Particle-in-Cell Technique with Monte Carlo Collisions for Plasma Simulation and Application to Fusion

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Summary

The particle-in-cell(PIC) technique [1,2,3] is a well-established computational method for the simulation of plasmas. This study will explore the potential for the PIC technique as a method of simulating plasmas which are undergoing nuclear fusion. The standard PIC framework is used, however collisions which are relevant to fusion are added using the Monte-Carlo model. The resulting neutron distribution, as well as the reaction rate for fusion events as a function of density and temperature are obtained, and compared to accepted results. The advantages and disadvantages of the PIC method for this application will be discussed.

1. Method

The particle-in-cell (PIC) technique is a method of modeling the motion and interactions of individual particles in a plasma. The particles' position and velocity are advanced at each time step in the simulation using the Lorentz force generated by the self consistent and external electromagnetic fields. The velocity of the particles can be further modified if a collision takes place. A Monte Carlo process is used to determine which particles (if any) undergo a collision.

The particles' position and velocity are continuous, however properties such as charge and current density are only considered at points on a discrete mesh grid [1]. The properties of the particles are weighted to these discrete grid points using a shape function, S(**x**-**X**), where **x** is the position of the particle, and **X** is the position of the grid point to which the particle's properties are being weighted to. A shape function must satisfy the conditions of space isotropy and charge distribution [2]. A popular shape function is the first order weighting. In this method the particle's properties are linearly interpolated to the four nearest grid points [1], see Figure 1.

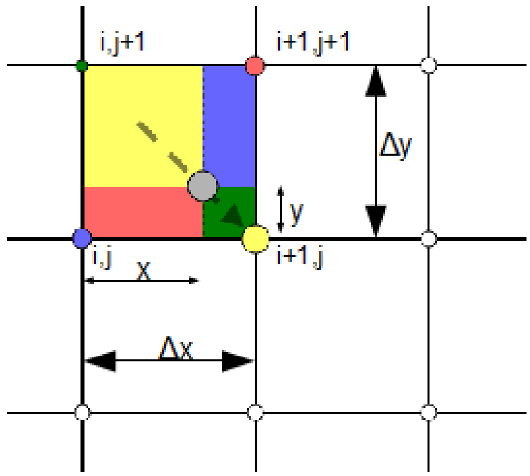

Figure 1: Linear interpolation particle weighting scheme. Adapted from [4].

The self-consistent electromagnetic fields can now be calculated numerically at the grid points using Maxwell's equations. In many situations the particles are moving slow enough that they can be approximated as static, and therefore only Poisson's equation is solved; this is known as an electrostatic PIC simulation. There are many methods for solving Poisson's equation including; relaxation methods, matrix inversion methods, and solving in Fourier space [2]. In this simulation the relaxation method is used. If the approximation of static particles does not hold, such as in a very hot plasma, then the full set of Maxwell's equations must be solved; this is know as an electromagnetic PIC simulation. Since the goal of this program is to simulate a plasma undergoing fusion, which must be very hot, an electromagnetic PIC method is used. The numerical method used to solve the full set of Maxwell's equations is the finite-difference time-domain (FDTD) method on a Yee's grid [5]. The self induced fields are then added to the external fields, to provide the total electric and magnetic fields at each grid point.

The fields found at the grid points are now weighted back to each particle in a manner inversely analogous to the particle weighting (Figure 1). The particle's velocities and positions are changed according to the equations of motion:

$$m\frac{d\vec{v}}{dt}=\vec{F} \quad , \quad \frac{d\vec{x}}{dt}=\vec{v} \qquad (1)$$

Where the force considered is the Lorentz force, which is found using the electric and magnetic fields at the particle's position:

$$\vec{F}=q[\vec{E}+(\vec{v}\times\vec{B})] \qquad (2)$$

This set of coupled differential equations is solved using the Boris method [6]. This technique involves solving the leap frog discretized versions of Equations 1 and 2 by separating the electric and magnetic forces.

