Heat bath algorithm for lattice gauge theories with fermions

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Abstract. The heat bath algorithm is applied to the lattice gauge theories with fermions.

Introduction.

Early lattice gauge theories simulations [1-4] were done for the pure gauge and made use of Monte-Carlo algorithms: the Metropolis algorithm [5] and the heat bath algorithm [6,7]. With the introduction of fermions the lattice gauge theories simulations had to deal with the fermionic determinant and it was still possible to use the Metropolis algorithm but not the heat bath algorithm. Later with the introduction of the pseudofermions [8,9] it was possible to deal directly with the fermionic matrix and the microcanonical algorithm which is a deterministic algorithm introduced earlier for the pure gauge simulations [10] was well suited for the simulations of lattice gauge theories with fermions [11,12]. To improve the ergodicity in the microcanonical algorithm some randomization was added to it which lead to the hybrid algorithm [13,14]. Another algorithm based on the hybrid algorithm but differs sufficiently from it was introduced elsewhere [15]. Later a global Monte-Carlo step was added to it to culminate into the hybrid Monte-Carlo [16]. In parallel to these developments an algorithm based on the Langevin equation was developped elsewhere [17-20].

Heat bath algorithm with fermions.

As it's mentionned above the heat bath algorithm was applied only to the pure gauge, in the following it will be shown that it can be applied to lattice gauge theories with fermions. The starting point is the Φ algorithm in ref. [15] whose conventions, notations and definitions will be adopted in the following. The equations (13-14) in ref. [15] for the H field are given by

$$i\dot{H}_{j,\mu} = \left[\frac{\beta}{3}U_{j,\mu}V_{j,\mu} - 2\,U_{j,\mu}\left(\sum_{\nu} U_{j+\mu,\nu}P_{j+\mu+\nu,j} - \sum_{\nu\neq\mu} U^{\dagger}_{j+\mu-\nu,\nu}P_{j+\mu-\nu,j}\right)\right]_{TA}$$

$$i\dot{H}_{j,\mu} = \left[\frac{\beta}{3}U_{j,\mu}V_{j,\mu} - 2\,U_{j,\mu}\left(\sum_{\nu} P_{j+\mu,j-\nu}U_{j-\nu,\nu} - \sum_{\nu\neq\mu} P_{j+\mu,j+\nu}U^{\dagger}_{j,\nu}\right)\right]_{TA}$$

for even and odd sites, respectively. The first equation above is corrected for a mistake in ref. [15].
These two equations can be recast in the following form

$$i\dot{H}_{j,\mu} = \left\{\frac{\beta}{3}U_{j,\mu}\left[V_{j,\mu} - \frac{6}{\beta}\left(\sum_{\nu} U_{j+\mu,\nu}P_{j+\mu+\nu,j} - \sum_{\nu\neq\mu} U^{\dagger}_{j+\mu-\nu,\nu}P_{j+\mu-\nu,j}\right)\right]\right\}_{TA}$$

$$i\dot{H}_{j,\mu} = \left\{\frac{\beta}{3}U_{j,\mu}\left[V_{j,\mu} - \frac{6}{\beta}\left(\sum_{\nu} P_{j+\mu,j-\nu}U_{j-\nu,\nu} - \sum_{\nu\neq\mu} P_{j+\mu,j+\nu}U^{\dagger}_{j,\nu}\right)\right]\right\}_{TA}$$

One then remarks that the first term in the RHS between brackets is the staples matrix of the pure gauge while the two terms between parentheses are the contribution of the fermionic sector to the staples matrix. One then defines an effective staples matrix given by

$$V'_{j,\mu} = V_{j,\mu} - \frac{6}{\beta}\left(\sum_{\nu} U_{j+\mu,\nu}P_{j+\mu+\nu,j} - \sum_{\nu\neq\mu} U^{\dagger}_{j+\mu-\nu,\nu}P_{j+\mu-\nu,j}\right)$$

$$V'_{j,\mu} = V_{j,\mu} - \frac{6}{\beta}\left(\sum_{\nu} P_{j+\mu,j-\nu}U_{j-\nu,\nu} - \sum_{\nu\neq\mu} P_{j+\mu,j+\nu}U^{\dagger}_{j,\nu}\right)$$

