Generalized Hybrid Monte-Carlo

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Abstract

We propose a modification of the Hybrid Monte-Carlo method to sample equilibrium distributions of continuous field models. The method allows an efficient implementation of Fourier acceleration and is shown to reduce completely critical slowing down for the Gaussian model, i.e., \( z = 0 \).
The development of efficient numerical algorithms to study equilibrium properties of field-theoretical models near second order phase transitions is a very important subject in particle and statistical physics\[1, 2, 3, 4, 5\]. For that purpose, several methods such as Molecular Dynamics, Langevin and Monte–Carlo (MC) have been used. While the first two methods suffer from systematic step–size time discretization errors which may affect the computed mean values of observables, the only errors present in MC methods are of statistical origin and can be easily controlled, in principle, by varying the number of samplings. In practice, however, it turns out that for many problems of interest the number of configurations necessary to achieve a given small error is very large and grows as some power of the system size, thus requiring too much computer time.

In its simplest form, MC introduces a stochastic dynamics which involves the proposal of a random new local field configuration plus an acceptance/rejection step. This method can be inefficient to implement in some systems. The Hybrid Monte Carlo (HMC) algorithm first proposed by Duane et al. \[6\], uses Molecular Dynamics to propose new configurations then requiring a single acceptance/rejection step every time the whole system is updated, which is a substantial improvement over other MC methods. The usual implementation of HMC relies on an appropriate numerical integration of the corresponding Hamiltonian dynamics of the system.

In this paper, we present a generalization of HMC which is based upon the numerical integration of a non-hamiltonian dynamics which, however, conserves the energy of the system\[7\]. Our method turns out to be closely related to the use of a time-step matrix in a Langevin integration scheme \[8\] and thus can be regarded as an exact version of this method in the sense of not being affected by step-size errors. We first define our generalized algorithm showing that it obeys correctly the detailed balance condition. As an application, we study the Gaussian model. The simplicity of the model enables us to carry a systematic analytic study of correlation times. We also show that the optimal implementation of our method for the Gaussian model is actually a Fourier acceleration scheme which completely reduces critical slowing down (CSD).

CSD theory\[9\] tells us that near second–order phase transitions the correlation time, \(\tau_{\hat{O}}\), of a measured observable \(\hat{O}\), increases as \(\tau_{\hat{O}} \sim \xi^z\), being \(\xi\) the correlation length and \(z\) the dynamical critical exponent. \(\tau_{\hat{O}}\) can be defined as some measure of
the relaxation time of the correlation function of the observable $\hat{O}$:

$$
C_\hat{O}(t) = \frac{\langle \hat{O}(t)\hat{O}(0) \rangle - \langle \hat{O}(t) \rangle \langle \hat{O}(0) \rangle}{\langle \hat{O}^2(0) \rangle - \langle \hat{O}(0) \rangle^2}
$$

(1)

In a numerical simulation of a d–dimensional system the computer time, $T_\hat{O}$, required to measure the observable $\hat{O}$ at a given error behaves as $T_\hat{O} \equiv t_\hat{O} L^d \sim L^{d+c}(2\tau_\hat{O} + 1)$. The factor $L^d$ is always present as we simulate a system of size $N = L^d$ as a consequence of the increase of the number of degrees of freedom. The factor $L^c$, present in HMC, is a consequence of the fact that simulations at a constant correlation length at bigger sizes may require an additional computer effort in order to keep the acceptance probability within reasonable limits. The last factor $(2\tau_\hat{O} + 1)$ takes into account the number of effectively independent configurations produced by the algorithm. For finite systems close enough to the critical point, the correlation time $\tau_\hat{O}$ increases with system size as $\tau_\hat{O} \sim L^z$. For the local updating schemes such as heat-bath or Metropolis the exponent $z$ being near 2 strongly demands on computer time (although the above defined exponent $c$ is actually 0 for these algorithms). For spin models the collective updating scheme of Swendsen and Wang [10] has proven quite successful in reducing the dynamical critical exponent and overcoming CSD. For continuous models a Multigrid Monte-Carlo Method [11] was proposed which can also reduce CSD in certain cases. Also the time-step matrix Langevin method [8] can be helpful for some models if an appropriate matrix is chosen. The last two algorithms were shown to reduce the exponent $z$ for the Gaussian model but it is not clear if some reducing can be achieved in interacting models such as the $\phi^4$ model. The standard implementation of HMC was not observed to ameliorate CSD for the $\phi^4$ model [12] and for the Gaussian model it was shown [13] that the algorithm reduces $z = 1$ if an appropriate tuning of the trajectory length is taken. For an application of the standard HMC to study the two dimensional XY model see [14]. Yet another algorithm also used for simulation of these models is Overrelaxation (see [4] and references therein) which was also shown to produce $z = 1$ for the Gaussian model [15]. The modified HMC we propose allows to reduce $z = 0$ for the Gaussian model.

