Particle Trajectory Error in Finite Element Particle-in-Cell Kinetic Plasma Simulations

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Abstract—Particle-In-Cell (PIC) algorithms are widely used for kinetic plasma simulations. In PIC algorithms, it's crucial to understand the resultant approximation errors due to the underlying space and time field discretization. Here, we examine the error in particle trajectories produced by a finite-element (FE) based PIC algorithm on unstructured meshes. We study the convergence of such error against two basic parameters: the FE mesh resolution and the matrix solver approximation.

Index Terms—Finite element, harmonic oscillator, kinetic plasma, particle-in-cell, sparse approximate inverse, unstructured mesh.

I. INTRODUCTION

PARTICLE-IN-CELL (PIC) algorithms [1], [2], [3], [4] are widely used for the numerical simulation of kinetic plasmas. PIC algorithms consist of four cyclic steps at each time step: a solver for the field quantities (field update), interpolation of field values to each particle location (field gather), updating the position and velocity of each particle through the equations of motion (particle pusher), and mapping the updated particle information into a current and charge densities on the computational mesh (scatter) [5]–[8]. A finite element (FE) field solver based on unstructured meshes enables greater geometrical flexibility when it comes to discretizing the domain of interest as opposed to finite difference solvers on regular meshes [9], [10]. When applying a FE-PIC algorithm, it is important to understand and analyze the sources of numerical error [11], [12]. In this work, we examine the error in particle trajectory due to the underlying space and time FE discretization. Two parameters are considered and varied to discern their effects on the trajectory perturbation: Mesh resolution and matrix solver approximation.

The ground truth trajectory corresponds to the trajectory produced by a confining parabolic electric potential along with an axial magnetic field. The resultant trajectory forms a closed orbit. Analytic investigations of such a problem can be found in [13], [14]. In this case, perturbations in the trajectory produced by the PIC-FE algorithm become visually apparent due to the formation of bounded orbits with a spurious precession rather than exact closed orbits.

II. METHODOLOGY AND RESULTS

A. Confining fields and simulation setup

The applied external electric and magnetic fields are of the form: \( E_o = (\hat{x} E_o, \hat{y} E_o) \), \( B = \hat{z} B_o \). If only one of the fields is zero and given certain initial conditions, the particle trajectory is periodic with period \( T_e = 2\pi \sqrt{m/(qE_o)} \) or \( T_m = 2\pi m/(qB_o) \), where \( T_e \) is the period due to the application of the electric field only and \( T_m \) is the period due to the application of the magnetic field only. When both fields are present, periodicity is not guaranteed but if \( E_o \neq 0 \) and \( B_o \neq 0 \), then periodicity is achieved as long as \( T_e/T_m \in \mathbb{Z} \) or \( T_m/T_e \in \mathbb{Z} \).

The domain of interest \( \Gamma \) is a square reference domain of size \( 1 \times 1 \) m\(^2\). We assume vacuum conditions. In order to study the behavior of the error against the mesh resolutions, different meshes are constructed to discretize \( \Gamma \) such that the \( m^n \) mesh contains \( 100 \times 2^{m-1} \) elements for \( m = 1, 2, \ldots, 10 \). When considering the field update step in the FE-PIC algorithm, the solution of a sparse linear system is required. A sparse approximation inverse (SPAI) [6], [15] is utilized to approximate the system inverse. The SPAI algorithm is controlled by a sparsity level parameter denoted here as \( \kappa \) [15]. Once a mesh resolution and SPAI solver level \( \kappa \) are specified, the associated trajectory errors can be computed.

B. Reference trajectory

As noted, in order to obtain a periodic trajectory, \( E_o \) and \( B_o \) are chosen such that \( T_e/T_m = 1 \). By fixing \( E = -(\hat{x} x + \hat{y} y) \times 10^7 \) V/m this results in \( B = \hat{z} 0.00754 T \). The particle charge and mass are set to that of an electron and the initial position is \( (x_0, y_0) = (0.4, 0) m \) with zero initial velocity. Five periods of the resultant trajectory is considered.

C. Numerical results

Fig. 1 shows the particle trajectories for various \( m \) (mesh resolution) and \( \kappa \) (FE solver approximation level). For each pair \( (m, \kappa) \), the numerical trajectory (red) and the ground truth trajectory (blue) are superimposed. It can be observed that as \( m \) (row index) and \( \kappa \) (column index) are increased, the numerical trajectory approaches the ground truth. With that said, the error does not converge monotonically because for any given \( (m, \kappa) \), errors due to \( m \) and errors due to \( \kappa \) might have opposite effects. Further, the error is not only dependent on the number of elements in the mesh, but also on the particular geometry of the mesh. That is, in order to produce a more monotonic decrease in error, the result must be averaged over multiple meshes with different geometry for any given \( (m, \kappa) \) pair [16]. Note also that for \( \kappa = 1 \), convergence is not observed with \( m \) due to the poor approximation of the inverse FE matrix.
Fig. 1: Approximate particle trajectory for various \((m, \kappa)\) pairs (red) and ground truth trajectory (blue)

III. CONCLUSION

In this work, a qualitative study was performed to evaluate the errors associated with perturbed particle trajectories in FE-based PIC algorithms. A useful visualization of the numerical perturbations on the particle trajectory was made possible by considering trajectories produced by parabolically confining potential and an axial magnetic field, which form perfectly closed orbits under certain conditions. It was shown that the numerical trajectories converge to the ground truth with a sufficiently fine mesh and accurate FE matrix solver.

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REFERENCES