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# Princeton Plasma Physics Laboratory

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# Canonical symplectic particle-in-cell method for long-term large-scale simulations of the Vlasov-Maxwell system

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## Abstract

Particle-in-Cell (PIC) simulation is the most important numerical tool in plasma physics and accelerator physics. However, its long-term accuracy has not been established. To overcome this difficulty, we developed a canonical symplectic PIC method for the Vlasov-Maxwell system by discretizing the Marsden-Weinstein bracket. A fast local algorithm to solve the symplectic implicit time advance is discovered without root researching or global matrix inversion, enabling applications of the proposed method to very large-scale plasma simulations with many, e.g.,  $10^9$ , degrees of freedom.

In modern plasma physics and accelerator physics, numerically solving the Vlasov-Maxwell (VM) equations using the Particle-In-Cell (PIC) method has become the most important tool [1, 2] for theoretical studies in the last half century. Many innovative algorithms, such as the Boris scheme for advancing particles [3, 4] and Villasenor-Buneman's charge-conserving deposition scheme [5], have been developed and successfully applied. Recently, new geometric numerical methodology has been adopted for PIC simulations. This exciting trend begins with the discovery of symplectic algorithms for Hamiltonian equations that govern charged particle dynamics [6–17]. The Boris algorithm was discovered to be volume-preserving [18, 19] and high-order volume-preserving methods have been found [20]. In addition, the Vlasov-Maxwell system [21–24] and the Vlasov-Poisson system [25] have been discretized from a variational symplectic perspective that preserves symplectic structures and exhibits excellent long-term accuracy and fidelity.

In this letter, we develop a new canonical symplectic PIC method for solving the VM equations by discretizing the canonical Marsden-Weinstein bracket for the VM equations [26]. The distribution function  $f$  is first discretized in phase space through the Klimontovich representation by a finite number of Lagrangian sampling points  $(\mathbf{X}_i, \mathbf{P}_i)$  ( $i = 1, \dots, N$ ), where  $\mathbf{X}_i$  and  $\mathbf{P}_i$  are the position and canonical momentum of the  $i$ -th particle, and  $N$  is the total number of sampling points. The electromagnetic field is discretized point-wise on a given spatial grid, and the Hamiltonian functional is expressed as a function of the sampling points and the discretized electromagnetic field. This procedure generates a finite-dimensional Hamiltonian system with a canonical symplectic structure. The number of degrees of freedom of the discrete system is  $D = 3N + 3M$ , where  $M$  denotes the total number of the discrete grid-points.

In general, for a Hamiltonian function whose momentum dependence and position dependence are not separable, it is not possible to make symplectic integration algorithms explicit [9, 15]. For the discrete Hamiltonian system developed here for the VM equations, the dimension of system is usually very large, and root searching algorithms required by implicit methods are too time-consuming to be practical. However, we discovered that if the symplectic Euler algorithm [9] is applied to the discrete VM Hamiltonian system at hand, the implicit time advance can be carried out as inexpensively as an explicit method by just inverting a  $3 \times 3$  matrix for every particle separately. The resulting canonical symplectic PIC method for the VM system inherits all the good numerical features of canonical symplec-

tic algorithms, such as the long-term bound on energy-momentum error. Being symplectic means that the numerical solution satisfies  $D(2D - 1)$  constraints as the exact solution does. Since  $D$  is a large number, the symplectic condition is much stronger than a few constraints on global energy and momentum. The symplectic condition is almost as strong as imposing local conservation everywhere in phase space.

As an example of applications, the nonlinear Landau damping is simulated. The discrete VM Hamiltonian system for this study has more than  $2.69 \times 10^8$  degrees of freedom. The damping rate from the numerical results agrees exactly with the theoretical result. The long-term simulation reveals that the phase mixing dynamics in velocity space is the physical mechanism of the nonlinear Landau damping, as recently proved by Mouhot and Villani [27, 28] for the Vlasov-Poisson system and conjectured by Villani [29] for the Vlasov-Maxwell system. It is the long-term accuracy and fidelity of the canonical symplectic PIC algorithm that enables us to numerically confirm Mouhot and Villani's theory and conjecture over several orders of magnitude.