We now describe the generalized HMC algorithm. Let us consider a system $(\phi_1, \phi_2, \ldots, \phi_N) \equiv [\phi]$, of $N = L^d$ scalar variables, whose statistical equilibrium properties are defined through the Gibbs factor $\exp(-\mathcal{H})$, by its Hamiltonian $\mathcal{H}[\phi]$. The variables $[\phi]$ are considered to be generalized coordinates and a set of conjugate momenta $(p_1, p_2, \ldots, p_N) \equiv [p]$ associated with a kinetic energy $\mathcal{H}_K = \sum_{i=1}^N p_i^2 / 2$ is
introduced. The variable \( p_i \) can be in general a vector variable with \( D \) components, 
\[ p_i = (p_{i1}, p_{i2}, \ldots, p_{iD}) \]. The total Hamiltonian is \( \hat{H} = H + H_K \). We propose the following dynamics:

\[
\frac{d\phi_i}{dt} = \sum_{s=1}^{D} \sum_{j=1}^{N} (A^s)_{ij} p^s_j \\
\frac{dp^s_i}{dt} = \sum_{j=1}^{N} (A^s)_{ji} F_j, \quad s = 1, \ldots, D
\]

or, written in more compact vector notation:

\[
\frac{d\phi}{dt} = \sum_{s=1}^{D} A^s p^s \\
\frac{dp^s}{dt} = (A^s)^T F, \quad s = 1, \ldots, D
\]

where the \( A^s \) are some linear operators which can be represented as a matrix, and \( F_j \) represents the force as computed from the Hamiltonian \( -\frac{\partial}{\partial \phi_j} H \). The standard HMC substitutes the above dynamics by the Hamiltonian dynamics which can be obtained from the above set of equations by considering \( D = 1 \) and \( A \) equal to the identity operator.

It is an essential property that can be easily verified that the proposed dynamics in equations (3) exactly conserves energy, i.e., \( d\hat{H}/dt = 0 \). For the approximate integration of the previous equations of motion the “leap–frog” scheme can be used, introducing a discrete mapping \([\phi(t), p(t)] \rightarrow [\phi(t + \delta t), p(t + \delta t)] = G^{\delta t}([\phi(t), p(t)])\) of phase space, dependent on the time step \( \delta t \) chosen. The total energy, as a result of the time discretization used in the leap–frog scheme, is no longer conserved and its variation can be controlled by varying \( \delta t \). The leap-frog approximation reads:

\[
\phi' = \phi + \delta t \sum_{s=1}^{D} A^s p^s + \frac{(\delta t)^2}{2} \sum_{s=1}^{D} A^s (A^s)^T F([\phi]) \\
p'^s = p^s + \frac{\delta t}{2} (A^s)^T (F([\phi]) + F([\phi']))
\]

We define yet another mapping obtained from \( n \) iterations of the previous mapping, i.e. \( G = (G^{\delta t})^n \). The configuration obtained when one applies \( G \) is then accepted or rejected in such a way that detailed balance is verified in order to sample the canonical distribution for the Hamiltonian \( H \). As in the standard HMC the momenta variables are refreshed after every acceptance/rejection step according to the Gaussian distribution of independent variables \( \exp(-H_K) \). The evolution given by \( G \) \((n \text{ leap–frog steps})\)
steps) and the acceptance/rejection step constitute what is called 1 MC trial. Detailed balance is obeyed if one requires $G^{st}$ to be time reversible and area preserving and if one accepts the new configuration with probability $\min[1, \exp(-\Delta \hat{H})]$, where $\Delta \hat{H} = \hat{H}(G([\phi, p])) - \hat{H}([\phi, p])$. The time reversibility $G^{st}([\phi', -p']) = [\phi, -p]$ can be easily verified to be obeyed by equations (4). One can also proof that the area preserving property is verified by these equations. The above properties are satisfied for arbitrary matrices $A^s$ provided the associated mapping $G^{st}$ remains a one to one mapping in phase-space. We have defined a variety of HMC–type methods characterized by a particular choice of matrices $A^s$. One can then choose the matrices $A^s$ that better suit a particular problem. We have shown before how a particular version of the above generalized HMC can be used to simulate conserved order parameter systems[16].

