve the link variable U_l was

$$\frac{\partial U_l}{\partial \tau} = -\beta \sum_{l \in \square} (\square / l) \sin U_{\square} + \eta_l \ , \tag{4}$$

where l labels a link, $(\square / l) = \pm 1$ depending on the orientation of the plaquette relative to l, and the noise η_l is Gaussian. This equation may be discretized to give

$$U_l(n+1) = U_l(n) - \delta\tau\beta f_l(n) + \sqrt{2\delta\tau}\, r_l(n) \ , \tag{5}$$

where n labels the step, $\delta\tau$ is the time increment, and

$$f_l(n) = \sum_{l \in \square} (\square / l) \sin U_{\square}(n), \quad \overline{r_l(n) r_k(m)} = \delta_{lk}\delta_{nm} \ . \tag{6}$$

The Monte Carlo simulation, on the other hand, changes the link variable U_l by a uniformly distributed amount between $\pm\delta U_{\max}$ where $\delta U_{\max} = \epsilon\pi$. The probability that a change δU is accepted is given by

$$P(\delta U_l) = \theta(e^{-\delta S} - 1) + e^{-\delta S}\theta(1 - e^{-\delta S}) \ , \tag{7}$$

where δS is the change in the action induced by δU_l:

$$\delta S = \beta \sum_{l \in \square} (\square / l) \sin U_{\square} \delta U_l = \beta f_l \delta U_l \ . \tag{8}$$

For small δS Eq. (7) gives

$$P(\delta U_l) = 1 - \beta f_l \delta U_l \theta(\beta f_l \delta U_l) \ . \tag{9}$$

Note that this is not the same as the probability of acceptance found by Meakin, Metiu, Petschek, and Scalapino, because they used an alternative acceptor algorithm

$$P(\delta U_l) = \frac{\exp(-\delta S)}{\exp(-\delta S) + 1} \ . \tag{10}$$

The probability that a coordinate change in the range $[a,b]$ occurs as a result of a Monte Carlo trial is then $\int_a^b w(x)dx$, where (dropping terms of higher order in $\delta U_{\max}$)

$$w(x) = \frac{1}{2\delta U_{\max}} [1 - \beta f_l x \theta(\beta f_l x)] \ . \tag{11}$$

We thus find

$$\bar{x} = \int_{-\delta U_{\max}}^{\delta U_{\max}} x w(x) = -\frac{\beta f_l (\delta U_{\max})^2}{6} \ . \tag{12}$$

The central limit theorem now assures us that, after a large number of trials N (Ref. 1),

$$w(z) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-(z-\mu)^2 / 2\sigma^2] \ , \tag{13}$$

where $w(z)$ is the probability of finding a total change in the range $z \to z + \delta z$ after N trials and $\mu = N\bar{x}$, $\sigma^2 = N(\overline{x^2} - \bar{x}^2)$.

Now Eq. (13) also provides a solution to the Langevin equation (4), with

$$\mu = -\beta f_l \delta\tau \ , \tag{14}$$

so we find, equating the two μ after M Langevin time steps,

$$N(\delta U_{\max})^2 = 6M\delta\tau \ . \tag{15}$$

If we had used Eq. (10) for our acceptance criterion we would have found

$$N(\delta U_{\max})^2 = 12M\delta\tau \ . \tag{16}$$

We should perhaps make two parenthetical observations about the above derivation. First, the force f_l depends on U_l and we have taken it as a constant, but this is justified for the small variations under consideration. Second, the derivation is not invalidated by Elitzur's theorem[4] which states that the mean equilibrium value of the U_l is zero because thermal fluctuations can induce gauge rotations at no cost in energy. We are considering the trajectory of a single-link variable moving towards equilibrium in incremental steps rather than the equilibrium average. To test Eqs. (15) and (16) we ran a two-dimensional Abelian gauge theory on a 16×16 lattice at $\beta=1$ and measured the equilibration of the mean plaquette energy from a cold start for both Monte Carlo and Langevin simulations. We used the acceptance criterion of Eq. (7) for results in Fig. 1 and that of Eq. (10) for the results in Fig. 2. Equations (15) and (16) would lead us to expect that 182 and 365 Metropolis sweeps, respectively, for Figs. 1 and 2, should match 300 Langevin steps, which is indeed what was observed. The graphs were drawn from the average of five trajectories and the number of points plotted adjusted to give a good visual fit.

