A backward Monte-Carlo method for solving parabolic partial differential equations

Johan Carlsson

Oak Ridge National Laboratory, P.O. Box 2009, Oak Ridge, TN 37831–8071, USA

Abstract

A new Monte-Carlo method for solving linear parabolic partial differential equations is presented. Since, in this new scheme, the particles are followed backward in time, it provides great flexibility in choosing critical points in phase-space at which to concentrate the launching of particles and thereby minimizing the statistical noise of the sought solution. The trajectory of a particle, $X_i(t)$, is given by the numerical solution to the stochastic differential equation naturally associated with the parabolic equation. The weight of a particle is given by the initial condition of the parabolic equation at the point $X_i(0)$. Another unique advantage of this new Monte-Carlo method is that it produces a smooth solution, i.e. without $\delta$-functions, by summing up the weights according to the Feynman-Kac formula.

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Key words: Linear parabolic partial differential equation; Feynman-Kac formula; Monte-Carlo method; Weighting

1 Introduction

The Monte-Carlo method was conceived at the Los Alamos National Laboratory during the Manhattan Project as a numerical method for solving the Boltzmann equation governing the neutron distribution function in fissile material [1]. Since then it has found numerous other uses across many fields of science. Overviews of its areas of applicability can be found in any of a number of textbooks, see e.g. Ref. [2]. In plasma physics the Monte-Carlo method has a long history of being used for solving the Fokker-Planck equation; see Ref. [3] for some of the earliest examples. It has two main advantages: it keeps small the incremental effort of solving a higher-dimensional problem,
and it makes easy satisfying boundary conditions. The Monte-Carlo method is typically worth consideration for three- or higher-dimensional problems, or already in two dimensions if there are internal boundary conditions imposed. The biggest disadvantage is the unavoidable statistical noise caused by the use of random numbers. This noise scales as the inverse square root of the number of particles followed (and hence the number of arithmetic operations and memory accesses required). The poor scaling is somewhat offset by the fact that the Monte-Carlo method “can be applied by many computers working in parallel and independently” as Metropolis and Ulam pointed out more than half a century ago [1]. In many cases, e.g. when a tail distribution forms, low-density regions of phase space are of particular interest. An example of such a case from plasma physics is when high-power radio waves are launched into the plasma and absorbed through resonance with the gyration of ions around magnetic field lines, resulting in the formation of a tail of high-energy ions. The Monte-Carlo method has been used on numerous occasions to solve the quasilinear Fokker-Planck equation, which models such wave absorption [4]. Due to the inverse-square-root scaling, the relative statistical error is worst in exactly these interesting low-density regions. Increasingly sophisticated weighting (i.e. splitting of particles), and reweighting, schemes [5] have been suggested to make the relative statistical error more constant throughout phase space.

The $\delta f$-method [6] also exists in a collisional version [7–9]. There seem to be two different schools of thought on how to include the collisions: by making the particle trajectories stochastic [7] or by letting the collisions enter the weight equation [8,9]. With the latter approach the spreading of the weight causes a gradual increase of the statistical error for a fixed number of particles. This makes simulations problematic on timescales longer than a few collision times. A potential cure for this particular ailment has recently been suggested [9]. Since the $\delta f$-method assumes that the solution is a weak perturbation of the equilibrium solution everywhere in phase space, it cannot be used when the distribution function develops a tail.

The new Monte-Carlo method presented here is firmly based on the well-established Feynman-Kac formula, which is briefly introduced in section 2. The Feynman-Kac formula puts the solution of a parabolic partial differential equation on the form of a conditional expectation value of a function of a stochastic variable. In section 3 it is shown how the numerical evaluation of this expectation value takes the form of a Monte-Carlo method stepping backward in time. Going backward in time allows us to choose the exact points in phase space, e.g. on an equidistant grid, at which we calculate the solution. It also allows us to redistribute the statistical noise to regions of phase space where it does the least harm. Finally, a comparison with the traditional Monte-Carlo method can be found in section 4.
2 The Feynman-Kac formula

There is an intimate connection between linear parabolic partial differential equations (PDEs) and stochastic differential equations (SDEs). Let us illustrate by using the regular diffusion equation as an example:

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial f}{\partial x}, \quad x \in \mathbb{R}, \quad 0 \leq t \leq T,$$

