Pure Monte Carlo Method: a Third Way for Plasma Simulation

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We bring a totally new concept for plasma simulation, other than the conventional two ways: Fluid/Kinetic Continuum (FKC) method and Particle-in-Cell (PIC) method. This method is based on Pure Monte Carlo (PMC), but far beyond traditional treatments. PMC solves all the equations (kinetic, fluid, field) and treats all the procedures (collisions, others) in the system via MC method. As shown in two paradigms, many advantages have been found. It has shown the capability to be the third importance approach for plasma simulation or even completely substitute the other two in the future. It’s also suitable for many unsolved problems, then bring plasma simulation to a new era.

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Introduction—The original of Monte Carlo (MC) method for computations can back to hundreds of years ago, e.g., the Buffon’s needle experiment. With the emergence of the modern computer in 1940s and pioneer works by John von Neumann, Stanislaw Ulam and Nicholas Metropolis, this method brings amounts of practical applications. The famous and classical [Metropolis1953] paper is said mainly contributed by the hero of plasma physics, M. N. Rosenbluth. However, up to now, MC for physics is mainly on statistical physics, and only in merely special cases for plasma physics.

Some people had known that, in fact, the PIC method can be seen a type of MC method. [1] provides a unified MC interpretation of particle simulations, which then treat a fluid edge pedestal transport model and the kinetic 1D electrostatic problem as paradigms.

PMC Method—In plasma simulation, MC has been used to many complex procedures, such as collisions and impurities transport, which has been widely known. So, here, we need not talk too much about that, and all the old MC methods in plasma simulation can be inherited by PMC method naturally. The new steps of PMC are to tell how we solve the fluid and field equations.

Using MC to solve PDEs can back to two pivotal papers, [3] and [4], the former uses probabilistic interpretations for linear elliptic and parabolic equations, the latter gives MC methods for solving integro-differential equations occur in various branches of the natural sciences.

Feynman-Kac formula—Many types of plasma equations (e.g., transport equations, Vlasov equation) have the form:

\[
\frac{\partial f}{\partial t} + \mu(x,t)\frac{\partial f}{\partial x} - \frac{\sigma^2}{2} \frac{\partial^2 f}{\partial x^2} - V(x,t)f + p(x,t) = 0.
\]

Feynman-Kac formula [5] [9] tells us, Eq. (1) is equivalent to SDE when \( V, p = 0 \) (\( V, p \neq 0 \) case can also find),

\[
dX = \mu(X, t)dt + \sigma(X, t)dW_t,
\]

where \( W_t \) is Wiener process (Brownian motion), which is described by normal (Gaussian) distribution. Eqs. (1) and (2) are easily general to high dimensions or more variables, e.g., \( (x, v, t) \). The above descriptions are also shown by Itô’s lemma [8], a classical work in SDE.

Now, we solve the convection-diffusion equation as example to show how to use this formula, which is standard steps and well known by SDE people but may not familiar by plasma community. At this case, \( a = \mu \) and \( D = \sigma^2/2 \), are constants. For \( f(x, 0) = f_0(x) \), we start with a set \( N \) samples \( \xi^1, \cdots, \xi^N \) from \( f_0(x) \). A sample for every next step is

\[
\xi_i^{t+dt} = \xi_i^t + adt + \sqrt{2Ddt}\eta_i, \quad i = 1, \cdots, N.
\]

where \( \eta_i \) is normal distribution with zero mean and unit variance. For \( a = 0 \), we get pure diffusion, and for \( D = \)}
0, pure convection. In fact, integral form explicit exact solution is

\[ f(x, t) = \int G_t(x - y)f_0(y - at)dy = G_t \ast f_0(x - at), \]

(4)

\[ G_t(x - y) = \frac{1}{(4\pi Dt)^{1/2}}e^{-\frac{(x-y)^2}{4Dt}}. \]

If we use MC to integral (4) directly, and use \( N \) samples for particles and \( M \) points in space, the total cost will be \( O(N^3 \times M) \). While using (3), the total cost is \( O(N) \). We write (4) here for benchmark.