It is clear that a similar relation to Eq. (1) will also hold for the non-Abelian case, the only new element being what we mean by hit size. The action for the non-Abelian SU(N) gauge theory is given by

$$S = \beta \sum_{\square} \left[1 - \frac{1}{N} \mathrm{Re\,Tr} U_{\square} \right] , \tag{17}$$

where $U \in \mathrm{SU}(N)$ is now the link variable and $U_{\square}$ denotes the product of U's around a plaquette. The Langevin equation that is used to evolve a link variable is now[5]

$$U_l^{-1} \frac{\partial U_l}{\partial \tau} = -T^a \nabla_l^a S(U_l) + T^a \eta_l^a \ , \tag{18}$$

where T^a is an anti-Hermitian generator of SU(N), normalized so that $\mathrm{Tr}(T^a T^b) = -\frac{1}{2}\delta^{ab}$ and

$$\nabla_l^a = i(U_l T^a)_{ij} \frac{\delta}{\delta (U^a)_{ij}} \ , \tag{19}$$

is the right Lie derivative on SU(N). This may be discretized in a similar manner to the Abelian equation.

The Monte Carlo algorithm used for comparison generated a table of 50 SU(2) matrices and their inverses, exponentially weighted about the identity with some large parameter α, and then multiplied a given test SU(3) matrix in each of its SU(2) subgroups by an element of the table. The acceptance criterion of Eq. (7) was then used to accept or reject the new configuration. [This is rather similar to the Cabibbo-Marinari[6] heat-bath algorithm for SU(3) but in our case the parameter α is fixed and the table is not refreshed.] The SU(2) subgroup was parametrized as the surface of a sphere

$$a_0^2 + |\mathbf{a}|^2 = 1 \ ,$$

where the SU(2) group elements were given by $a_0 \mathbf{1} + i\mathbf{a}\cdot\boldsymbol{\sigma}$, with $\boldsymbol{\sigma}$ being a vector of Pauli matrices.

A rough measure of the hit size is given by the size of one of the off-diagonal elements $a_i \in \mathbf{a}$. The mean of a_i with the acceptance criterion of Eq. (7) and the exponential weighting of a_0 is given approximately by

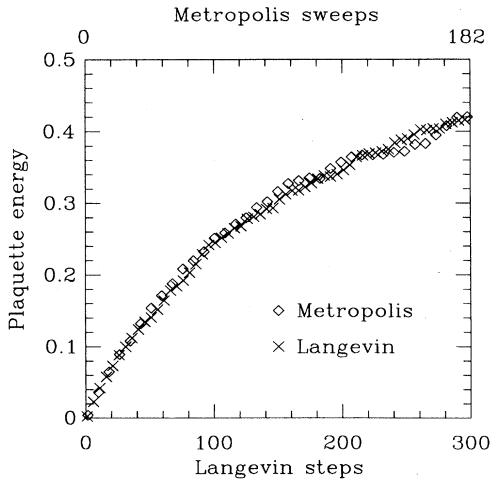

FIG. 1. The mean plaquette energy is plotted against the number of steps for Monte Carlo and Langevin evolution in a two-dimensional Abelian gauge theory on a 16×16 lattice. The acceptance criterion is given by Eq. (7), $\beta=1$, $\delta\tau=0.0001$, and $\epsilon=0.01$.

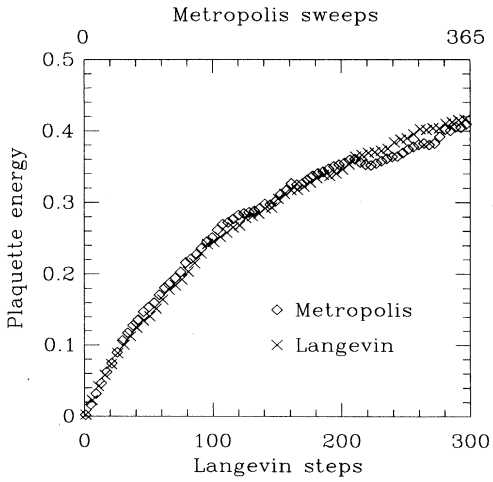

FIG. 2. As Fig. 1 but the acceptance criterion is now given by Eq. (10).