(1)

with some initial condition $f(x,0) = \Phi(x)$. Now, let the process $X(\tau)$ be governed by the SDE,

$$dX = \mu \, d\tau + \sigma \, dW,$$

(2)

where $W$ is a Wiener process, $\tau = T - t$, and we impose the initial condition $X(0) = x$. Using Itô’s formula [see Eq. (A.7) in appendix A] to differentiate $f(X(\tau), \tau)$, we get:

$$f(X(0), 0) = f(X(T), T) + \int_0^T \left\{ \frac{\partial f}{\partial \tau} + \mu \frac{\partial f}{\partial x} + \frac{\sigma^2}{2} \frac{\partial^2 f}{\partial x^2} \right\} \, d\tau + \int_0^T \sigma \frac{\partial f}{\partial x} \, dW.$$

(3)

(To make this article more self-contained a brief introduction to stochastic calculus and a mathematically somewhat questionable, but hopefully elucidating, derivation of Itô’s formula is presented in appendix A for those who are unfamiliar with the formalism). By defining,

$$\mu = \frac{\partial D}{\partial x}, \quad \sigma = \sqrt{2D},$$

(4)

we make Eq. (2) the naturally associated SDE of the linear parabolic PDE (1). Using the definition (4), Eq. (1), and the initial conditions $f(x,t=0) = \Phi(x)$ and $X(\tau=0) = x$, Eq. (3) becomes:

$$f(x,t=T) = \Phi(X(t=0)) + \int_0^T \sigma \frac{\partial f}{\partial x} \, dW.$$

Taking the expectation value of both sides we obtain:

$$f(x,t=T) = \mathbb{E}[ \Phi(X(t=0)) \mid X(t=T) = x ],$$

(5)

which is known as the stochastic Feynman-Kac representation of $f(x,T)$, or the Feynman-Kac formula for short. (See Ref. [10] for a thorough presentation of stochastic calculus and the Feynman-Kac formula).
3 Backward Monte-Carlo method

In general, the expectation value on the RHS of Eq. (5) must be calculated numerically. We first integrate the SDE (2):

\[
\int_{\tau}^{\tau + \Delta t} dX = \int_{\tau}^{\tau + \Delta t} \mu d\tau + \int_{\tau}^{\tau + \Delta t} \sigma dW \Rightarrow X(\tau + \Delta t) - X(\tau) = \mu [1 + \mathcal{O}(\sqrt{\Delta t})] \Delta t + \\
\sigma [1 + \mathcal{O}(\sqrt{\Delta t})] [W(\tau + \Delta t) - W(\tau)].
\]

The \( \mathcal{O}(\sqrt{\Delta t}) \) error terms come from the variation of \( \mu \) and \( \sigma \) during the time step \( \Delta t \). By the definition of a Wiener process (see appendix A), \( W(\tau + \Delta t) - W(\tau) \in \mathcal{N}(0, \sqrt{\Delta t}) \) and we can write:

\[
X(\tau + \Delta t) = X(\tau) + \mu \Delta t + \zeta \sigma \sqrt{\Delta t} + \mathcal{O}(\Delta t),
\]

where \( \zeta \) is a zero-mean, unit-variance Gaussian random number, \( \zeta \in \mathcal{N}(0, 1) \). The numerical approximation of the Feynman-Kac formula (5) is simply:

\[
f(x, t = T) = N^{-1} \sum_{i=1}^{N} \Phi(X_i(t=0)) + \mathcal{O}(\Delta t) + \mathcal{O}(N^{-1/2}),
\]

(6)

where \( \mathcal{O}(N^{-1/2}) \) is the statistical error and the stochastic variables \( X_i(t=0) \) are found by following the stochastic trajectories given by:

\[
X_i(t - \Delta t) = X_i(t) + \mu \Delta t + \zeta \sigma \sqrt{\Delta t}, \quad X_i(t = T) = x, \ i = 1, \ldots, N. \quad (7)
\]

A very simple algorithm, illustrated in Fig. 1, can now be used to solve Eq. (1). Assume that we want the solution at time \( t = T \) at the points \( x = x_j, \ j = 1, \ldots, n \). Then, for each \( j \), we simply launch \( N \) particles at \( x = x_j \) and let them evolve according to the backward Monte-Carlo equation of motion (7). As they reach \( t = 0 \), we sample \( \Phi(x) \) at their respective locations, \( X_i(t=0) \), and calculate the solution \( f(x = x_j, t = T) \) as the average of the sampled values, \( \Phi(X_i(t=0)) \), just as prescribed by Eq. (6).

