

New Physical Principle for Monte-Carlo simulations

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Abstract: New physical principle for Monte-Carlo simulations has been introduced. It is based upon *coupling* of dynamical equations and the corresponding Liouville equation. The proposed approach does not require a random number generator since randomness is generated by instability of dynamics triggered and controlled by the feedback from the Liouville equation. Direct simulation of evolutionary partial differential equations have been proposed, discussed, and illustrated.

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1. Introduction

Monte-Carlo is one of the most powerful computational tools for solving high-dimensional problems in physics, chemistry, economics, and information processing. It is especially effective for problems in which the computational complexity grows exponentially with the dimensionality (PDE, NP-complete problems). The main advantage of the Monte-Carlo simulations over other computational techniques is independence of the computational resources upon the problem dimensionality. There are many modifications of this method such as "classical" Monte Carlo, (samples are drawn from a probability distribution), "quantum" Monte Carlo, (random walks are used to compute quantum-mechanical energies and wavefunctions), "path-integral" quantum Monte Carlo, (quantum statistical mechanical integrals are computed to obtain thermodynamic properties), "simulation" Monte Carlo, (stochastic algorithms are used to generate initial conditions for quasiclassical trajectory simulations), etc. However, success of this approach depends upon effi-

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cient implementations of multi-dimensional stochastic processes with prescribed density distribution, and that necessitates a fast and effective way to generate random numbers uniformly distributed on the interval $[0,1]$. It should be noticed that often-used computer-generated numbers are not really random, since computers are deterministic. In particular, if a random number seed is used more than once, one will get identical random numbers every time. Therefore, for multiple trials, different random number seeds must be applied. The proposed modification of the Monte-Carlo method is free of such limitation since it is based upon randomness that is generated by instability of dynamics triggered and controlled by the feedback from the Liouville equation. The approach is motivated by the mathematical formalism of coupled Liouville-Langevin equations being applied to modeling active systems,[1], as well as by the Madelung version of quantum mechanics, [2]. Our strategy exploits different feedbacks from the Liouville equation to the corresponding dynamical ODE. These feedbacks may be different from those used for modeling active or quantum systems and their choice is based upon computational efficiency rather than upon a physical meaning of the underlying models.

2. Destabilizing Liouville Feedback

For mathematical clarity, we will start here with a one-dimensional motion of a unit mass under action of a force f depending upon the velocity x and time t

$$\dot{x} = f(x, t), \quad (1)$$

If initial conditions are not deterministic, and their probability density is given in the form

$$\rho_0 = \rho_0(X), \quad \text{where } \rho \geq 0, \quad \text{and} \quad \int_{-\infty}^{\infty} \rho dX = 1 \quad (2)$$

while ρ is a single-valued function, then the evolution of this density is expressed by the corresponding Liouville equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial X}(\rho f) = 0 \quad (3)$$

The solution of this equation subject to initial conditions and normalization constraints (2) determines probability density as a function of X and t

$$\rho = \rho(X, t) \quad (4)$$

Let us now specify the force f as a feedback from the Liouville equation

$$f(x, t) = \varphi[\rho(x, t)] \quad (5)$$

and analyze the motion after substituting the force (5) in to Eq.(1)

$$\dot{x} = \varphi[\rho(x, t)], \quad (6)$$

This is a fundamental step in our approach. Although theory of ODE does not impose any restrictions upon the force as a function of space coordinates, the Newtonian physics does: equations of motion are never coupled with the corresponding Liouville equation. Moreover, as shown in [3], such a coupling leads to non-Newtonian properties of the underlying model. Indeed, substituting the force f from Eq. (5) into Eq. (3), one arrives at the *nonlinear* equation for evolution of the probability density

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial X} \{ \rho \varphi[\rho(X, t)] \} = 0 \quad (7)$$

Regardless of a physical meaning of the underlying model, we will exploit the mathematical property of this equation for simulation of a prescribed probability density.