We start from the canonical Marsden-Weinstein bracket and Hamiltonian for the Vlasov-Maxwell equations [26],

$$\{F, G\} \equiv \int f \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}_{\mathbf{x}\mathbf{p}} d\mathbf{x}d\mathbf{p} + \int \left( \frac{\delta F}{\delta \mathbf{A}} \frac{\delta G}{\delta \mathbf{Y}} - \frac{\delta G}{\delta \mathbf{A}} \frac{\delta F}{\delta \mathbf{Y}} \right) d\mathbf{x}. \quad (1)$$

$$H(f, \mathbf{A}, \mathbf{Y}) = \frac{1}{2} \int (\mathbf{p} - \mathbf{A})^2 f d\mathbf{x}d\mathbf{p} + \frac{1}{2} \int [\mathbf{Y}^2 + (\nabla \times \mathbf{A})^2] d\mathbf{x}. \quad (2)$$

Here,  $F$ ,  $G$ , and the Hamiltonian  $H$  are functionals of the distribution function  $f$ , vector potential  $\mathbf{A}$ , and  $\mathbf{Y} \equiv \partial \mathbf{A} / \partial t$ . The bracket  $\{h, g\}_{\mathbf{x}\mathbf{p}}$  inside the first term on the right hand side of Eq. (1) is the canonical Poisson bracket for functions  $h$  and  $g$  of canonical phase space  $(\mathbf{x}, \mathbf{p})$ . The temporal gauge, i.e.,  $\phi = 0$ , has been explicitly chosen for this Poisson bracket to be valid. The Poisson bracket defined in Eq. (1) can be formally derived from the point of view of co-adjoint orbit theory [26], and can be used to derive the non-canonical Morrison-Marsden-Weinstein bracket in the  $(f, \mathbf{E}, \mathbf{B})$  and  $(\mathbf{x}, \mathbf{v})$  coordinates [26, 30, 31]. First, we discretize the distribution function using the Klimontovich representation

$$f(\mathbf{x}, \mathbf{p}, t) = \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{X}_i) \delta(\mathbf{p} - \mathbf{P}_i), \quad (3)$$

where  $(\mathbf{X}_i, \mathbf{P}_i)$  ( $i = 1, \dots, N$ ) are particles' coordinates in phase space. Under this discretiza-

tion, it can be shown that

$$\frac{\delta F}{\delta \mathbf{X}_i} = \int \delta(\mathbf{x} - \mathbf{X}_i) \delta(\mathbf{p} - \mathbf{P}_i) \frac{\partial}{\partial \mathbf{x}} \left( \frac{\delta F}{\delta f} \right) d\mathbf{x} d\mathbf{p}, \quad (4)$$

$$\frac{\delta F}{\delta \mathbf{P}_i} = \int \delta(\mathbf{x} - \mathbf{X}_i) \delta(\mathbf{p} - \mathbf{P}_i) \frac{\partial}{\partial \mathbf{p}} \left( \frac{\delta F}{\delta f} \right) d\mathbf{x} d\mathbf{p}, \quad (5)$$

from which we obtain

$$\frac{\delta F}{\delta \mathbf{X}_i} \frac{\delta G}{\delta \mathbf{P}_i} - \frac{\delta G}{\delta \mathbf{X}_i} \frac{\delta F}{\delta \mathbf{P}_i} = \int \delta(\mathbf{x} - \mathbf{X}_i) \delta(\mathbf{p} - \mathbf{P}_i) \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}_{\mathbf{x}\mathbf{p}} d\mathbf{x} d\mathbf{p}. \quad (6)$$

It then follows that the first term on the right-hand side of Eq. (1) is

$$\int f \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}_{\mathbf{x}\mathbf{p}} d\mathbf{x} d\mathbf{p} = \sum_{i=1}^N \left( \frac{\delta F}{\delta \mathbf{X}_i} \frac{\delta G}{\delta \mathbf{P}_i} - \frac{\delta G}{\delta \mathbf{X}_i} \frac{\delta F}{\delta \mathbf{P}_i} \right). \quad (7)$$