Notice that the relative statistical error should be roughly constant if \( N \) is the same for every \( j \). Alternatively, as is indicated in Fig. 1, we can concentrate the launching of particles to exactly those points where a low-noise solution is desirable. In this sense, the backward Monte-Carlo method offers a perfect weighting scheme.
The backward Monte-Carlo method. The trajectories as given by the backward Monte-Carlo difference equation of motion (7).

The equivalents of Eqs. (6) and (7) when Eq. (1) is replaced by a more general linear parabolic PDE can be found in appendix B.

4 Discussion

The algorithm we arrived at in the previous section has a striking similarity to the conventional Monte-Carlo method, but there are also some fundamental differences. When comparing the conventional Monte-Carlo difference equation of motion:

\[ Y_i(t + \Delta t) = Y_i(t) + \mu \Delta t + \zeta \sigma \sqrt{\Delta t}, \quad i = 1, \ldots, N, \]

(8)

to Eq. (7), it is evident that they both describe identical trajectories, but for Eq. (7) these trajectories are traversed backward in time. Since we are dealing with parabolic equations, moving backward in time raises questions about time reversibility and the change of entropy. The form of the solution (6) also raises some suspicion; \( f \) on the left-hand side is a macroscopic quantity and so is \( \Phi \) on the right-hand side, whereas \( X_i(t = 0) \) is microscopic. In itself the backward Monte-Carlo difference equation of motion (7) is perfectly legitimate; at the microscopic level the motion is time-reversible since the entropy is undefined. The potential danger lies in macroscopic information spilling over into the microscopic world; i.e. if the particles carried any information about the solution with them going backward in time, then clearly the second law of thermodynamics would be violated. Fortunately, the form of Eq. (6) guarantees that this will not happen since the particle weight \( \Phi(X_i(t = 0)) \) is undefined until \( t = 0 \). Despite the superficial similarity between the Monte-Carlo difference equations of motion, (7) and (8), this is quite different from
a conventional, forward Monte-Carlo method where the particle weights are known at all times, $t \geq 0$.

Another difference between the backward and the forward Monte-Carlo method is the very different character of the solutions. With the forward Monte-Carlo method an obvious weighting scheme would be to use the same weights as in the backward method and launch the particles with $Y_i(t = 0)$ uniformly distributed over some sub-interval of $y$ (see Fig. 2). The solution then looks like

$$f(y, t = T) = N^{-1} \sum_{i=1}^{N} \Phi(Y_i(t = 0)) \delta(y - Y_i(t = T)).$$

Just to do something as simple as plotting the solution, the particles have to be distributed in bins to smooth out the jaggedness and the solution interpolated. This obviously means that a trade-off between resolution and noisiness is unavoidable. With the backward method, the solution [see Eq. (6)] is given as a numerical value at a point in phase space; it does not contain any $\delta$-functions. Points can be arbitrarily close together to give the desired resolution without increasing the noise (see Fig. 1). It is also worth noting that the backward method makes it trivial to calculate the solutions for a whole set of initial conditions, $f(x, t = 0) = \Phi_m(x)$, once the trajectories have been traced back to $t = 0$ and the $X_i(t = 0)$ are known. This makes the summing of samples $\Phi(X_i(t = 0))$ in Eq. (6) somewhat similar to the convolution of a Green function with $\Phi(x)$.

Fig. 2. Conventional, forward Monte-Carlo method with the same weights as the backward method. The trajectories as given by the forward Monte-Carlo difference equation of motion (8).
In the forward Monte-Carlo method, the drift $\mu$ and the diffusion function $\sigma$ are derived by taking moments of the single-particle distribution function [11], and the forward stochastic Monte-Carlo difference equation of motion (8) is normally seen as something rather artificial. From section 3 we see that in the backward Monte-Carlo method, the Monte-Carlo difference equation of motion (7) has a more natural interpretation as the numerical solution to the SDE (2) naturally associated with the parabolic equation (1) that we wish to solve.

Finally, since it has a tendency to appear in contexts similar to this, a very brief comment on the Langevin equation, and why its use is deprecated, is made in appendix C.

5 Summary

A backward Monte-Carlo method for solving parabolic differential equations has been introduced. As compared to the conventional, forward Monte-Carlo method, which is derived by taking moments of the single-particle distribution function, the improved method originates from quite a different starting point: the Feynman-Kac formula.