Now we will demonstrate the destabilizing effect of the feedback (6). For that purpose, it should be noted that the derivative $\partial \rho / \partial x$ must change its sign, at least once, within the interval $-\infty < x < \infty$, in order to satisfy the normalization constraint (2). But since

$$\text{Sign} \frac{\partial \dot{x}}{\partial x} = \text{Sign} \frac{d\varphi}{d\rho} \text{Sign} \frac{\partial \rho}{\partial x} \quad (8)$$

there will be regions of x where the motion is unstable, and this instability generates randomness with the probability distribution guided by the Liouville equation (7).

3. Simulation of Stochastic Processes with Prescribed Probability Distributions

Most of the Monte-Carlo simulations require generation of stochastic processes having prescribed probability density distribution. In this section we propose to generate such processes using controlled instability of the ODE driven by a feedback from the corresponding Liouville equation.

Let us consider Eqs. (1) and (7) defining f as the following function of probability density

$$f = \frac{1}{\rho(x, t)} \int_{-\infty}^x [\rho(\zeta, t) - \rho^*(\zeta)] d\zeta \quad (9)$$

Then these equations take the form, respectively

$$\dot{x} = \frac{1}{\rho(x, t)} \int_{-\infty}^x [\rho(\zeta, t) - \rho^*(\zeta)] d\zeta \quad (10)$$

$$\frac{d\rho}{dt} + \rho(t) - \rho^* = 0 \quad (11)$$

The last equation has the analytical solution

$$\rho = (\rho_0 - \rho^*) e^{-t} + \rho^* \quad (12)$$

Subject to the initial condition

$$\rho(t = 0) = \rho_0 \quad (13)$$

this solution converges to a prescribed stationary distribution $\rho^*(x)$.

Substituting the solution (12) in to Eq. (10), one arrives at the ODE that simulates the stochastic process with the probability distribution (12),

$$\dot{x} = \frac{e^{-t}}{[\rho_0(x) - \rho^*(x)]e^{-t} + \rho^*(x)} \int_{-\infty}^x [\rho_0(\zeta) - \rho^*(\zeta)]^d \zeta \quad (14)$$

As notices above, the randomness of the solution to Eq. (14) is caused by instability that is controlled by the corresponding Liouville equation. It should be emphasized that in order to run the stochastic process started with the initial distribution ρ_0 and approaching a stationary process with the distribution ρ^* , one should substitute into Eq. (14) *analytical expressions* for these functions.

It is reasonable to assume that the solution (12) starts with sharp initial condition

$$\rho_0(X) = \delta(X) \quad (15)$$

As a result of that assumption, all the randomness is supposed to be generated *only* by the controlled instability of Eq. (14). Substitution of Eq. (15) in Eq. (14) leads to two different domains, [4]

$$\int_{-\infty}^x \rho^*(\zeta) d\zeta = \frac{C_1}{e^{-t} - 1}, \quad x \neq 0 \quad (16)$$

$$x \equiv 0 \quad (17)$$

Eq. (17) represents a singular solution, while Eq. (16) is a regular solution that includes arbitrary constant C_1 . The regular solution is unstable at $t=0$, $|x| \rightarrow 0$ where the Lipschitz condition is violated

$$\frac{d\dot{x}}{dx} \rightarrow \infty \quad \text{at} \quad t \rightarrow 0, \quad |x| \rightarrow 0 \quad (18)$$

and therefore, an initial error always grows generating *randomness*. This type of non-Lipschitz instability has been introduced and analyzed in [3]. The solutions (15) and (16) describe an irreversible motion: it is characterized by the “beginning of time” where all the trajectories intersect (that results from the violation of Lipschitz condition at $t = 0$, while the backward motion obtained by replacement of t with $(-t)$ leads to imaginary values of velocities. As follows from Eq. (14),

$$\dot{x} \rightarrow 0 \quad \text{at} \quad t \rightarrow \infty \quad \text{for} \quad -\infty < x < \infty \quad (19)$$

If Eq. (14) is run for fixed initial conditions, i.e. for fixed values of the arbitrary constant C_1 , the solution (16) produces a sample of the corresponding stochastic process. If the same equation (14) is run at different values of C_1 , the solution produces the whole

ensemble characterizing the underlying stochastic process. Due to the condition (19), eventually the process becomes stationary as it prescribed by the solution of Eq. (12).

