Chapter 20

Particle-In-Cell Simulation of Plasma: A Basic Overview

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20.1 Introduction

Plasma consists of charged particles- ions and electrons, and hence, the behaviour of plasma, in principle, can be evaluated by calculating the forces the constituent particles exert on one another using the Coulomb's law. In an ensemble of N charged particles, a particle will interact with other (N-1) particles creating $N(N-1)/2$ number of interacting pairs. For a plasma of volume 1 cm^3 and density $1 \times 10^8 cm^{-3}$, total number of charged particles is $N = 2 \times 10^8$. If at least 10 arithmetic operations are required in the evaluation of the Coulomb force, then the number of operations in a time-step will be of the order of 10^{16} to 10^{17}. If one operation takes 10^{-9} seconds to execute, one time-step will take about 2780 hours (for 10^{16} operations). In LIS-related [165, 229, 230] plasma simulation, the number of time-steps required to cover a few tens of microseconds of plasma propagation is in the range of 10^4 to 10^5. For 10^4 time-steps, the total time required for execution will be 2780×10^4 hours, i.e. more than 3000 years which is clearly impractical.

To overcome this problem, the concept of super-particles (or macro-particles) was introduced for plasma simulation. A super-particle is a computational particle which may represent millions of ions (or electrons) of a plasma. Secondly, a spatial grid was utilised such that the electric potential due to the charges of the super-particles as well as the applied voltages to the electrodes would be calculated only on the nodes of the grid, not at the location of the super-particles. This method of computation is generally referred to as the Particle-In-Cell (PIC) simulation of plasmas [231, 232]. It reduces the number of operations per time-step to N log(N) from N^2 earlier [231–233].

20.2 Governing Equations

Plasma simulation involves motion of the constituent charged particles under the influence of any applied electric field as well as the electric field produced by the distribution of the charged particles themselves. The two main steps involved in the simulation are: calculation of the electric potential (and subsequently, electric field) and calculation of the particles' position and velocity coordinates under the influence of that electric field.

The electric potential (V) or field ($\vec{E}$) can be calculated using Maxwell's equations. In the area of laser isotope separation, the problem is electrostatic in nature and hence simplifies to solving Gauss law which states that the electric flux (φ) through a closed surface area (A) is proportional to the total charge (Q) enclosed by the area:

$$\varphi = \oint \vec{E}.d\vec{A} = \frac{Q}{\varepsilon_0} \tag{20.1}$$

Using the differential form of the Gauss law

$$\vec{\nabla}.\vec{E} = -\frac{\rho}{\varepsilon_0} \tag{20.2}$$

where ρ is the charge density, one arrives at the following equation for potential (V), which is known as the electrostatic Poisson equation:

$$\nabla^2 V = -\frac{\rho}{\varepsilon_0}, \tag{20.3}$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ in 3D Cartesian coordinates. The Poisson equation is then discretized using the finite difference method. For an initial distribution of the super particles, potentials are calculated at the nodes of the spatial grid using the discretized Poisson equation [231, 232, 234]. Electric field at the location of a super-particle is then calculated using potentials at the nearby nodes via an interpolation scheme. Due to the effect of this electric field, the super-particle is moved to a new location. The new position ($\vec{r}$) and velocity ($\vec{v}$) coordinates of the particle with mass m and charge q are obtained by using the Lorentz equation,

$$m\frac{d\vec{v}}{dt} = q\left\{\vec{E} + \vec{v} \times \vec{B}\right\}, \tag{20.4}$$

solved with an implicit method called the leap-frog method [231, 232]. Here, $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields, respectively, in the particle location. Boris (explicit) method is also often used to solve for the position and velocity using the above equation [231, 232].

For the new the distribution of the charged particles, the potentials at the nodes of the spatial grid are re-calculated. The electric fields at the particles' locations are then evaluated and the particles are subsequently moved to newer locations using the leap-frog method. This process is continued repeatedly for several thousand time-steps until the simulation progresses to the desired dynamics of the plasma.