The stochastic Monte-Carlo difference equations of motion, including the drift $\mu$ and the diffusion function $\sigma$, are identical in the conventional and the new scheme, except for one vital difference: in the new scheme the particles are followed backward in time. The similarity should make it easy to retrofit the backward method to existing Monte-Carlo codes.

The solutions found with the forward Monte-Carlo method and the backward one, however, take completely different forms. In the backward scheme, the solution is smooth, unlike the jagged sum of $\delta$-functions associated with the forward Monte-Carlo method. By default, the backward method also yields a solution with a roughly constant relative statistical error throughout phase space. In addition, it offers great flexibility in redistributing the statistical noise to corners of phase space where it does minimal harm. This latter capability makes the backward method particularly well suited for cases where we are only interested in the solution in a small part of phase space.
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A Stochastic calculus and Itô’s formula

We start with the stochastic differential equation (2), repeated here for convenience:

\[ dX = \mu \, d\tau + \sigma \, dW, \tag{A.1} \]

where \( W \) is a Wiener process. Ordinary stochastic variables are just mappings from one probability space to another; stochastic processes are time dependent. A stochastic process \( W(\tau), \tau \geq 0 \) is a Wiener process if:

- \( W(0) = 0 \)
- the increment \( W(\tau + \Delta \tau) - W(\tau), \Delta \tau > 0 \), is independent of \( W(s), s \leq \tau \)
- \( W(\tau + \Delta \tau) - W(\tau) \in N\left(0, \sqrt{\Delta \tau}\right) \)
- \( W(\tau) \) has continuous trajectories

We will first derive a differential identity that will be needed later in this appendix. We first define \( \Delta \tau = \tau_{j+1} - \tau_j \) and \( \Delta W_j = W(\tau_{j+1}) - W(\tau_j) \) with \( \tau_j = j \tau/n, j = 0, 1, \ldots, n-1 \). We are now ready to introduce the stochastic variable \( S_n(\tau) \),

\[ S_n(\tau) = \sum_{j=0}^{n-1} (\Delta W_j)^2. \tag{A.2} \]

If \( dW/d\tau \) had existed, then clearly \( S_n(\tau) \) would tend to zero as \( n \) goes to infinity. But the derivative \( dW/d\tau \) is undefined everywhere, so we have to actually calculate the limit value. We take a congenially probabilistic approach...
to this task. The expectation value $E[S_n]$ is trivial:

$$
E[S_n] = \sum_{j=0}^{n-1} E[(\Delta W_j)^2] = \sum_{j=0}^{n-1} V[\Delta W_j] = \sum_{j=0}^{n-1} \Delta \tau_j = \sum_{j=0}^{n-1} (\tau/n) = \tau .
$$  \hspace{1cm} (A.3)

To establish that the expectation value (A.3) is really the sought limit of (A.2), we must show that the variance $V[S_n]$ goes to zero when $n$ goes to infinity. We will start by calculating $E[X^4], X \in N(0, \sigma)$,

$$
E[X^4] = (2\pi\sigma^2)^{-1/2} \int_{-\infty}^{\infty} x^4 e^{-x^2/2\sigma^2} dx \ldots
$$  \hspace{1cm} (A.4)

where (\ldots) is an integration by parts. With the help of the identity (A.4) we find

$$
V[S_n] = \sum_{j=0}^{n-1} V[(\Delta W_j)^2] = \sum_{j=0}^{n-1} \left( E[(\Delta W_j)^4] - E[(\Delta W_j)^2]^2 \right)
$$

$$
= 2 \sum_{j=0}^{n-1} V[(\Delta W_j)^2] = 2 \sum_{j=0}^{n-1} (\Delta \tau_j)^2 = 2 \sum_{j=0}^{n-1} (\tau/n)^2 = 2\tau^2/n .
$$  \hspace{1cm} (A.5)

Now, since $V[S_n] \to 0, n \to \infty$ and $E[S_n] \to \tau, n \to \infty$, we will be bold enough to draw the conclusion (inspired by the limit sum):

$$
\lim_{n \to \infty} S_n(\tau) = \lim_{n \to \infty} \sum_{j=0}^{n-1} (\Delta W_j)^2 = \tau \Rightarrow \int_{0}^{\tau} (dW)^2 = \int_{0}^{\tau} d\tau .
$$  \hspace{1cm} (A.6)

