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Studies of particle wake potentials in plasmas

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ABSTRACT

A detailed understanding of electron stopping and scattering in plasmas with variable values for the number of particles within a Debye sphere is still not at hand. Presently, there is some disagreement in the literature concerning the proper description of these processes. Theoretical models assume electrostatic (Coulomb force) interactions between particles and neglect magnetic effects. Developing and validating proper descriptions requires studying the processes using first-principle plasma simulations. We are using the particle-particle particle-mesh (PPPM) code ddcMD and the particle-in-cell (PIC) code BEPS to perform these simulations. As a starting point in our study, we examine the wake of a particle passing through a plasma in 3D electrostatic simulations performed with ddcMD and BEPS. In this paper, we compare the wakes observed in these simulations with each other and predictions from collisionless kinetic theory. The relevance of the work to Fast Ignition is discussed.

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1. Introduction

Particle-in-cell (PIC) and particle-particle particle-mesh (PPPM) simulations are both useful for studying stopping and scattering of electrons in plasmas, and in Fast Ignition (FI) [1] targets in particular. PIC codes such as OSIRIS [2] can simulate the transport of supra-thermal electrons from the edge of the target to the core [3]. PPPM codes such as ddcMD [4], while more computationally expensive than traditional PIC, accurately resolve pair-wise interactions. Such simulations can be used to study the role of electron scattering in FI and resolve the dispute over the proper description of electron stopping in plasmas [5–8]. In addition, an electrostatic or Darwin PIC code might be useful to study collisions from first principles if the cell size is significantly smaller than a Debye length.

We begin our stopping and scattering studies with a study of particle wake potentials. Wakes play an important role in charged particle stopping [9] and provide a convenient starting point for our studies. They also provide a way for us to observe some of the differences between PIC and PPPM simulations.

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2. PIC & PPPM methods

The PIC method [10,11] is simple in concept. The point of the method is to accurately model collective behavior of plasmas while achieving a speed-up over the traditional molecular dynamics algorithm by smoothing out interactions that occur inside a grid spacing (often a Debye length). We achieve this smoothing and speed-up by solving for the fields on a spatial grid rather than solving for the force on each particle from all the other particles directly. Since PIC uses a grid, we often say that the particles have a finite size. Typically, the grid spacing is on the order of a Debye length, so interactions on smaller spatial scales are unresolved. However, the grid spacing can be smaller [12].

Each iteration in the PIC method contains four steps. First, given the positions and velocities of the particles in the system, interpolate the charge and current to the grid points. Second, solve for the electric and magnetic fields on the grid. Third, interpolate to find the values of the electric and magnetic fields at the particle positions. Finally, push the particles using the Lorentz force law. The process is demonstrated visually in Fig. 1. This process gives us an O(N) algorithm, where N is the number of particles, as opposed to the $O(N^2)$ algorithm of molecular dynamics.

The PPPM method [13] is designed to maintain computational efficiency and take into account pair-wise interactions between particles. It calculates the smooth long-range forces using a grid like PIC does for computational efficiency, then only computes pair-



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Fig. 1. The cycles used in the PIC method (top) and the PPPM method (bottom). Conceptually, the two cycles are identical except for the additional step in the PPPM method, which takes into account pair-wise interactions.

wise interactions within a cutoff sphere specified by the user. Computing the pair-wise interactions typically makes the PPPM method more computationally intensive than PIC. We have again demonstrated the steps visually in Fig. 1. The PPPM method has the advantage over PIC of more accurately simulating processes in which collisions play an important role.

3. Collisionless kinetic theory of particle wakes

We derive the time-dependent potential of a particle in a plasma following Decyk [14]. The potential generated by a charge density ρ in a plasma (in CGS units) is

$$\phi(\vec{k},\omega) = \frac{4\pi\rho(\vec{k},\omega)}{k^2\varepsilon(\vec{k},\omega)},\tag{1}$$

where $\varepsilon(\vec{k}, \omega)$ is the collisionless plasma dielectric. If we assume an electron plasma with a Maxwellian velocity distribution and immobile ions, the dielectric is given by

$$\varepsilon(\vec{k},\omega) = 1 - \frac{\omega_{pe}^2}{2k^2 v_{th}^2} Z' \left(\frac{\omega}{\sqrt{2k}v_{th}}\right),\tag{2}$$

where $v_{th} = \sqrt{T_e/m_e}$ is the electron thermal speed and Z'(s) = dZ/ds. Z'(s) must be calculated numerically, and is typically found by first computing Z(s), which is known as the plasma dispersion function. The two are related by the differential equation, Z'(s) + 2sZ(s) + 2 = 0. Z(s) is related to the error function by

$$Z(s) = i\sqrt{\pi}e^{-s^{2}}[1 + erf(is)].$$
 (3)