The second term on the right-hand side of Eq. (1) can be discretized point-wise on a Eulerian spatial grid as

$$\int \left( \frac{\delta F}{\delta \mathbf{A}} \frac{\delta G}{\delta \mathbf{Y}} - \frac{\delta G}{\delta \mathbf{A}} \frac{\delta F}{\delta \mathbf{Y}} \right) d\mathbf{x} = \sum_{J=1}^M \left( \frac{\partial F}{\partial \mathbf{A}_J} \frac{\partial G}{\partial \mathbf{Y}_J} - \frac{\partial G}{\partial \mathbf{A}_J} \frac{\partial F}{\partial \mathbf{Y}_J} \right) \frac{1}{\Delta V}, \quad (8)$$

where the discrete fields  $\mathbf{A}_J(t)$  and  $\mathbf{Y}_J(t)$  are the fields evaluated on the grid-point  $\mathbf{x}_J$ , and the subscript  $J$  is the index of the grid-point, and  $M$  is the total number of the grid-points. The volume of each cell  $\Delta V$ , which is taken to be a constant in the present study. Finally, the discrete Poisson Bracket for the VM system is

$$\{F, G\}_d = \sum_{i=1}^N \left( \frac{\partial F}{\partial \mathbf{X}_i} \cdot \frac{\partial G}{\partial \mathbf{P}_i} - \frac{\partial G}{\partial \mathbf{X}_i} \cdot \frac{\partial F}{\partial \mathbf{P}_i} \right) + \sum_{J=1}^M \left( \frac{\partial F}{\partial \mathbf{A}_J} \cdot \frac{\partial G}{\partial \mathbf{Y}_J} - \frac{\partial G}{\partial \mathbf{A}_J} \cdot \frac{\partial F}{\partial \mathbf{Y}_J} \right) \frac{1}{\Delta V}, \quad (9)$$

for functions  $F$  and  $G$  of the particles  $(\mathbf{X}_i, \mathbf{P}_i)$  and the discretized field  $(\mathbf{A}_J, \mathbf{Y}_J)$ .

Next, we need to express the Hamiltonian functional in terms of  $(\mathbf{X}_i, \mathbf{P}_i)$  and  $(\mathbf{A}_J, \mathbf{Y}_J)$ . The particles' total kinetic energy is the sum of each particle's kinetic energy. The vector potential at a particle's position can be interpolated from  $\mathbf{A}_J(t)$  as

$$\mathbf{A}(\mathbf{X}_j, t) = \sum_{J=1}^M \mathbf{A}_J(t) W(\mathbf{X}_j - \mathbf{x}_J), \quad (10)$$

where  $W(\mathbf{X}_j - \mathbf{x}_J)$  is a chosen interpolation function. The Hamiltonian then becomes

$$\begin{aligned} \tilde{H}(\mathbf{X}_i, \mathbf{P}_i, \mathbf{A}_J, \mathbf{Y}_J) = & \frac{1}{2} \sum_{i=1}^N \left( \mathbf{P}_i^2 - 2\mathbf{P}_i \cdot \sum_{J=1}^M \mathbf{A}_J W(\mathbf{X}_i - \mathbf{x}_J) \right. \\ & \left. \sum_{J,L=1}^M \mathbf{A}_J \cdot \mathbf{A}_L W(\mathbf{X}_i - \mathbf{x}_J) W(\mathbf{X}_i - \mathbf{x}_L) \right) + \frac{1}{2} \sum_{J=1}^M \left[ \mathbf{Y}_J^2 + (\nabla_d \times \mathbf{A})_J^2 \right] \Delta V \quad (11) \end{aligned}$$

where  $(\nabla_d \times \mathbf{A})_J$  is the discrete curl operator acting on the discrete vector potential evaluated at the  $J$ -th grid-point. Finally, the discrete Hamiltonian (11) and discrete Poisson structure (9) form a canonical symplectic discretization of the original continuous Vlasov-Maxwell system. The ordinary differential equations for the canonical system are

$$\dot{\mathbf{X}}_i = \{\mathbf{X}_i, \tilde{H}\}_d = \mathbf{P}_i - \sum_{J=1}^M \mathbf{A}_J W(\mathbf{X}_i - \mathbf{x}_J), \quad (12)$$

$$\dot{\mathbf{A}}_J = \{\mathbf{A}_J, \tilde{H}\}_d = Y_J, \quad (13)$$

$$\dot{\mathbf{P}}_i = \{\mathbf{P}_i, \tilde{H}\}_d = \sum_{J=1}^M (\mathbf{P}_i \cdot \mathbf{A}_J) \nabla W(\mathbf{X}_i - \mathbf{x}_J) - \sum_{J,L=1}^M (\mathbf{A}_J \cdot \mathbf{A}_L) W(\mathbf{X}_i - \mathbf{x}_J) \nabla W(\mathbf{X}_i - \mathbf{x}_L), \quad (14)$$