If collisions are considered, then the properties of the particles undergoing collisions must be further modified as a result of the collision. The Monte Carlo Collision method is used to determine which particles participate in collisions [3]. In general this method uses randomly generated numbers to calculate the time between collisions. The probability of a collision occurring in a time step Δt is calculated using the collision's cross section $\sigma(\varepsilon)$, the speed of the incident particle v_i, and the density of the target species $n(\mathbf{r})$, using the relation seen below [7]:

$$P_i = 1 - e^{-v_i \Delta t\, \sigma(\epsilon) n(\vec{r})} \qquad (3)$$

A uniform random number between 0 and 1 is now generated and compared to the value of the probability found using Equation 3. If this number is less than the calculated probability a collision will occur. The effect of the collision on the properties of the particles involved will depend on the specific type of collision taking place. In typical particle-in-cell simulations most collisions are of the scattering type and therefore only the velocity of the particles is modified. However, since fusion collisions are also being considered in this simulation the particle's mass and charge may also be changed. The fusion collisions which have been simulated are shown below [8, 9]:

$$
\begin{aligned}
&{}^{2}\mathrm{D} + {}^{3}\mathrm{T} \rightarrow {}^{4}\mathrm{He}(3.5\,\mathrm{MeV}) + {}^{1}\mathrm{n}(14.1\,\mathrm{MeV}) \\
&{}^{2}\mathrm{D} + {}^{2}\mathrm{D} \rightarrow {}^{3}\mathrm{He}(0.82\,\mathrm{MeV}) + {}^{1}\mathrm{n}(2.45\,\mathrm{MeV}) \\
&{}^{2}\mathrm{D} + {}^{3}\mathrm{T} \rightarrow {}^{4}\mathrm{He}(3.5\,\mathrm{MeV}) + {}^{1}\mathrm{n}(14.1\,\mathrm{MeV}) \\
&{}^{2}\mathrm{D} + {}^{3}\mathrm{He} \rightarrow {}^{4}\mathrm{He}(3.67\,\mathrm{MeV}) + {}^{1}\mathrm{H}(14.68\,\mathrm{MeV})
\end{aligned}
$$

The process of computing the electromagnetic fields, collisions, and movement of the particles is repeated for each time step. A diagram outlining the entire process taking place during each time step can be seen in Figure 2.

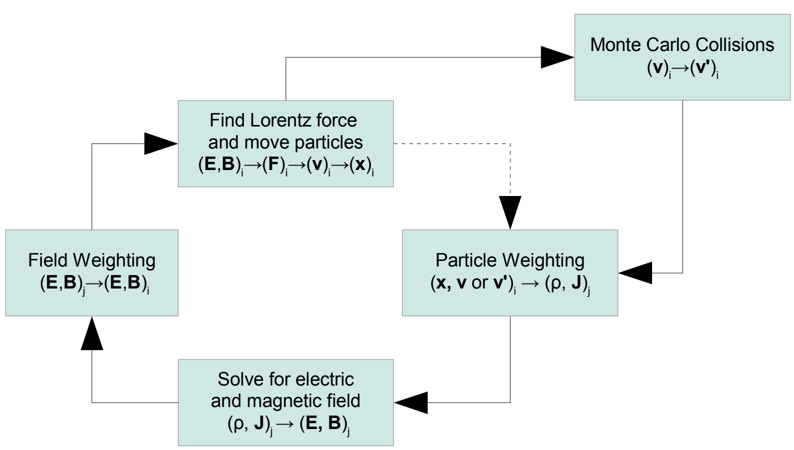

Figure 2: Flow chart of the PIC technique. The process is repeated for each time step. Individual particles are i, grid indices are j. Adapted from [2].

2. Results and Expected Results

Thus far the results gained from the simulation have been to test the various components of the PIC technique. For instance, the electric potential and field surrounding a single electron have been computed using the simulator in order to test the Poisson equation solver. These results can be seen in the image below (Figure 3):