Using (3), a result is show in FIG.1. We can see that the MC result reproduces the exact solution very well, when we using larger \( N \) and \( M \), the result can be even better. Here, \( M \) is not for calculation but just for reconstructing the grids for \( f \).

FIG. 1: (Color online) Solve convection-diffusion equation using (3), as example to show PMC method.

The above is a summary of SDE for our usage, which is a key fundament of our PMC method, the applications to plasma examples will be shown at below.

Poisson equation—We may meet Poisson equation frequently in plasma physics, for example, in the electrostatic kinetic case or the electromagnetic gyrokinetic case. The equation is as the form

\[ \nabla^2 \phi(x) = -\rho(x), \ x \in D. \]

(5)

If \( \rho = 0 \), gives Laplace equation, which can be found solved by MC in many places, e.g., [12]. A good introduction of MC methods for Poisson equation can find in [3]. The method can also take from an extended Feynman-Kac formula. For Dirichlet boundary, \( \phi(x) = f(x), x \in \partial D \). Standard solution for position \( x_0 \) using SDE notation is

\[ \phi(x_0) = \frac{1}{2}E \left[ \int_0^{\tau_{OD}} \rho(W_t) \ dt \right] + E \left[ f(W_{\tau_{OD}}) \right], \]

(6)

where, \( \tau_{OD} = \inf \{ t : W_t \in \partial D \} \) is the first-passage time and \( W_{\tau_{OD}} \) is the first-passage location on the boundary, \( E \) is average. Using floating random walk, the results for 2D are show in FIG.2. The MC method here has another advantage that we can obtain the solution at a few points directly instead of calculating the whole range, and even if there are steep gradients or irregular boundary. Some updates of MC for Poisson equation may also find in recent literatures, such as for Neumann boundary, improving efficiencies, or reducing errors.

Other equations—There are many other types of PDEs in plasma physics. Scalar conservation law equation \( \partial u/\partial t + \partial F(u)/\partial x = 0 \), e.g., Burgers’ equation, can find be solved generally in [9]. Navier-Stokes (vector) equation for turbulence can find in [2]. For ODE, we often need just the standard MC integral. Some more MC methods and details for electromagnetic problems are introduced in [16]. One can also refer [11] for some general descriptions.

The types of equations mentioned at above have contented many of the main plasma physics equations.

Application Paradigms—We use the above methods to solve two practical plasma problems.

Simple fluid edge pedestal transport model—The simplest model for calculating pedestal width can find in [18] or [20], the inner range of SOL (Scrape-Off Layer, for divertor or limiter) is mainly slowly perpendicular transport, and the outer range is mainly fast parallel (to the magnetic field line, mainly on toroidal \( \varphi \) direction) transport and the particles travel at most \( L \) \( (2\pi R \) or \( 2\pi qR) \) then hit the target with the thermal velocity, where \( R \) is the major radius, \( q \) is edge safety factor, and the thermal velocity is equal to acoustic velocity \( c_s \) at edge from sheath calculations.

We can write the inner range transport equation as

\[ \frac{\partial n}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r D \frac{\partial n}{\partial r} \right) + S(n, r, t) = \frac{D}{r} \frac{\partial n}{\partial r} + D \frac{\partial^2 n}{\partial r^2} + S. \]

(7)

For simplification, we only use the density diffusion equation and treat the coefficient \( D \) as constant, and also ignore the source term \( S \). For outer range, we find quickly that we cannot easily write a 1D equation combine to the inner range equation. Even though we write down the outer range equation, we will quickly meet the singularity problem at the last closed (magnetic) flux surface.
A special treatment for transport barriers can be found in [19], which rewrites the transport equations to new form. However, using PMC, we can avoid the above problems automatically.