The approach is generalized to n-dimensional case simply by replacing x with a vector

$$x = x_1, x_2, \dots, x_n \quad (20)$$

Application of the results described in this section to finding global maximum of an integrable (but not necessarily differentiable) function has been introduced in [2].

Remark 1. It has been assumed that both probability distributions, ρ^* and ρ_0 satisfy the normalization constraints

$$\int_{-\infty}^{\infty} \rho^*(X) dX = 1, \quad \int_{-\infty}^{\infty} \rho_0(X) dX = 1 \quad (21)$$

Then, integrating Eq. (11) over X , with reference to Eqs. (19), one obtains

$$\frac{d}{dt} \int_{-\infty}^{\infty} \rho(X) dX = 0, \quad (22)$$

Therefore, if the probability distribution satisfies the normalization constraint at $t = 0$, it will satisfy the same constraint for $t > 0$.

Remark 2. In order to control the speed of convergence to the stationary distribution, one can modify Eq. (9) by introducing a control parameter a

$$f = \frac{a}{\rho(X, t)} \int_{-\infty}^x [\rho(\zeta, t) - \rho^*(\zeta)] d\zeta \quad (23)$$

4. Example

Turning to the solution (16), let us choose the final distributions ρ^* as following

$$\rho^*(X) = \frac{1}{\sqrt{2\pi}} e^{-\frac{X^2}{2}} \quad (24)$$

Substituting the expressions (21) into Eq. (16) at $X = x$, one obtains

$$x = \operatorname{erf}^{-1}\left(\frac{C_1}{e^{-t} - 1} - 1\right) \quad (25)$$

5. Direct Simulation of Parabolic PDE

Computational complexity of deterministic numerical methods for solving PDE grows exponentially with the growth of the problem dimensionality, and that make such problems intractable. On the other hand, the Monte-Carlo methods, which are based upon simulation of a random walk, are free of this major limitation. However, simulating of a

random work with prescribed probability distribution has its own limitations. (Actually, the approach proposed above can be applied for that purpose). In this section we will demonstrate direct simulations of the solutions to parabolic PDE using a feedback from the Liouville equation. The main idea of the proposed approach is to consider a given parabolic PDE (to be solved) as a Liouville equation for some dynamical system described by random ODE, and thereby, to replace solution of PDE by a system of random ODE. The first candidate for the demonstration of the proposed approach is a multi-dimensional Fokker-Planck equation. The computational complexity of integrating this equation is on the order of $(1/\varepsilon)^\ell$ — that is, the reciprocal of the error threshold raised to a power equal to the number of variables that is exponential in ℓ . In contradistinction to that, the resources for simulations by Monte-Carlo (MC) method is on the order of $(1/\varepsilon^2)$, i.e., they do not depend upon the dimensionality of the problem.

There is another advantage of MC-simulations of the Fokker-Planck equation: suppose that we are interested in behavior of the solution in a local region of the variables $\{x\}$; then, in case of computing, one has to find the global solution first, and only after that the local solution can be extracted, while the last procedure requires some additional integrations in order to enforce the normalization constraints. On the other hand, in case of MC simulations, one can project all the simulations onto a desired sub-space $j_\alpha \otimes j_\beta$ of the total space $j_1 \otimes \dots \otimes j_\ell$ and directly obtain the local solution just disregarding the rest of the space.

All these advantages of MC method are preserved in the proposed approach that is based upon *new physical principle* of generating randomness.