We compare now our method with the one introduced in reference [8] based upon the numerical integration of a Langevin equation using a matrix time–step. This method is based upon the observation that the stationary probability distribution of the Langevin equation:

$$\frac{\partial \phi_i(\tau)}{\partial \tau} = -\frac{\delta \hat{H}}{\delta \phi_i} + \sqrt{2} \xi_i(\tau)$$

is precisely exp($-\hat{H}$). Here $\xi_i(\tau)$ are stochastic Gaussian random variables of mean zero and correlations $< \xi_i(\tau)\xi_j(\tau') > = \delta_{ij}\delta(\tau - \tau')$. The solution of the equation is approximated by:

$$\phi_i(\tau + \delta \tau) = \phi_i(\tau) + \sum_j \left[ -\delta \tau \epsilon_{ij} \frac{\delta \hat{H}}{\delta \phi_j} + \sqrt{2\delta \tau} \epsilon_{ij} \eta_j \right]$$

(6)

Where $\epsilon_{ij}$ is an arbitrary matrix and $\eta_j$ is a Gaussian variable of mean zero and correlations $< \eta_i \eta_j > = \delta_{ij}$. This corresponds exactly to the one step leap–frog approximation of the generalized HMC introduced above (equation (4) with $D = 1$) if we identify: $(\delta \tau)^2/2 = \delta \tau$ and $AA^T = \epsilon$. The main difference between the two methods is the presence of an acceptance/rejection step in the generalized HMC absent in the numerical integration of the Langevin equation. In that sense, we can say that the generalized HMC method introduced in this paper makes exact (in the sense that averages are not biased by the choice of the time step) the numerical integration of the Langevin equation using a matrix time step introduced in reference [8].

As an application we have considered the Gaussian model defined by the following Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \left[ \frac{\mu}{2} \dot{\phi}_i^2 + \frac{1}{2} | \nabla_L \phi_i |^2 \right]$$

(7)
index $i$ runs over the $N = L^2$ sites of a 2-dimensional square lattice, with periodic boundary conditions (a similar analysis can be carried out in any spatial dimension but we refer to the case $d=2$ for simplicity). $\nabla_L$ is the usual lattice discretized version of the gradient operator. This problem can be better analyzed in Fourier space. The total Hamiltonian $\hat{H}$ in terms of the Fourier transform of fields and momenta space is:

$$\hat{H} = \sum_{k=1}^{N} \left[ \frac{\omega_k^2}{2} |\hat{\phi}_k|^2 + \frac{1}{2} |\hat{p}_k|^2 \right]$$

where $\omega_k$ is given by $\omega_k^2 = \mu + 4(\sin^2(k_x/2) + \sin^2(k_y/2))$ and $\hat{\phi}_k$ and $\hat{p}_k$ stand for the fields and momenta variables in Fourier space. We choose the number of momenta variables associated to a given field equal to 1, $D = 1$. Suppose that we choose for the matrix $A_k$, generating the dynamics, a diagonal matrix in Fourier space. Then after $n$ leap-frog steps, equation (4) implies that:

$$\begin{bmatrix} \omega_k \hat{\phi}_k(n\delta t) \\ \hat{p}_k(n\delta t) \end{bmatrix} = M_k^n \begin{bmatrix} \omega_k \hat{\phi}_k(0) \\ \hat{p}_k(0) \end{bmatrix}$$

for $k = 1, \ldots, N$. Matrices $M_k^n$ are given by:

$$M_k^n = \begin{bmatrix} \cos(n\theta_k) & \sin(n\theta_k) / \cos(\theta_k/2) \\ -\cos(\theta_k/2) \sin(n\theta_k) & \cos(n\theta_k) \end{bmatrix}$$

where we have introduced $\theta_k = \cos^{-1}(1 - c_k^2/2)$ and $c_k = \hat{A}_k \omega_k \delta t$ and $\hat{A}_k$ denoting the diagonal elements of the matrix $A$ in Fourier space. In this model the different modes evolve independently of each other and the evolution equations are linear (this is similar to the standard HMC with $A = 1$). For the stability of the leap-frog integration, the eigenvalues of $M_k$ should lie on the unit circle of the complex plane which happens to be the case if $c_k$ is between 0 and 2.