20.3 Simulation Parameters of Crucial Importance

20.3.1 Debye length for spatial grid

The electrons tend to surround an isolated ion in a plasma because of the potential created by it. The sphere of this electron cloud is known as Debye sphere and the radius of this

sphere is known as Debye length (λ_D) [235]. It is given by:

$$\lambda_D = \sqrt{\frac{\varepsilon_0 T_e[eV]}{ne}} \tag{20.5}$$

where T_e [eV] is the electron plasma temperature in eV and n is the plasma density (all the units are in SI except for T_e). Debye length is the maximum distance up to which the ions and the electrons can be separated while still maintaining the state of plasma.

In PIC simulation, the cell size of the spatial grid has to be less than or equal to the Debye length in order to fully include the effect of external perturbation. The recommended value of the grid size is (0.5 - 1.0) $\times$ λ_D. Grid size more than 3.3 $\times$ λ_D can lead to numerical instability and non-physical gain of temperature of the plasma.

20.3.2 Plasma period for simulation time-step

When a plasma is perturbed, for example, with an external electric field, the electron cloud which is dispersed among the less-mobile ions, is slightly displaced from the mean position and it starts to oscillate about it. The angular frequency of this oscillation, called the electron plasma frequency (ω_{pe}), is related to Debye length (λ_D) and the electron thermal velocity (v_{Te}) with the following relation:

$$\omega_{pe} = \frac{v_{Te}}{\lambda_D} \tag{20.6}$$

The corresponding time-period (τ_e) is the characteristic time within which the plasma responds to any external field [235]. It is expressed as:

$$\tau_e = 2\pi\sqrt{\frac{\varepsilon_0\ m_e}{ne^2}} \tag{20.7}$$

where m_e is the mass of the electron. External oscillatory electric fields with frequency higher than the plasma frequency can thus penetrate the plasma. On the other hand, for fields with frequency lower than the plasma frequency, the electrons with their rapid response try to shield the plasma from the external fields. In plasma simulation, therefore, the time-step required has to be less than that of the plasma oscillation time period. The recommended value for the time-step is $0.25/\omega_{pe}$.

Ions, like electrons, also exhibit an oscillation under an external perturbation and have a characteristic oscillation time-period (τ_i). But their oscillation is very slow compared to that of the electrons and thus, the simulation time-step is determined by τ_e.

20.3.3 Plasma generation and initialization of simulation

In laser isotope separation, one isotopic species in the atomic vapor beam is ionised by pulsed lasers. This process generates a plasma consisting of ions of the species of interest. Let us suppose, Yb-176, which has potential application for production of medically important radio-isotope Lu-177, needs to be separated from the atomic vapor beam of Yb, containing all its isotopes [229, 230]. For a vapor column of width 1 cm, and charge exchange cross-section of the order of 10^{-14} cm^2, the density (n_0) of Yb atomic beam should not exceed 10^{12} cm^{-3}, beyond which charge exchange between the isotope of interest and the other isotopes in the original atomic beam becomes significant [165, 236]. Considering a vapor density of $n_0 = 2 \times 10^{11}\ cm^{-3}$, the density of Yb-176 ions in the laser produced plasma can be calculated as $n_i = n_0\ A_N \times \alpha = 2 \times 10^{11}\ cm^{-3} \times 12.7 \times 10^{-2} \times 30 \times 10^{-2} = 7.6 \times 10^9\ cm^{-3}$, where A_N is the natural abundance of Yb-176 (12.7%); α is the ionisation efficiency of laser and is considered to be 30%.

The electron temperature (T_e) of the plasma is also a crucial parameter in deciding plasma behaviour. For isotopes with no low-lying meta-stable states, e.g. Yb-176, T_e is equivalent to the kinetic energy carried away by the released electron in the laser ionization process which is nearly equal to the difference between the photon energy and the ionization potential. In case of transient plasma generated by laser, ions do not achieve thermal equilibrium with the electrons during the process time-scale and have far less temperature than the electrons ($T_i < T_e$). But plasma expansion in free space is decided by the temperature of the electrons, and not of the ions as the ambipolar expansion velocity [235, 237] is given by $v_B = \sqrt{kT_e/m_i}$, where T_e is the temperature of the electrons, m_i is the mass of the ion and k is the Boltzmann constant. Therefore, the dynamics of the extraction process is dominated by T_e and not T_i. For the ionization schemes, generally adopted for photo-ionization of Yb-176, T_e is approximately 0.25 eV.