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for even and odd sites, respectively.
For a given SU(N) gauge group the effective staples matrix is given by

$$V'_{j,\mu} = V_{j,\mu} - \frac{2N}{\beta}\left(\sum_{\nu} U_{j+\mu,\nu}P_{j+\mu+\nu,j} - \sum_{\nu\neq\mu} U^{\dagger}_{j+\mu-\nu,\nu}P_{j+\mu-\nu,j}\right)$$

$$V'_{j,\mu} = V_{j,\mu} - \frac{2N}{\beta}\left(\sum_{\nu} P_{j+\mu,j-\nu}U_{j-\nu,\nu} - \sum_{\nu\neq\mu} P_{j+\mu,j+\nu}U^{\dagger}_{j,\nu}\right)$$

for even and odd sites, respectively.
One then use the effective staples matrix in the heat bath algorithm as in ref. [6] to update the links for SU(2) gauge group or the heat bath algorithm as in ref. [7] to update the links for SU(N) gauge group with N $\geq$3.
The new algorithm proceeds as follows
0-Generate a starting links configuration U
1-Generate a vector of random complex numbers R living on all sites and distributed according to $e^{-R^{\dagger}R}$
2-Compute $\Phi = M^{\dagger}R$ with Φ living on even sites
3-Solve $\left(M^{\dagger}M\right)X = \Phi$ for X
4-Compute $P_{i,j}$
5-Compute the effective staples matrix $V'_{j,\mu}$
6-Apply the heat bath algorithm
7-Go to 1

The ref. [15] proposes another algorithm called the R algorithm which is claimed to be applicable to any number (even non-integer) of flavors of fermions just like in the Langevin algorithm [20]. The equations (46-47) in ref. [15] for the H field in the R algorithm are given by

$$i\dot{H}^{R}_{j,\mu} = \left[\frac{\beta}{3}U_{j,\mu}V_{j,\mu} - \frac{1}{2}N_f U_{j,\mu}\left(\sum_{\nu} U_{j+\mu,\nu}P^{R}_{j+\mu+\nu,j} - \sum_{\nu\neq\mu} U^{\dagger}_{j+\mu-\nu,\nu}P^{R}_{j+\mu-\nu,j}\right)\right]_{TA}$$

$$i\dot{H}^{R}_{j,\mu} = \left[\frac{\beta}{3}U_{j,\mu}V_{j,\mu} - \frac{1}{2}N_f U_{j,\mu}\left(\sum_{\nu} P^{R}_{j+\mu,j-\nu}U_{j-\nu,\nu} - \sum_{\nu\neq\mu} P^{R}_{j+\mu,j+\nu}U^{\dagger}_{j,\nu}\right)\right]_{TA}$$

for even and odd sites, respectively. The first equation above is corrected for a mistake in ref. [15].
One then extracts the effective staples matrix

$$V''_{j,\mu} = V_{j,\mu} - \frac{3}{2\beta}N_f\left(\sum_{\nu} U_{j+\mu,\nu}P^{R}_{j+\mu+\nu,j} - \sum_{\nu\neq\mu} U^{\dagger}_{j+\mu-\nu,\nu}P^{R}_{j+\mu-\nu,j}\right)$$

$$V''_{j,\mu} = V_{j,\mu} - \frac{3}{2\beta}N_f\left(\sum_{\nu} P^{R}_{j+\mu,j-\nu}U_{j-\nu,\nu} - \sum_{\nu\neq\mu} P^{R}_{j+\mu,j+\nu}U^{\dagger}_{j,\nu}\right)$$

for even and odd sites, respectively.
For a given SU(N) gauge group the effective staples matrix is given by

$$V''_{j,\mu} = V_{j,\mu} - \frac{N}{2\beta}N_f\left(\sum_{\nu} U_{j+\mu,\nu}P^{R}_{j+\mu+\nu,j} - \sum_{\nu\neq\mu} U^{\dagger}_{j+\mu-\nu,\nu}P^{R}_{j+\mu-\nu,j}\right)$$

$$V''_{j,\mu} = V_{j,\mu} - \frac{N}{2\beta}N_f\left(\sum_{\nu} P^{R}_{j+\mu,j-\nu}U_{j-\nu,\nu} - \sum_{\nu\neq\mu} P^{R}_{j+\mu,j+\nu}U^{\dagger}_{j,\nu}\right)$$

for even and odd sites, respectively.
The different steps of the R algorithm are given by eqs. (48-54) in ref. [15] and an adaptation to the heat bath algorithm proceeds as follows