By using the evolution equations together with the assumption that the field variables $\hat{\phi}_k(0)$ are in thermal equilibrium and, therefore, follow the distribution $\exp(-\hat{H})$, one can compute the equilibrium average discretization error as:

$$< \hat{H}(n\delta t) - \hat{H}(0) > \equiv < \Delta \hat{H} > = \sum_{k=1}^{N} \frac{c_k^4}{32 - 8c_k^2} \sin^2(n\theta_k)$$

In reference [17] it was shown that, to a good approximation, the average acceptance probability $< p_A >$ is related to the average discretization error $< \Delta \hat{H} >$ by:

$$< p_A > = \text{erfc}(\frac{1}{2}\sqrt{< \Delta \hat{H} >})$$
We now turn to the question of the optimal choice for the matrix \( \mathbf{A} \). From equation (9) it is immediately seen that if we choose the matrix \( \mathbf{A} \) such that \( \hat{A}_k = 1/\omega_k \) the iteration equations get independent of the mass \( \mu \) and all the modes are equally updated. This is, in effect, an exact implementation of the method of Fourier acceleration. This choice of the matrix clearly reduces completely CSD \( (z = 0) \) in the sense that correlation times are independent of the mass even when the mass goes to zero and the model becomes critical. The standard HMC corresponds here to the choice \( \hat{A}_k = 1 \), independent of \( k \) \[13\].

Let us compute the computational effort needed to achieve a given statistical error. In order to make further analytical calculations, it is convenient to introduce a set of random variables \( \sigma_m \) which take the value 1 or 0 if the configuration proposed after \( m \) MC trials has been accepted or not, respectively. Using this variable we can write an expression for the field variable after \( m \) MC trials, \( \hat{\phi}_k(m \, n\delta t) \), as
\[
\omega_k \hat{\phi}_k(m \, n\delta t) = \sigma_m \left[ \cos(n\theta_k) \omega_k \hat{\phi}_k((m-1) \, n\delta t) + \frac{\sin(n\theta_k)}{\cos(\theta_k/2)} \hat{p}_k((m-1) \, n\delta t) \right]
+ (1 - \sigma_m) \omega_k \hat{\phi}_k((m-1) \, n\delta t) \tag{13}
\]
The momenta \( \hat{p}_k(m \, n\delta t) \) are the independent random variables following a Gaussian distribution which are drawn after the \( m \)-th acceptance/rejection step. This equation can be iterated to obtain \( \hat{\phi}_k(m \, n\delta t) \) in terms of \( \hat{\phi}_k(0) \) and all the momenta generated during the evolution.

The variables \( \sigma_m \) are Bernoulli variables with probability of being equal to 1 equal to the acceptance probability, \( \min[1, \exp(-\Delta \hat{H}(m))] \). This probability depends on the total change in energy at the \( m \)-th MC trial, \( \Delta \hat{H}(m) \) which is a function of the initial field configuration and of the momenta generated at the \( j \)-th MC trial and variables \( \sigma_j \) such that \( j < m \). To proceed we make the approximation that the \( \sigma \) variables are all independently distributed variables with the probability of being equal to one equal to the average acceptance probability \( p = < p_A > \), given by \[12\]. This means that we consider the probability to accept or reject the whole configuration at a given step to be independent of the previous “time-history” of the system. The approximation is reasonably good as we will see later. Within this approximation, the correlation function for the magnetization is:
\[
\bar{C}_M(m) = C_M(m \, n\delta t) = \left[ 1 - 2p \sin^2\left(\frac{n\theta_0}{2}\right) \right]^m \tag{14}
\]
The obtained correlation function is exponential with a correlation time equal to \( \tau_M = -1/\log(|\bar{C}_M(1)|) \) in units of MC trials. The relaxation time of other modes is
obtained replacing in the previous equation $\theta_0$ by $\theta_k$. For the optimal matrix, $\theta_k \equiv \theta$ is independent of $k$ and so all the modes relax in the same way.

In figure 1 we compare $\bar{C}_M(1)$ given by the above correlation function for the magnetization with simulation results for the case $L = 32$ and $n = 4$ as a function of $\delta t$. The excellent agreement between the analytical expression and the simulation results shows that the previous approximation works extremely well for the calculation of the correlation function for the magnetization. The agreement between simulation and this approximation actually improves with increasing system size. We note the following features (see figure 1): the value of $\tau_M$ as a function of $\delta t$ for a given $n$ shows a minimum for small values of $\delta t$ and then $n - 1$ zeros for $n$ odd and $n$ zeros for $n$ even. This minimum disappears for $n$ larger than a given value. We discuss now how the parameters $n$ and $\delta t$ should be optimized in order to minimize the computer effort for the magnetization $t_M = (2\tau_M + 1)n$.

