Journal of Statistical Physics, Vol. 43, Nos. 5/6, 1986

Langevin Simulations of Lattice Field Theories Using Fourier Acceleration

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KEY WORDS: Lattice field theory; lattice QCD; fourier acceleration; critical slowing-down; conjugate gradient algorithm; numerical gauge fixing.

We have been studying the Langevin equation as a means of simulating lattice field theories.[1] In its simplest form the Langevin procedure for updating a scalar field with action $S[\phi]$ is

$$\phi(x) = \phi(x) + \Delta\phi(x) \tag{1}$$

where

$$\Delta\phi(x) = -\varepsilon \frac{\delta S}{\delta\phi(x)} - \sqrt{\varepsilon}\,\eta(x) \tag{2}$$

Here η is a random number (usually Gaussian) with $\langle \eta(x)^\dagger \eta(y) \rangle = 2\delta_{x,y}$ and ε is the step size. Without the noise term the algorithm would be simply a technique for finding the minima of $S[\phi]$ by the gradient method. The noise term simulates quantum fluctuations about these classical configurations.

In common with other techniques, the Langevin simulation according to (2) will suffer from critical slowing down for large lattices and long correlation lengths ξ. This is because the components of ϕ with highest momenta evolve ξ^2 times faster than those with the lowest momenta and therefore the amount of computing time required to study the infrared structure of configurations on the lattice grows as (volume)$\cdot \xi^2$.

The remedy to this problem is a technique known as Fourier acceleration. One simply chooses a larger step size ε for low p relative to

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0022-4715/86/0600-1073$05.00/0

high p. The rates of evolution of the different momentum components of the field become decoupled and they can all be made to change at the same rate. Equation 2 is replaced by

$$\Delta\phi(x) = -\hat{F}\left\{\varepsilon(p)\,\hat{F}^{-1}\frac{\delta S}{\delta\phi(y)} + \sqrt{\varepsilon(p)}\,\eta(p)\right\} \tag{3}$$

where $\hat{F}$ represents a fast Fourier transform. The algorithm now resembles an improved Newton's method for finding the minima of $S[\phi]$.

In a simulation of the XY model on a $16 * 16$ lattice, results were obtained 25 times faster with Fourier acceleration than without it.[1] The method works both in the perturbative regime where $\varepsilon(p)$ is proportional to the lattice propagator and in the nonperturbative regime where $\varepsilon(p)$ cannot be calculated but must be chosen from preliminary measurements of the decorrelation times of different momentum components.

Such acceleration can be used in simulating gauge theories as well, provided that some sort of complete gauge fixing is applied to the configurations between updates. Without gauge fixing there is no simple correlation between different momenta and different length scales and Fourier acceleration becomes useless. This suggests that smooth gauges, like $\partial \cdot A = 0$, are the best.

The gauge that we use is defined by first fixing the configuration into an axial gauge, which ensures the gauge invariance of the simulation when ε becomes dependent on p. We then reduce $\partial \cdot A$ by successive gauge transformations to some small value. The gauge transformation $G(x)$ is chosen to maximize the sum over the lattice of the trace of the link field $U_\mu(x)$. A simple gradient algorithm for this procedure suffers again from a kind of critical slowing down; the low momentum components of $\partial \cdot A(p)$ decay much more slowly than the high momentum ones and so the number of gauge fixing iterations required grows as the lattice size increases. This problem is also alleviated by Fourier acceleration. The size of the gauge transformation $w(x)$ $\{G(x) = \exp[iw(x) \cdot T]\}$ is made inversely proportional to p^2. Results on an 8^4 lattice for QCD show that with Fourier acceleration all momentum components of $\partial \cdot A(p)$ decay at the same rate, providing a considerable increase in the speed of the algorithm.[2]

Another problem with simulations of QCD on the lattice is the inclusion of fermions. The full action for the theory becomes

$$S = S_g[U] - \mathrm{tr}\ln M[U] \tag{4}$$

where $S_g[U]$ is the gauge action and $M[U] = \gamma_5(D \cdot \gamma + m)$. A Langevin

update of a link variable U is obtained by multiplying by exp(-if) where schematically

$$f = \varepsilon \left\{ \frac{\delta S_g}{\delta U} - \mathrm{tr}\left[\frac{1}{M} \frac{\delta M}{\delta U} \right] \right\} + noise \tag{5}$$

The tr term is replaced by an estimator

$$\eta_q^+ \left[\frac{1}{2M} \frac{\delta M}{\delta U} \right] \eta_q \tag{6}$$

which reproduces the correct term when averaged over the Gaussian random variable η_q.

The evaluation of the term in (6) requires solving $M(U)\,\psi = \eta_q$ once per sweep, which we do with the conjugate gradient algorithm. This again suffers from critical slowing down for very small quark masses, and again the solution is to invert M in Fourier space. Results on an 8^4 lattice at $\beta = 6.2$ show that one quarter the number of iterations of the algorithm are required when Fourier acceleration is used.[2]

We conclude that the technique of Fourier acceleration shows great promise for the future and will significantly reduce the computation time for simulations on large lattices.

REFERENCES

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