Structure-preserving geometric particle-in-cell algorithm suppresses finite-grid instability – Comment on “Finite grid instability and spectral fidelity of the electrostatic Particle-In-Cell algorithm” by Huang et al.

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Abstract

A recent paper by Huang et al. [Computer Physics Communications 207, 123 (2016)] thoroughly analyzed the Finite Grid Instability (FGI) and spectral fidelity of standard Particle-In-Cell (PIC) methods. Numerical experiments were carried out to demonstrate the FGI for two PIC methods, the energy-conserving algorithm and the momentum-conserving algorithm. The paper also suggested that similar numerical experiments should be performed to test the newly developed Structure-Preserving Geometric (SPG)-PIC algorithm. In this comment, we supply the results of the suggested numerical experiments, which show that the SPG-PIC algorithm is able to suppress the FGI.
Huang et al. recently provided an in-depth analysis of the Finite Grid Instability (FGI) and spectral fidelity of standard Particle-In-Cell (PIC) methods [1]. The spectral errors, especially the aliased spatial modes, from charge deposition and field interpolation schemes were rigorously quantified. Numerical experiments were carefully designed and carried out to demonstrate the FGIs of the Momentum-Conserving (MC)-PIC algorithm [2] and the Energy-Conserving (EC)-PIC algorithm [3]. Simulation results using a Particle-And-Spectrum (PAS) method [4] was also given for comparison and benchmark. The paper suggested performing similar numerical experiments to test the newly developed Structure-Preserving Geometric (SPG)-PIC algorithm [5–14]. In this comment, we supply the results of the suggested numerical experiments using the specific implementation of the SPC-PIC algorithm reported in Ref. [7].

The parameters for the numerical experiments are the same as in Ref. [1], which are listed as follows. The simulation domain is a $L \times 1 \times 1$ periodic box where $L = 33$, $\Delta x = 1$, and $\omega_p = 2\pi/L$. The time step is set to $\Delta t = 0.2\omega_p^{-1}$. The numbers of sampling points per grid for both electron and ions are 300, and the mass ratio and charge ratio between electrons and ions are 1 : 3672 and $-1 : 1$, respectively. Initially the ions are equally spaced and their velocities are set to 0. Electrons are equally spaced with a sinusoidal displacement $\delta x(x_p0) = LA \cos(2\pi M x_p0/L) / (2\pi M)$, and their velocities are $v_x(x) = 0.01c + LA \omega_p \sin(2\pi M x/L) / (2\pi M)$, where $A = 0.01$ and $M = 9$. Initial electric field is $E_x(x) = -Lq_e A \cos(2\pi M x/L) / (2\pi M)$.

The simulation first is performed to $t = 220\omega_p^{-1}$. The resulting mode spectrum, final velocity distribution, energy and momentum evolution are plotted in Figs.1 and 2 which correspond to Fig. 3 and Fig. 4 of Ref. [1], respectively. These results show that even though mode alias still exists in the SPG-PIC algorithm, the FGI is suppressed. While mode alias effect, as an error of spatial discretization, is inevitable in any spatial grid, its existence does not necessarily imply unstable numerical eigenmodes will be exited. Note that when a unstable numerical eigenmode is excited, all components of the dynamics, especially the dominant ones, of the discrete system will grow exponentially. Unfortunately, such FGIs do exist in the standard PIC methods. As demonstrated in Ref. [1], in about 30 plasma oscillation periods $(200\omega_p^{-1})$, the total energy error for the MC-PIC algorithm exceeds 200%, and the total momentum error for the EC-PIC algorithm exceeds 70%. On the other hand, Fig.2 shows that for the SPG-PIC algorithm, the total energy error is less than 1%, and the
The observed suppressing of FGI for the SPG-PIC algorithm can be attributed to the structure-preserving nature of its spatial discretization. The charge deposition and field interpolation are derived from a variational principle using the techniques of Whitney interpolation forms [5, 10, 14] or finite element discrete exterior calculus [9, 13], which preserves the discrete gauge symmetry and the discrete exterior calculus structure of the electromagnetic field. As a result, physical laws, such as the charge conservation and \( \nabla \cdot \mathbf{B} = 0 \), are satisfied exactly by the discrete system. This result is consistent with Ref. [1]'s conclusion that charge deposition and field interpolation can be optimally designed to suppress or reduce FGIs.

Another feature of the SPG-PIC algorithm is the preserving of non-canonical symplectic structure for time-integration, which in general bounds simulation errors on conserved quantities for a very long time. We run the simulation for 500 longer to \( t = 10000 \omega_p^{-1} \), and the result is plotted in Fig. 3. Over this long simulation time, the total energy error and total momentum error are bounded by 1% and 2%, respectively.

We finish this comment with two footnotes. First, the SPG-PIC algorithm used is for Vlasov-Maxwell system in 3D configuration space. For the simplified geometry and simulation parameters of the present numerical experiments, the dominated modes of the discrete system are longitudinal electrostatic modes. Secondly, for the PAS methods, symplectic time-integration can also be adopted. For example, Cary and Doxas [15, 16] first applied a canonical symplectic algorithm to simulate the particle-and-mode Hamiltonian models [17, 22] for the Vlasov-Poisson system.

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Figure 1. Mode spectrum simulated by the SPG-PIC algorithm. Full mode spectrum $\log(|\text{fft}(E)|)$ as a function of time is shown in the left figure, and evolution of the mode amplitude for mode number $k = 9, 15, 6$ is shown in the right figure.

Figure 2. Electron distribution at $t = 200\omega_p^{-1}$ (left) and the evolution of energy and momentum (right).

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Figure 3. Long term evolution of spectrum (left), total energy and momentum (right) simulated by the SPG-PIC algorithm.

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