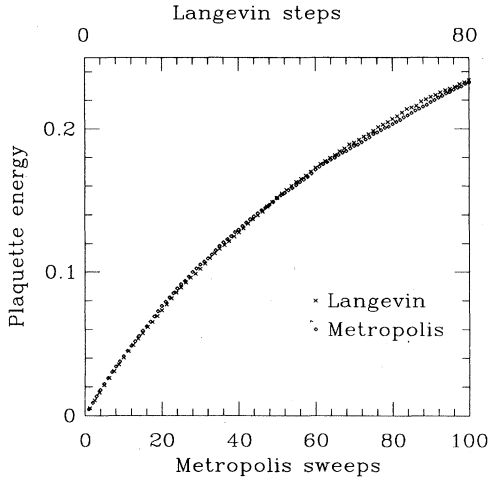

FIG. 3. The mean plaquette energy is plotted against the number of steps for Monte Carlo simulation and Langevin evolution in a four-dimensional SU(3) gauge theory on a 4^4 lattice. The acceptance criterion is given by Eq. (7), $\beta=5$, $\delta\tau=0.001$, and $\alpha=2500$.

$$\bar{a}_i \approx \frac{\int_{-1}^{1}[1-\theta(\beta f a_i)\beta f a_i]a_i \exp(\alpha\sqrt{1-a_i^2})da_i}{\int_{-1}^{1}[1-\theta(\beta f a_i)\beta f a_i]\exp(\alpha\sqrt{1-a_i^2})da_i}\ , \tag{20}$$

where we ignore the contribution of the other two elements of **a**, and use the fact that $\delta S \ll 1$. We would expect an answer to be correct up to factor ~ 1. As we take α large, the main contribution to the integral comes from $a_i \approx 0$ so we can rewrite Eq. (20) as

$$\bar{a}_i \approx \frac{\int_{-\infty}^{\infty}[1-\theta(\beta f a_i)\beta f a_i]a_i \exp\left[-\frac{\alpha}{2}a_i^2\right]da_i}{\int_{-\infty}^{\infty}[1-\theta(\beta f a_i)\beta f a_i]\exp\left[-\frac{\alpha}{2}a_i^2\right]da_i}\ , \tag{21}$$

which gives

$$\bar{a}_i \approx -\frac{\beta f}{\alpha}\ . \tag{22}$$

The same reasoning as in the Abelian case now allows us to derive an equation of the form

$$\frac{N}{\alpha} = cM\delta\tau\ , \tag{23}$$

where N is the number of Monte Carlo simulation sweeps, M is the number of Langevin steps, $\delta\tau$ is the Langevin step size, and c is some constant ~ 1.

To test the validity of Eq. (23) we ran a pure SU(3) gauge-theory simulation on a 4^4 lattice at $\beta=5$, using both a Monte Carlo procedure with various values of α, and a Langevin procedure with $\delta\tau=0.001$.

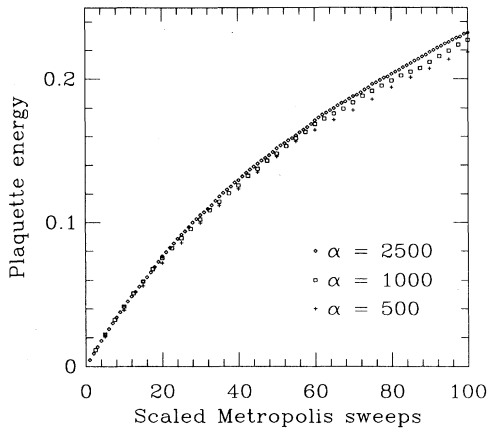

FIG. 4. The mean plaquette energy is plotted against 100 Monte Carlo steps at $\alpha=2500$, 40 steps at $\alpha=1000$ and 20 steps at $\alpha=500$ to confirm the $1/\alpha$ behavior. The SU(3) gauge theory was run once again at $\beta=5$ on a 4^4 lattice.

In Fig. 3 we show the mean plaquette energy at each iteration from a cold start, averaged over five runs. We have adjusted the number of points plotted to obtain a good visual fit between the Monte Carlo and Langevin curves. We found that the numerical constant c was given by 0.5. To confirm the expected $1/\alpha$ behavior we have also plotted in Fig. 4 the mean plaquette energy at each iteration for 100 sweeps at $\alpha=2500$, 40 sweeps at $\alpha=1000$, and 20 sweeps at $\alpha=500$ using the Monte Carlo procedure, finding a good match [according to Eq. (23) they should be identical]. Runs at lower values of β reproduced the value of c and the $1/\alpha$ behavior. The large values of α were chosen to ensure that δS was, indeed, small.

In summary, we have confirmed that the linear relation between Monte Carlo and Langevin "time" in lattice gauge theories that was suggested by the analysis of Ref. 1, and assumed in deriving the error bounds of Ref. 2 does, in fact, exist both for Abelian and non-Abelian gauge theories.

The SU(3) runs were carried out on the 128-mode Caltech/JPL Mark II hypercube, using code originally developed by Martin, Otto, and Flower.

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