In principle, since there is always a value of $\delta t$ that yields $\tau_M = 0$ for $n = 2$, these are obviously the optimal choices. The corresponding computational effort $t_M = 2$ is independent of the system size corresponding to an exponent $c = 0$. However, a closer look shows that as the system size grows the precise $\delta t$ value at which the correlation time is zero is very difficult to locate in the sense that a slight error in the chosen value puts the system in a region of high (negative) correlations (see figure 1). Furthermore the corresponding correlation times of the energy would not be optimized, increasing enormously as the system size grows. This becomes apparent when one discusses the correlation function of the energy. The obtained approximation for the correlation function of the energy is:

$$\bar{C}_H(m) \equiv C_H(m \ n\delta t) = [1 - p\sin^2(n\theta)]m$$

The correlation time is $\tau_H = -1/\log(\bar{C}_H(1))$. In figure 2 we have compared $\bar{C}_H(1)$ given by the above correlation function to simulation results. The agreement here, although still reasonable, is not as good as it was in the case of the magnetization. However, one can still obtain precise quantitative conclusions from this figure. The value of $\bar{C}_H(1)$ has no zeros as a function of $\delta t$ for a given $n$, in contrast to what happens with $\bar{C}_M(1)$. It still shows, however, an absolute minimum at a given $\delta t$ which approaches zero as $n$ is increased. We have used this minimum in the correlation function of the energy as a function of $\delta t$ to find the optimal $n$ for a given system size that minimizes the computer effort $(2\tau_H + 1)n$. Although we have been unable to obtain an analytical expression for the optimal values for $n$ and $\delta t$, a numerical
study of equations (11), (12) and (15) allows us to conclude that the optimal value for \( n \) increases with system size as \( L^{1/2} \) whereas the optimal \( \delta t \) behaves as \( L^{-1/2} \). The obtained optimal values of \( n \) were such that \( \bar{C}_M(1) \) still has the local minimum as a function of \( \delta t \) mentioned above and which is near the absolute minimum of the energy. For large \( L \), the corresponding correlation times \( \tau_M \) and \( \tau_H \) turn out to be \( L \)-independent and are given by \( \tau_M = 2.5 \), \( \tau_H = 1.5 \) approximately. The optimal acceptance probability \( p \approx 0.67 \) and the product \( n \delta t \approx 1 \) are also independent of the system size.

In summary, the computational effort both for the magnetization and the energy behaves as \( t_M, t_H \sim L^{1/2} \), corresponding to an exponent \( c = 1/2 \). This can be understood in the following way: In order to keep the acceptance probability constant as we increase the system size, \( \delta t \) has to be varied as \( L^{-d/4} \). Thus one needs to increase \( n \) as \( L^{d/4} \) in order that the product \( n \delta t \) appearing on the correlation function remains also unchanged as the system size grows. The same picture was also seen to apply to a study of the \( \phi^4 \) model performed with the standard HMC method\[12\]. One should also note that an explicit implementation of the method of Fourier acceleration needs the calculation of Fourier transforms that involve an additional computer effort of order \( \log L \).

In conclusion, we have proposed a generalized version of HMC that is an exact implementation of time-step matrix Langevin methods. We have considered the Gaussian model as a test-case of the algorithm. The optimal matrix \( A \) is a diagonal matrix in Fourier space with diagonal elements \( \hat{A}_k = 1/\omega_k \) (Fourier acceleration). This matrix reduces completely CSD in the sense that the correlation times are mass independent, \( z = 0 \). We have proposed an approximation for the calculation of the correlation functions of energy and magnetization that improves as the system size gets larger. Using this approximation we have discussed the optimization of the parameters of the algorithm. The optimal computer effort grows as \( L^{d/4} \) due to the decrease of the acceptance probability with the system size and the need to keep the trajectory length, \( n \delta t \), constant at different system sizes.

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Figures Captions

Figure. 1.- Comparison of $\bar{C}_M(1)$ as obtained from our analytical approximation (continuous line) from equation (14), for a system of size $L = 32$ and $n = 4$ with simulation results (rhombi).

Figure. 2.- Comparison of $\bar{C}_H(1)$ (continuous line) from equation (15), with simulation results (rhombi) for the same system size and number of leap-frog steps used in figure 1.