$$\begin{aligned} \dot{\mathbf{Y}}_J = \{\mathbf{Y}_J, \tilde{H}\}_d &= \sum_{i=1}^N \mathbf{P}_i W(\mathbf{X}_i - \mathbf{x}_J) \frac{1}{\Delta V} - \sum_{i=1}^N \sum_{L=1}^M \mathbf{A}_L W(\mathbf{X}_i - \mathbf{x}_J) W(\mathbf{X}_i - \mathbf{x}_L) \frac{1}{\Delta V} \\ &\quad - (\nabla_d \times \nabla_d \times \mathbf{A})_J. \end{aligned} \quad (15)$$

This equation system consists of  $6(M+N)$  equations describing the dynamics of  $N$  particles and fields on  $M$  discrete grid-points. In Eq. (15), we have used the fact that for well-chosen spatial grids, such as Yee's grid [32],

$$(\nabla_d \times \nabla_d \times \mathbf{A})_J = \frac{\partial}{\partial A_J} \frac{1}{2} \sum_{L=1}^M (\nabla_d \times \mathbf{A})_L^2. \quad (16)$$

It is clear from Eqs. (12)-(15) that the particles and fields interact through the interpolation function  $W(\mathbf{X}_i - \mathbf{x}_J)$ . The function  $W(\mathbf{X}_i - \mathbf{x}_L)/\Delta V$  distributes particles' charge over the grid-points as if they are "charged clouds" with finite-size [1].

Once the canonical symplectic structure is given, canonical symplectic algorithms can be readily constructed using well-developed methods [6–14]. For a reason soon to be clear, we adopt the semi-explicit symplectic Euler method for time advance. The symplectic Euler method for a generic canonical Hamiltonian system is

$$p^{n+1} = p^n - \Delta t \frac{\partial H}{\partial q}(p^{n+1}, q^n), \quad (17)$$

$$q^{n+1} = q^n + \Delta t \frac{\partial H}{\partial p}(p^{n+1}, q^n). \quad (18)$$

where  $\Delta t$  is the time-step, and the superscript  $n$  in  $p^n$  and  $q^n$  denotes that they are the value at the  $n$ -th time step. It is implicit for  $p$ , but explicit for  $q$ . Making use of this algorithm, the iteration rules for Eqs. (12) -(15) are

$$\frac{\mathbf{X}_i^{n+1} - \mathbf{X}_i^n}{\Delta t} = \mathbf{P}_i^{n+1} - \sum_{J=1}^M \mathbf{A}_J^n W(\mathbf{X}_i^n - \mathbf{x}_J), \quad (19)$$

$$\frac{\mathbf{A}_J^{n+1} - \mathbf{A}_J^n}{\Delta t} = \mathbf{Y}_J^{n+1}, \quad (20)$$

$$\frac{\mathbf{P}_i^{n+1} - \mathbf{P}_i^n}{\Delta t} = \sum_{J=1}^M (\mathbf{P}_i^{n+1} \cdot \mathbf{A}_J^n) \nabla W(\mathbf{X}_i^n - \mathbf{x}_J) - \sum_{J,L=1}^M (\mathbf{A}_J^n \cdot \mathbf{A}_L^n) W(\mathbf{X}_i^n - \mathbf{x}_J) \nabla W(\mathbf{X}_i^n - \mathbf{x}_L), \quad (21)$$

$$\begin{aligned} \frac{\mathbf{Y}_J^{n+1} - \mathbf{Y}_J^n}{\Delta t} = & \sum_{i=1}^N \mathbf{P}_i^{n+1} W(\mathbf{X}_i^n - \mathbf{x}_J) \frac{1}{\Delta V} - \sum_{i=1}^N \sum_{L=1}^M \mathbf{A}_L^n W(\mathbf{X}_i^n - \mathbf{x}_J) W(\mathbf{X}_i^n - \mathbf{x}_L) \frac{1}{\Delta V} \\ & - (\nabla_d \times \nabla_d \times \mathbf{A}^n)_J, \end{aligned} \quad (22)$$

These difference equations furnish a canonical symplectic PIC method for the Vlasov-Maxwell equations.