For the purpose of mathematical clarity, we will start with a simplest case of the one-dimensional Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \sigma^2 \frac{\partial^2 \rho}{\partial X^2} \quad (26)$$

The solution of Eq. (26) subject to the sharp initial condition is

$$\rho = \frac{1}{2\sigma\sqrt{\pi t}} \exp\left(-\frac{X^2}{4\sigma^2 t}\right) \quad (27)$$

Let us now find a dynamical equation for which Eq. (26) plays the role of the corresponding Liouville equation. It can be verified that such an equation is the following

$$\dot{x} = -\sigma^2 \frac{\partial}{\partial X} \ln \rho, \quad (28)$$

Substituting the solution into Eq. (28) at $X = x$ one arrives at the differential equation with respect to $x(t)$

$$\dot{x} = \frac{x}{2t} \quad (29)$$

and therefore,

$$x = C\sqrt{t} \quad (30)$$

where C is an arbitrary constant. Since $x = 0$ at $t = 0$ for any value of C , the solution (30) is consistent with the sharp initial condition for the solution (27) of the corresponding

Liouville equation (26). As the solution (15) and (16), the solution (30) describes the simplest irreversible motion: it is characterized by the “beginning of time” where all the trajectories intersect (that results from the violation of Lipschitz condition at $t = 0$, Fig. 1), while the backward motion obtained by replacement of t with $(-t)$ leads to imaginary values of velocities. One can notice that the probability density (27) possesses the same properties.

For a fixed C , the solution (29) is *unstable* since

$$\frac{d\dot{x}}{dx} = \frac{1}{2t} > 0 \quad (31)$$

and therefore, an initial error always grows generating *randomness*, (compare to Eq.(25)). Initially, at $t = 0$, this growth is of infinite rate since the Lipschitz condition at this point is violated

$$\frac{d\dot{x}}{dx} \rightarrow \infty \quad \text{at} \quad t \rightarrow 0 \quad (32)$$

Considering first Eq. (30) at fixed C as a sample of the underlying stochastic process (28), and then varying C , one arrives at the whole ensemble characterizing that process, (see Fig. 1). One can verify that, as follows from Eq. (27), the expectation and the variance of this process are, respectively

$$Mx = 0, \quad Dx = 2\sigma^2 t \quad (33)$$

The same results follow from the ensemble (30) at $-\infty \leq C \leq \infty$. Indeed, the first equality in (33) results from symmetry of the ensemble with respect to $x = 0$; the second one follows from the fact that

$$Dx \propto x^2 \propto t$$

It is interesting to notice that the stochastic process (30) is an alternative to the following Langevin equation, [5]

$$\dot{x} = \Gamma(t), \quad M\Gamma = 0, \quad D\Gamma = \sigma \quad (34)$$

that corresponds to the *same* Fokker-Planck equation (26).

Here $\Gamma(t)$ is the Langevin (random) force with zero mean and constant variance σ . Thus, the solution to Eq. (28) has a well-organized *structure*: as follows from Eq. (30) (Fig 1), the initial “explosion” of instability driven by the violation of the Lipschitz condition at $t = 0$ distributes the motion over the family of *smooth* trajectories with the probability expressed by Eq. (27). *Therefore, the solution (27) can be reconstructed from the solution (30) by taking cross-section over the ensemble at fixed t , and then computing the probability density for each t .* It should be emphasized that in this particular case, we have already known the solution (see Eq. (27)), and this solution was used to obtain the solution (30) in the analytical form. However, in the next example we will show that actually we need to know only the initial value of the solution (27).