The inner equation (7) can be solved using (2). The outer range needs an extra MC treatment: if a particle comes out to the outer range, we use the same equation as the inner range for perpendicular transport but in the same time let it vanish random in time $[0, T]$ if it is still in the outer range, with $T = L/c_s$.

Quickly, we can find when using (3) to treat (7), the drift velocity $a = -D/r \to \infty$ for the MC particles at $r = 0$. This problem is also met similarly in PIC when using polar coordinate, also in large scale PIC simulation as in GTC [13]. The conventional method to treat this problem is making a hollow and ignoring a small $r \to 0$ region. While, one can find in [16] other ways of MC implement transport equations and treat the $r \to 0$ problem (e.g., L’Hospital’s rule $\lim_{r \to 0} \rho f/\rho \sigma = \partial^2 f/\partial r^2$), which means that this won’t be a severe problem in PMC.

However, in fact, we will find MC can be a natural method to solve this geometry and complex boundary problems. The only reason why people using different coordinates is that we can use the symmetry of the system to make us treat (e.g., analytical calculations) or understand problem easier. People care but the great nature never cares the coordinates. The physics law won’t change in any coordinates. So, we can rewrite (7) from $(r, \theta)$ coordinate to Cartesian coordinate $(x, y)$ and use $\sqrt{x^2 + y^2} = r = r_b$ as boundary. MC is suitable for any complex boundaries, and the circle boundary is just one of them. Then, in use of PMC, people can use Cartesian coordinate always (in fact, as the circle symmetry case in FIG 2 we have already given an example), which will simplify many old complex coordinates (notable: the magnetic surface coordinate) or boundaries problems a lot. A 2D implement of PMC for this edge pedestal transport model is shown in FIG 3. In tokamak experiment, one can see lots of figures as FIG 3, i.e., the above simple model can model the experiment at least qualitatively.

**Kinetic 1D electrostatic (ES1D) problem**—For ES1D, the system is described by kinetic equation

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{qE}{m} \frac{\partial f}{\partial v} = C(f).$$

where, $q$ is the charge, $m$ is mass, $E = -\nabla \phi$ is the electrical field, $C(f)$ is collision term. The field equation is [3], with $\rho = \int (f_i - f_e) dv$ the charge density. All the variables has normalized in units of $e\phi/T_e, \omega_{pe}^{-1}, \lambda_{De}$. For 1D, (8) can rewrite to a more simple ODE form

$$dE/dx = \rho.$$  

Firstly, we can easily find [3] has the form of (1), gives

$$dx_i = v_i dt, \quad dv_i = (qE/m) dt,$$

which is totally the same as in PIC. Eq. (9) tells us that more dimensions won’t bring significant new time cost (note: higher dimensions we may need more particles for accuracy, which will bring some new time cost), while [3] will if we use DD. If the collision term has the form $C(f) = \alpha f + \beta \partial f/\partial v + \gamma \partial^2 f/\partial v^2$, the kinetic equation is still nothing else but [3]. We see here, for PIC simulation of collision, we need an extra MC step, while in PMC method, we can write this step to equation of motion [3] directly.

Here, we assume ions immobile for simplify and treat the collisionless (Vlasov) case, i.e., $C(f) = 0$, because that which is easy for benchmark.

For $f(x, v, t)$, $x$ and $v$ can be anywhere. For $E(x)$ or $\phi(x)$, the $x$ can also be anywhere. But, [3] and [9] are coupled. We should find out a way to connect the position $x$ and $E$. A naturally thought is calculating the $E(x)$ directly using MC for every $f$-particle one by one, but which is too much time consumed, especially when $f$-particles ($N_f$) and $\phi$-particles ($N_\phi$) are very large. An adjust way is using grids and then interpolating, which can reduce the time cost by an order of $O(N_\phi)$. We find this is just what PIC does, i.e., we re-deduce all the key steps of PIC method by PMC! The interpolating method is easy and has checked by PIC, however, one may also find other ways to implement this PMC step if can make sure they work.