As discussed above, symplectic algorithms for a Hamiltonian system with non-separable momentum and position dependence are implicit in general. This is indeed the case for the difference equations (19)-(22), because the right-hand sides of Eqs. (19)-(22) depend on values of the  $(n+1)$ -th time-step. However, they are semi-explicit, because Eqs. (19), (20), and (22) are explicit for  $\mathbf{X}_i^{n+1}$ ,  $\mathbf{A}_J^{n+1}$ , and  $\mathbf{Y}_J^{n+1}$ , respectively. Another good property of the system is that the only implicit equation (21) is linear in terms of  $\mathbf{P}_i^{n+1}$ , and it is only implicit for each particle, i.e., Eq. (21) does not couple  $\mathbf{P}_i^{n+1}$  and  $\mathbf{P}_k^{n+1}$  when  $i \neq k$ . Therefore, the system can be solved without root searching iterations as follows. We first solve the linear equation (21) for  $\mathbf{P}_i^{n+1}$  for every index  $i$  separately, which amounts to inverting a  $3 \times 3$  matrix for every  $i$ . Then  $\mathbf{X}_i^{n+1}$  and  $\mathbf{Y}_J^{n+1}$  are advanced explicitly according to Eqs. (19) and (22), and the last step is to advance  $\mathbf{A}_J^{n+1}$ , also explicitly, according to Eq. (20).

The preservation of the symplectic structure exerts  $D(2D-1)$  constraints on the numerical solution. Because  $D$  is a large number, preservation of symplectic structure is a very strong constraint and significantly reduces the errors of numerical solutions.

We now apply this canonical symplectic PIC scheme to simulate the nonlinear Landau damping process. The ions are treated as a uniform positively charged background, and the dynamics of electrons are simulated. The electron density is  $n_e = 1.149 \times 10^{16}/m^3$ , and the thermal velocity of electrons is  $v_T = 0.1c$ , where  $c$  is the light velocity in vacuum. The three-dimensional computational region is divided into  $896 \times 1 \times 1$  cubic cells. The size of grid is chosen to be  $\Delta x = 2.4355 \times 10^{-4}m$ , the time step  $\Delta t = \Delta x/2c$ . The interpolation



function is chosen to be 8'th order, i.e.,

$$W(\mathbf{x}) = W_1(x/\Delta x)W_1(y/\Delta x)W_1(z/\Delta x) , \quad (23)$$

$$W_1(q) = \begin{cases} 0, & q > 2 , \\ \frac{15}{1024}q^8 - \frac{15}{128}q^7 + \frac{49}{128}q^6 - \frac{21}{32}q^5 + \frac{35}{64}q^4 - q + 1, & 1 < q \leq 2 , \\ -\frac{15}{1024}q^8 - \frac{15}{128}q^7 + \frac{7}{16}q^6 - \frac{21}{32}q^5 + \frac{175}{256}q^4 - \frac{105}{128}q^2 + \frac{337}{512}, & 0 < q \leq 1 , \\ -\frac{15}{1024}q^8 + \frac{15}{128}q^7 + \frac{7}{16}q^6 + \frac{21}{32}q^5 + \frac{175}{256}q^4 - \frac{105}{128}q^2 + \frac{337}{512}, & -1 < q \leq 0 , \\ \frac{15}{1024}q^8 + \frac{15}{128}q^7 + \frac{49}{128}q^6 + \frac{21}{32}q^5 + \frac{35}{64}q^4 + q + 1, & -2 < q \leq -1 , \\ 0, & q < -2 , \end{cases} \quad (24)$$