Suppose we insert a test particle with charge q_t at \vec{x}_0 with velocity \vec{v} at t = 0. Then, the charge density takes the form,

$$\rho(\vec{x},t) = q_t \delta(\vec{x} - \vec{x}_0 - \vec{v}t), \quad t > 0$$
(4)

in real space and, performing a Fourier transform in position and a Laplace transform in time,

$$\rho(\vec{k},\omega) = \frac{q_t e^{-i\vec{k}\cdot\vec{x}_0}}{i(\vec{k}\cdot\vec{\nu}-\omega)}$$
(5)

in the transform space. Therefore,

$$\phi(\vec{k},\omega) = \frac{4\pi q_t e^{-i\vec{k}\cdot\vec{x}_0}}{ik^2(\vec{k}\cdot\vec{v}-\omega)\varepsilon(\vec{k},\omega)}.$$
(6)

We need $\phi(\vec{x}, t)$, so we first invert the Laplace transform, which gives,

$$\phi(\vec{k},t) = \frac{4\pi q_t e^{-i\vec{k}\cdot\vec{x}_0}}{k^2} \int_{-\infty-ic}^{\infty-ic} \frac{d\omega e^{-i\omega t}}{2\pi i(\vec{k}\cdot\vec{v}-\omega)\varepsilon(\vec{k},\omega)}, \quad t > 0.$$
(7)

The integrand has poles at $\omega = \vec{k} \cdot \vec{v}$ and $\omega = \omega_j(\vec{k})$, where $\omega_j(\vec{k})$ are the roots of $\varepsilon(\vec{k}, \omega) = 0$. Therefore, we can apply Cauchy's theorem, which yields,

$$\phi(\vec{k},t) = \frac{4\pi q_t e^{-i\vec{k}\cdot(\vec{x}_0+\vec{v}t)}}{k^2 \varepsilon(\vec{k},\vec{k}\cdot\vec{v})}$$
$$-\sum_j \frac{4\pi q_t e^{-i\vec{k}\cdot\vec{X}_0} e^{-i\omega_j t}}{k^2(\vec{k}\cdot\vec{v}-\omega_j)\frac{\partial\varepsilon(\vec{k},\omega)}{\partial\omega}\Big|_{\omega=\omega_j}}, t > 0.$$
(8)

We next apply the inverse Fourier transform and write $\phi(\vec{x},t) = \phi_D(\vec{x},t) + \phi_C(\vec{x},t)$, where

$$\phi_{D}(\vec{x},t) = 4\pi q_{t} \int_{-\infty}^{\infty} \frac{d\vec{k}}{(2\pi)^{n}} \frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}_{0}-\vec{v}t)}}{k^{2}\varepsilon(\vec{k},\vec{k}\cdot\vec{v})}, \quad t > 0$$
(9)

and

$$\phi_{C}(\vec{x},t) = -4\pi q_{t} \sum_{j} \int_{-\infty}^{\infty} \frac{d\vec{k}}{(2\pi)^{n}} \frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}_{0})}e^{-i\omega_{j}t}}{k^{2}(\vec{k}\cdot\vec{v}-\omega_{j})\frac{\partial\varepsilon(\vec{k},\omega)}{\partial\omega}\Big|_{\omega=\omega_{j}}}, t > 0,$$
(10)

where *n* is the spatial dimensionality. Decyk calls $\phi_D(\vec{x},t)$ the Debye cloud term and $\phi_C(\vec{x},t)$ the Cherenkov term. We shall see that we usually only need to keep the least damped root of $\varepsilon(\vec{k},\omega)$, even though $\phi(\vec{x},t)$ contains a sum over all roots.

4. The subtraction technique

Fluctuations in plasmas are large compared to the wake of a single particle. Particle simulations such as PIC and PPPM reproduce these fluctuations, so we must remove them from the data during analysis. The subtraction technique [14] removes the uncorrelated background through the use of two simulations. The first simulation includes the small perturbation, such as a test charge, while the second does not. The simulations are otherwise identical. Subtracting the second from the first reveals the response to the perturbation, as shown in Fig. 2.

5. PIC results and comparison with collisionless kinetic theory

We first study particle wakes by performing traditional PIC simulations using the 3D periodic electrostatic code BEPS [15]. BEPS solves for the potential and the electric fields in the plasma using FFTs, supports linear and quadratic particle shapes, and offers a relativistic and non-relativistic particle pusher. We use quadratic particle shapes and a non-relativistic particle pusher in all BEPS simulations in this paper.

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