0-Generate two starting links configurations $\mathrm{U}^{(1)}$ and $\mathrm{U}^{(2)}$
1-Generate a vector of random complex numbers R living on all sites and distributed according to $e^{-R^\dagger R}$
2-Compute $\Phi = M^\dagger \left(U^{(1)}\right) R$ with Φ living on even sites
3-Solve $\left[M^\dagger \left(U^{(2)}\right) M \left(U^{(2)}\right)\right] X^R = \Phi$ for X^R
4-Compute $P^R_{i,j} = X^R_i X^{R*}_j$
5-Compute the effective staples matrix $\mathrm{V}''_{j,\mu}$
6-Copy the configuration $\mathrm{U}^{(2)}$ to $\mathrm{U}^{(1)}$
7-Update the configuration $\mathrm{U}^{(2)}$ by the heat bath algorithm
8-Go to 1

Instead of the algorithm above one may simply use an algorithm similar to the first algorithm with $\mathrm{V}'_{j,\mu}$ replaced by $\mathrm{V}''_{j,\mu}$.
The different algorithms above are simple: a code for the heat bath [6] or [7] can be easily upgraded to include pseudofermions. Also, they should run faster than the hybrid algorithm [15] since there is no H field and the update of the links U in [15] costs a non-negligible amount of CPU time. Moreover, in the ref. [10] it is concluded that for the local Wilson action in SU(2) the standard heat bath algorithm [6] may be generally superior to the microcanonical algorithm.

Conclusion.

A heat bath algorithm for lattice gauge theories with fermions is proposed. This algorithm is simple and easy to code and may be faster than the hybrid algorithm. Due to the lack of computing means it was not possible to compute some observables and then to make comparisons with other algorithms.

References.

[1] M. Creutz, L. Jacobs and C. Rebbi, Phys. Rep. 95 (1981) 201.
[2] C. Rebbi, Lattice gauge theories and Monte-Carlo simulations, World Scientific, Singapore (1983).
[3] M. Creutz, Quarks, gluons and lattices, Cambridge University Press, Cambridge (1983).
[4] J.B. Kogut, Rev. Mod. Phys. 55 (1983) 775.
[5] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.
[6] M. Creutz, Phys. Rev. D21 (1980) 2308.
[7] N. Cabbibo and E. Marinari, Phys. Lett. B119 (1982) 387.
[8] F. Fucito, E. Marinari, G. Parisi and C. Rebbi, Nucl. Phys. B180 (1981) 369.
[9] D.H. Weingarten and D.N. Petcher, Phys. Lett. B99 (1981) 333.
[10] D. Callaway and A. Rahman, Phys. Rev. D28 (1983) 1506.
[11] J. Polonyi and H.W. Wyld, Phys. Rev. Lett. 51 (1983) 2257.
[12] J. Polonyi, H.W. Wyld, J.B. Kogut, J. Shigemitsu and D.K. Sinclair, Phys. Rev. Lett. 53 (1984) 644.
[13] S. Duane, Nucl. Phys. B257 (1985) 652.
[14] S. Duane and J.B. Kogut, Nucl. Phys. B275 (1986) 398.
[15] S. Gottlieb, W. Liu, D. Toussaint, R.L. Renken and R.L. Sugar, Phys. Rev. D35 (1987) 2531.
[16] S. Duane, A.D. Kennedy, B.J. Pendleton and D. Roweth, Phys. Lett. B195 (1987) 216.
[17] G. Parisi and Y.-S. Wu, Sci. Sin. 24 (1981) 483.
[18] A. Guha and S.-C. Lee, Phys. Rev. D27 (1983) 2412.
M. Falcioni, E. Marinari, M.L. Paciello, G. Parisi, B. Taglienti and Y.-C. Zhang, Nucl. Phys. B215 (1983) 265.
I.T. Drummond, S. Duane and R.R. Horgan, Nucl. Phys. B220 (1983) 119.
M.B. Halpern, Nucl. Phys. B228 (1983) 173.
H.W. Hamber and U.M. Heller, Phys. Rev. D29 (1984) 928.
M. Falcioni, M.L. Paciello, G. Parisi and B. Taglienti, Nucl. Phys. B251 (1985) 624.
[19] A. Ukawa and M. Fukugita, Phys. Rev. Lett. 55 (1985) 1854.
[20] G.G. Batrouni, G.R. Katz, A.S. Kronfeld, G.P. Lepage, B. Svetitsky and K.G. Wilson, Phys. Rev. D32 (1985) 2736.