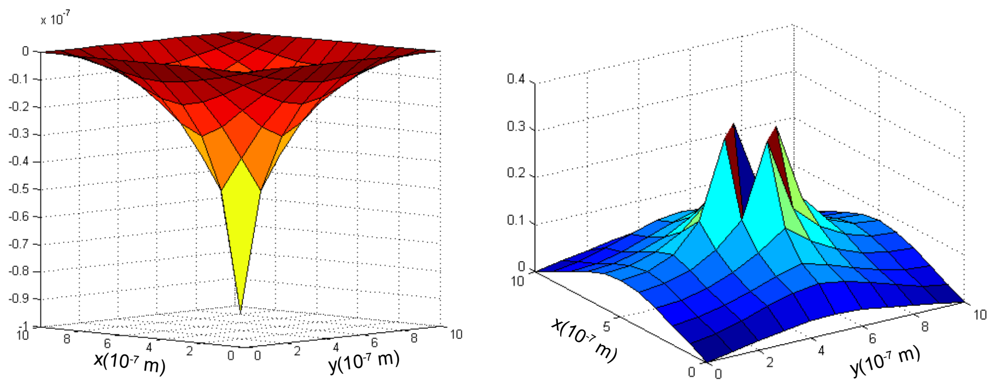

Figure 3: The computed electric potential (left) and electric field (right) surrounding an electron.

The Maxwell equation solver has been demonstrated by simulating the magnetic fields induced around a localized current in a single direction (i.e. a wire). The results can be seen in the image below (Figure 4):

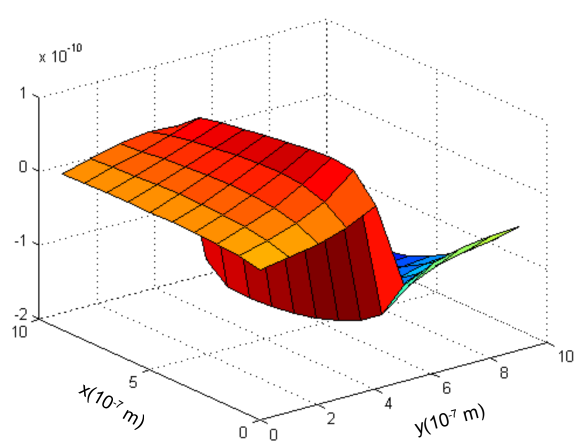

Figure 4: Magnitude of the magnetic field in the z-direction (arbitrary units) generated by the current through a wire.

As can be seen the magnetic field has opposite signs on either side of the wire, and decays in a $1/r$ fashion, as expected. The motion of a single electron in a magnetic field was also found (Figure 5), in order to verify the particle motion.

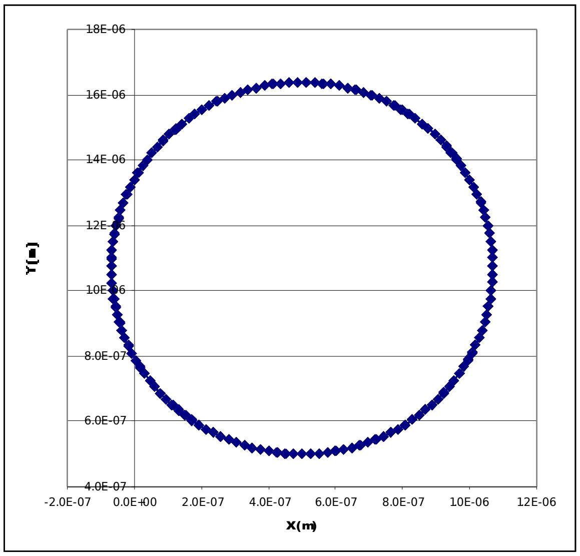

Figure 5: The motion of an electron on the x-y plane in a 0.01 T magnetic field in the z-direction.

As can be seen in Figure 5 the particles motion is circular as expected. The gyromagnetic period has also been found to be within uncertainty of the theoretical value.

The end goal of the simulation is to obtain relationships between the fusion reaction rates and particle density and temperature. These results will be compared to known theory, and the difference between the theoretical and computational results will be used as a metric to judge how successful the application of the PIC technique is for fusion plasmas. The expected reaction rate is [8]:

$$R_{ij} = a_{ij} n_i n_j \langle \sigma v \rangle \quad (4)$$

Where n_i and n_j are the densities of species i and j respectively, $\langle \sigma v \rangle$ is the reactivity, and a_{ij} is equal to 1 if the species are distinct, and ½ otherwise.

The simulator also handles neutron-charged collisions and therefore can be used to obtain the distribution of neutrons as a function of energy for various densities and temperatures. This is of great importance because a major portion of the energy transported to the working fluid is contained in the neutrons. The escaped neutrons also degrade the surrounding materials, and lead to impurities in the plasma.

3. References

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