Now we are ready to calculate the differential $df(X(\tau), \tau)$ and start by Taylor expanding $f$ to second order:

$$
df = f_x dX + f_\tau d\tau + \frac{1}{2} f_{xx} (dX)^2 + \frac{1}{2} f_{\tau \tau} (d\tau)^2 + f_{x\tau} dX d\tau .
$$

Substituting Eq. (A.1) for $dX$ and letting the identity (A.6) justify the ordering $dW \gg d\tau = (dW)^2 \gg dW d\tau \gg (d\tau)^2$, we get

$$
df = \left\{ f_\tau + \mu f_x + \frac{1}{2} \sigma^2 f_{xx} \right\} d\tau + \sigma f_x dW ,
$$  \hspace{1cm} (A.7)

where only the two lowest orders ($dW$ and $d\tau$) have been kept. This is the sought Itô’s formula, which is more rigorously derived in Ref. [10].
B  General linear parabolic PDE

The backward Monte-Carlo method introduced in section 3 can be used to solve much more general linear parabolic PDEs than Eq. (1). In this appendix we will generalize Eqs. (6) and (7) to solve the following equation:

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial x} D^{k\ell} \frac{\partial f}{\partial x^k} + \lambda f + S, \quad x^k \in \mathbb{R}, \quad 0 \leq t \leq T, \quad (B.1)$$

with the initial condition $f(x^k, 0) = \Phi(x^k)$, and $D^{k\ell} = D^{k\ell}(x^k, t)$, $\lambda = \lambda(x^k, t)$, and $S = S(x^k, t)$. We will again try to find the Feynman-Kac representation of $f(x^k, t)$, and to do so we need the naturally associated SDEs. The matrix $D^{k\ell}$ is in general not diagonal. In other words, the diffusion processes along the different axes are in general correlated to some degree and the SDEs take the form:

$$dX^k = \mu^k d\tau + A^{k\ell} dW^\ell.$$ 

Itô’s formula is trivial to generalize to multiple dimensions, and applying it to $f$ we find the identities:

$$\mu^k = \frac{\partial D^{k\ell}}{\partial x^\ell},$$

and

$$A^{km} A^{\ell m} = 2D^{k\ell}. \quad (B.2)$$

Finding the Feynman-Kac representation of the solution to Eq. (B.1) is straightforward, with $\Lambda(t) = \exp[\int_0^t \lambda(X^k(s), s) ds]$ we get

$$f(x^k, T) = E \left[ \Lambda(T) \Phi(X^k(0)) + \int_0^T \Lambda(t) S(X^k(t), t) dt \right| X^k(T) = x^k],$$

with the numerical approximation

$$f(x^k, T) = N^{-1} \sum_{i=1}^N \left\{ \Lambda(T) \Phi(X_i^k(0)) + \int_0^T \Lambda(t) S(X_i^k(t), t) dt \right\}, \quad (B.3)$$

where

$$X_i^k(t - \Delta t) = X_i^k(t) + \mu^k \Delta t + \zeta^\ell A^{k\ell} \sqrt{\Delta t}, \quad X_i^k(T) = x^k, \quad i = 1, \ldots, N. \quad (B.4)$$

Here, $\zeta^\ell$ are uncorrelated, zero-mean, unit-variance Gaussian random numbers, $\zeta^\ell \in N(0, 1)$, and the matrix elements $A^{k\ell}$ solve the system of algebraic Eqs. (B.2).
C Langevin equation

A literature review on Monte-Carlo methods for solving parabolic equations is impossible without occasionally coming across the Langevin equation [12,13]:

\[
\frac{dv}{dt} = -\beta v + A(t).
\]  

(C.1)

Here \( v \) is the velocity of a particle, and \( A(t) \) is a “fluctuating” acceleration. The Langevin equation was historically used to model Brownian motion [14].

The following assumptions are being made about the “fluctuating” term \( A(t) \):

- \( A(t) \) is independent of \( v \).
- \( A(t) \) varies extremely rapidly compared to the variations of \( v \).

It should come as no surprise that the second assumption is problematic. To quote Chandrasekhar [13]: “But we should draw attention even at this stage to the very drastic nature of assumptions implicit in the very writing of an equation of the form (C.1). For we have in reality supposed that we can divide the phenomenon into two parts, one in which the discontinuity of the events taking place is essential while in the other it is trivial and can be ignored”.

Since the theory of stochastic calculus [10] is on considerably firmer mathematical footing, the SDE (2) should be allowed to supersede the Langevin equation.
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