Using ODE (9) as field equation, for MC, which is just an integral from one side to another side, and we use random particles to do this, the errors of each step will cancel and average is zero. While, for DD (e.g., Euler, Runge-Kutta or else), the integral is summation and errors will accumulate. Using Poisson equation, the MC method is provided at before, an extra step is needed to calculate $E$ from $\phi$ by calculating gradient from the MC $\phi$-particles. Periodic boundary for the MC particles of $f$ is easy to implement, which is the same as PIC. We comment here, for $\phi$, the periodic boundary means $\phi(0) = \phi(L)$, but when we see $E$, which is not $E(0) = E(L)$ but average $<E(x)> = 0$ ([3] has known this). In fact, this implies
TABLE I: Comparison of FKC, PIC and PMC for kinetic plasma simulation.

|          | FKC                  | PIC                  | PMC                  |
|----------|----------------------|----------------------|----------------------|
| Approach | Continuum            | Particle + continuum | Only particle        |
| Equations| Only PDEs            | New method for eqn.  | Eqn. of motion brown from PIC, |
|          |                      | of motion,          | New method for field equation |
| Good     | Accurate             | Field eqn. brown     |                      |
|          |                      | from FKC             |                      |
| Bad      | Numerical unstability and dissipation | Noise | Crude, with error ∝ 1/√N |
| Philosophy| More mathematical | Half math, half first principle | More first principle |

that, we have added two charged slabs (not real ‘particles’, because this is 1D, or called ‘markers’ in PIC) at the boundary to cancel the extra E field! Few ES1D PIC researchers have seen this. Thinking in PMC way will bring us many new insights or re-thoughts.

For this ES1D problem, we can find, the conventional PIC treatment and new PMC treatment can be very similar. The implements can be close, but the concepts are totally different. PIC is fixed and nonadjustable. PMC provides more possibilities and can bring us new ways.

Using PMC to solving [8] and [9], a result is show in FIG. 4. Note that, due to noises, the phase space plotting will change for both PIC and PMC, even though under the same parameters (e.g., keep source code unchanged), especially in nonlinear stages. The above figure is a select from typical runs. The main feature of phase space holes is clearly in both PMC and PIC results. PMC is slightly slower than PIC in this case.

Summary and Comments—The above two paradigms have shown many new advantages. In fact, PMC is more powerful when problems are complicated. For example, many large scaled codes are possible be completely rewritten via this new method, an example is BOUT [21], gyrofluid. For large scaled gyro-kinetic, this method is also possible. Some complicated paradigms are beyond this short letter.

A comparison of FKC, PIC and PMC is listed in TABLE. [1] which can also shows that why we can call PMC be a third method for plasma simulation.

At present, many tools of PMC are brown from other fields. But the concept change is the key important thing. The unified viewpoint by combining everything in one provides us a totally new picture. In this new angle, we can see difficult old problems naturally and problems become simple. We can not only do new problems but also provide new insights or more efficient methods for old problems. For kinetic problems, PMC can be seen as advanced PIC; for fluid problems and complex procedures, PMC is new. Whatever, people may just concern that if an approach is useful and works well. PMC matches this. PMC is not a single fixed approach as PIC, but a combine of varies of old and new MC methods, flexible.

As far as the author (HSX) knows, Max-Planck-Institut für Plasmaphysik is developing MC methods for Stellarator edge transport physics, while it seems [17] has already or almost implemented a fully PMC ES2D code though they didn’t know this concept when they did that. New applications for resistive MHD tearing mode, Hasegawa-Mima equation, Grad-Shafranov equation and many other problems are on the way by the author or others. This letter has given/built the framework of PMC, which is enough for many practical applications. But, there may are still many new intelligent works need do for some special types of cases. Some unexpected problems may also meet when using to more complicated examples. The author does not know that yet. If also implemented well for the above untested several examples, this new approach is possible completely substitute the conventional two methods, FKC and PIC, and also suitable for solving many old unsolved or hard to solve problems, then bring plasma simulation to a new era.

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