Initially,  $10^5$  sampling points of electrons are distributed in each cell. The total number of particles is  $N = 8.96 \times 10^7$ , and the number of degrees of freedom is  $D = 2.69 \times 10^8$ . The initial electric field perturbation is  $\mathbf{E}_1 = E_1 \cos(kx) \mathbf{e}_x$ , where the wave vector is  $k = 2\pi/224\Delta x$ , and the amplitude of the perturbation electric field  $E_1 = 9.103 \times 10^4 V/m$ . The simulations are performed for 80000 time steps, during which a complete picture of the nonlinear Landau damping is revealed. As expected for symplectic algorithms, the numerical error of energy does not increase with time and is bounded within 1% for all time. The theoretical damping rate calculated from the dispersion relation is  $\omega_i = -1.3926 \times 10^9/s$ , and the theoretical real frequency is  $\omega_r = 9.116 \times 10^9/s$ . In Fig. 1, the slope of the green line is the theoretical damping rate, and the blue curve is the evolution of the electrical field observed in the simulation. It is evident that the simulation and theory agree perfectly. After  $t = 30/\omega_r$ , the energy of the wave drops below the level of numerical noise, and the damping process stops. The evolution of the electron distribution function is plotted in Fig. 2, which clearly demonstrates the mechanism of phase mixing in velocity space. We observe in Fig. 2 that the wave-number in velocity space increases with time, which results in a decrease in density perturbation and thus attenuation of the electrical field. More importantly, this mechanism of phase mixing is the dominant physics for the entire nonlinear evolution of the Landau damping, as proved by Mouhot and Villani [27, 28] recently for the electrostatic Vlasov-Poisson system. In addition, our simulation shows that this physical picture of nonlinear Landau damping is also valid for the electromagnetic Vlasov-Maxwell system, as Villani conjectured [29]. We emphasize that it is the long-term accuracy and fidelity of the canonical symplectic PIC algorithm that enables the confirmation of Mouhot and Villani's theory and conjecture over several orders of magnitude.

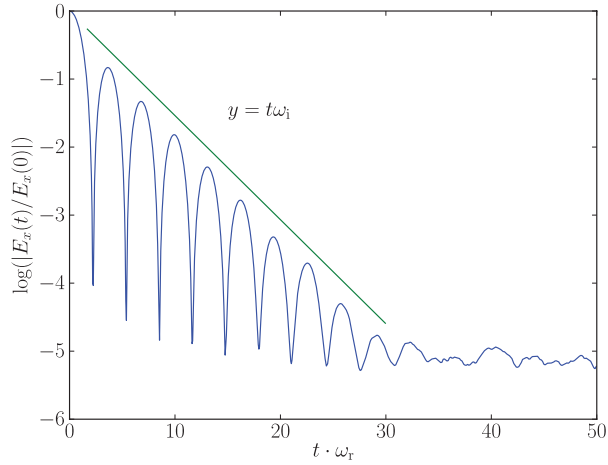


FIG. 1. Perturbed electric field as a function of time. The slope of the green line is the theoretical damping rate.

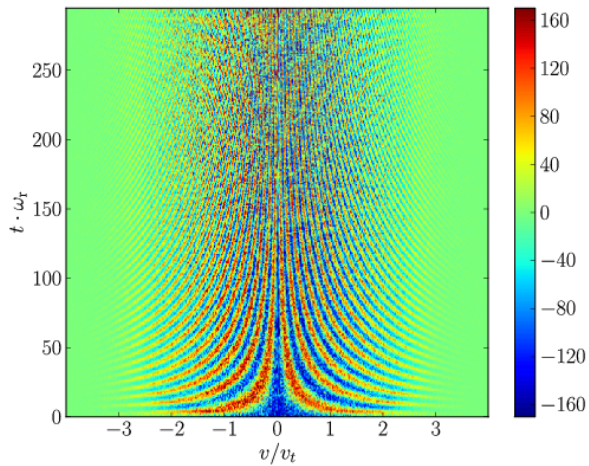


FIG. 2. Electron distribution function in velocity space as a function of time. Different colors denote the amplitude of the perturbation. The mechanism of phase mixing in velocity space is clearly demonstrated. The wave-number in velocity space increases with time, which results in a decrease in density perturbation and thus attenuation of the electrical field.

In conclusion, we have developed a canonical symplectic particle-in-cell simulation method for the Vlasov-Maxwell system by discretizing the canonical Marsden-Weinstein bracket. In phase space, the distribution function is discretized by the Klimontovich representation using Lagrangian markers, and the electromagnetic field is discretized point-wise

on a spatial grid. The resulting canonical Hamiltonian system with a large number of degrees of freedom is integrated by the symplectic Euler method. The Euler method's difference equations can be solved inexpensively by inverting a  $3 \times 3$  matrix locally for every particle. Implicit root searching and global matrix inversion are avoided entirely. This technique makes large-scale applications of the developed canonical symplectic PIC method possible. To suppress numerical noise caused by the coarse sampling, smoothing functions for sampling points can also be conveniently implemented in the canonical symplectic PIC algorithm. By incorporating the smoothing functions into the Hamiltonian functional before the discretization, we are able to rein in all the benefits of smoothing functions without destroying the canonical symplectic structure. Progress in this and other directions will be reported in future publications.

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