Let us turn now to the Fokker-Planck equation with a variable diffusion coefficient

$$\frac{\partial \rho}{\partial t} + \frac{\partial^2}{\partial X^2} [a(X)\rho] = 0 \quad (35)$$

to be solved subject to the following initial conditions

$$\rho(t = 0) = \rho_*(X) \quad (36)$$

First of all, we have to find such an ODE for which Eq. (35) plays the role of the corresponding Liouville equation. Although such an ODE is not unique, we will select the simplest one

$$\dot{x} = \frac{1}{\rho} \frac{\partial}{\partial x} [a(x)\rho(x)] \quad (37)$$

Substituting the initial value of the probability density (36) into Eq. (37), one finds an approximate solution to Eq. (37) within a small initial time interval Δt

$$x = x_0 + \frac{1}{\rho_*(x_0)} \left\{ \frac{\partial}{\partial x} [a(x)\rho_*(x)] \Big|_{x=x_0} \right\} t, \quad 0 < t < \Delta t \quad (38)$$

where x_0 is the initial value of x .

Varying this value as $-\infty < x_0 < \infty$, one obtains the whole ensemble of solutions during the initial time interval Δt . Then computing the probability density $\rho_{**}(x_1)$ at $t = \Delta t$ one arrives at the next approximation cycle that starts with the “initial” density $\rho_{**}(x_1)$, where

$$x_1 = x_0 + \frac{1}{\rho_*(x_0)} \left\{ \frac{\partial}{\partial x} [a(x)\rho_*(x)] \Big|_{x=x_0} \right\} \Delta t \quad (39)$$

etc. It should be emphasized that the solution is obtained *without* exploiting the original PDE (35). Nothing would change in the proposed methodology if

$$a = a(x, t, \rho, \frac{\partial \rho}{\partial x} \dots) \quad (40)$$

This would include a nonlinear version of the Fokker-Planck equation, the Burgers equation, the Korteweg-de-Vries equation, etc. A generalization to multi-dimensional case

$$\frac{\partial \rho}{\partial t} + \nabla \bullet [\nabla(a\rho)] = 0, \quad a = a(\{X\}, t, \rho, \dots) \quad (41)$$

where $\{X\} = X_1, X_2, \dots, X_n$ is n-dimensional vector, would require a system of n ODE to replace Eq. (37)

$$\{\dot{x}\} = \frac{1}{\rho} \nabla(a\rho), \quad a = a(\{x\}, t, \rho, \dots) \quad (42)$$

For this system, Eq.(41) plays the role of the Liouville equation, and the proposed methodology described above can be applied without significant modification.

Remark 3. It should be noticed that as in other modifications of the MC simulations, the normalization constraints imposed upon the probability density are implemented “automatically”, and this is another significant advantage of simulations over computations. However, if the variable of a PDE to be solved is not a probability density, the normalization constraint can be applicable only in special cases of mass or heat conservation, while in case of sinks or sources this constraint has to be modified.

6. Direct Simulation of Hyperbolic PDE

Let us modify Eq. (44) as following

$$\dot{x} = -\frac{1}{\rho} \frac{\partial(\sigma^2\psi)}{\partial x}, \quad \sigma = \sigma(x), \quad \dot{\psi} = \rho \quad (43)$$

Then the corresponding Liouville equation is

$$\frac{\partial\rho}{\partial t} = \frac{\partial^2}{\partial X^2}(\sigma^2\psi) \quad (44)$$

or, after differentiation with respect to time,

$$\frac{\partial^2\rho}{\partial t^2} = \frac{\partial^2}{\partial X^2}(\sigma^2\rho) \quad (45)$$

This is a hyperbolic equation describing elastic waves in strings, as well as longitudinal waves in bars, and its solution is simulated by the dynamical system (43). A generalization to multi-dimensional case is straightforward

$$\frac{\partial^2\rho}{\partial t^2} = \nabla^2(\sigma^2\rho), \quad \sigma = \sigma(\{X\}) \quad (46)$$

where $\{X\} = X_1, X_2, \dots, X_n$ is n-dimensional vector, would require a system of n ODE to replace Eq. (43)

$$\{\dot{x}\} = \frac{1}{\rho} \nabla(\sigma^2\psi), \quad \dot{\psi} = \rho \quad (47)$$

The waves with dispersion that is represented by the Klein-Gordon equation of quantum theory

$$\frac{\partial^2\rho}{\partial t^2} = \frac{\partial}{\partial X}(\sigma^2 \frac{\partial\rho}{\partial X}) - \beta^2\rho \quad (48)$$

are simulated by the following dynamical system

$$\dot{x} = -\frac{\sigma^2}{\rho} \frac{\partial\psi}{\partial x} + \frac{\beta^2}{\rho} \int_{-\infty}^x \rho dx, \quad \sigma = \sigma(x), \quad \dot{\psi} = \rho, \quad \beta = const \quad (49)$$

The same approach can be applied to non-hyperbolic wave equations. For instance, the equation for flexural vibration of a beam

$$\frac{\partial^2\rho}{\partial t^2} = -\gamma^2 \frac{\partial^4\rho}{\partial X^4} \quad (50)$$

is simulated by the dynamical system

$$\dot{x} = -\frac{\gamma^2}{\rho} \frac{\partial^3\psi}{\partial x^3}, \quad \dot{\psi} = \rho \quad (51)$$

However, the simulation strategy of these wave equations is different from the parabolic PDE described above since solutions of the hyperbolic equations do not have transitions

from a delta-function to distributed functions as the parabolic equations do. Therefore, such a transition should be introduced prior to simulation. We will illustrate the proposed strategy based upon Eqs.(43) and (44). Suppose that

$$\rho(t = 0) = \rho_0(x), \quad \psi(t = 0) = \psi_0(x) \quad (52)$$

and introduce an auxiliary dynamical system of the type (10)

$$\dot{x} = \frac{1}{\rho(x, t)} \int_{-\infty}^x [\rho(\zeta, t) - \rho^*(\zeta)] d\zeta, \quad \rho^*(x) = \frac{1}{\rho_0} \frac{d\psi_0}{dx} \quad (53)$$

that has the corresponding Liouville equation of the type (11)

$$\frac{\partial \rho}{\partial t} + \rho(t) - \rho^* = 0 \quad (54)$$

The simulation starts with the system (53) which approaches the stationary distribution of the probability $\rho^*(X)$ after the time period (see Eq. (17))

$$\tau \approx \ln \frac{1 - \rho^*}{\varepsilon \rho^*} \quad (55)$$

Using this solution as random initial conditions for Eqs.(43), one can start the simulation of Eqs. (43).

7. Direct Simulation of Elliptic PDE

Elliptic equations describe stationary processes, and in many cases they can be considered as a limit of the solutions of the corresponding parabolic equations. We will demonstrate the proposed strategy of the simulations using the solution of the Laplace equation

$$\nabla^2 \rho = 0 \quad (56)$$

as a limit of the solution to the corresponding Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \sigma^2 \nabla^2 \rho \quad \text{at } t \rightarrow \infty \quad (57)$$

taking advantage of the fact that the solution to Eq. (57) always tends to a stationary limit regardless of boundary conditions imposed upon the solution, [5].

Therefore, the dynamical system simulating the Laplace equation (56) can be presented as following

$$\{\dot{x}\} = \frac{1}{\rho} \nabla(\sigma^2 \rho), \quad \sigma = \sigma(\{x\}, t, \rho, \dots), \quad t \rightarrow \infty \quad (58)$$

The speed of convergence of the simulations (58) to a stationary solution can be control by a choice of the factor σ .

Conclusion

New physical principle for Monte-Carlo simulations has been introduced. It is based upon *coupling* of dynamical equations and the corresponding Liouville equation. The proposed approach does not require a random number generator since randomness is generated by instability of dynamics triggered and controlled by the feedback from the Liouville equation. Simulations of random processes with prescribed probability density as well as direct simulation of evolutionary partial differential equations have been proposed, discussed, and illustrated.

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