The choice on the number of super-particle is important for collecting sufficient statistical data [231, 232, 237]. To achieve necessary inter-particle interaction, more than ten super-particles per cell of the spatial grid are required [231, 232]. But that might not be sufficient enough for a smooth trend of a physical parameter, e.g. ion current recorded at a particular electrode near the plasma as a function of time. This, therefore, needs to be chosen on the basis of the required level of precision.

The charge-to-mass ratio of a super-particle of a particular species of particles is identical to the charge-to-mass ratio of the real particles of that species. That is, the charge-to-mass ratio of an electron super-particle and that of an electron is the same. Similarly, the charge-to-mass ratio of an ion super-particle and an ion is the same. Because of this, the trajectory of an electron is identical to the trajectory of an electron super-particle. The same holds for ions, too.

The super-particles are considered to follow the Maxwell-Boltzmann distribution of speed in addition to an upward velocity corresponding to the flow velocity of the atomic vapor beam. Considering a vapour source temperature of 800 K, this flow velocity of the vapour is estimated to be ∼300 m/s at the laser-atom interaction region. The main parameters of the photo-plasma are summarised in table 20.1 along with their typical values.

Table 20.1: Plasma parameters for the Yb-176 photo-plasma.

Plasma parameters	**Typical values**
Plasma density	7.6×10^9 cm^{-3}
Electron temperature	0.25 eV
Plasma frequency	4.92×10^9 rad s^{-1} (= 0.78 GHz)
Debye length	0.04 mm
Ion drift velocity	300 m/s
Ion mass	176 u
Plasma volume	$1 \times 4 \times 14$ cm^3

20.4 Case study: Plasma Evolution With and Without External Electric Field

The schematic diagram of a typical ion extractor set-up [212] is shown in Fig. 20.1. This corresponds to the first and second runs of Yb-176 separation at the ATLA facility in Hall-6. The laser-generated plasma has a dimension of 1 cm x 4 cm x 14 cm, located symmetrically between a pair of meshes. The meshes have a separation of 55 mm between them and the geometrical transmission of each of them is ∼90%. A voltage of -1.5 kV is applied to one

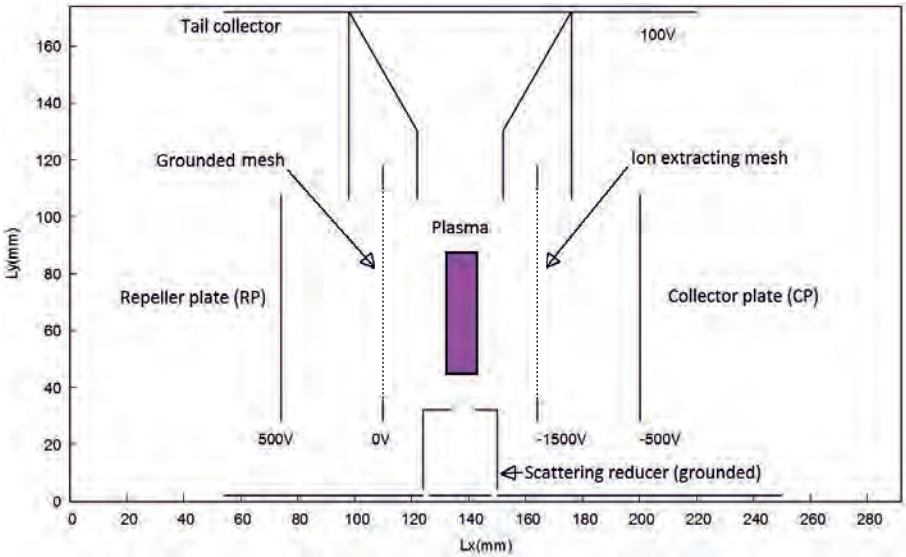

Figure 20.1: 2D schematic diagram of the ion extractor assembly used for the first and second runs of Yb-176 separation at the ATLA facility in Hall-6 along with the applied voltages to different components.

of the meshes, while the other is kept at ground, creating a cathode-anode pair. The mesh at -1.5 kV is expected to extract the ions from the plasma and transmit them through it onto a plate located at a distance of 40 mm from it. This plate, called the collector plate (CP), is generally kept at a potential of -500 V. On the other side, another plate, located at a distance of 40 mm from the grounded mesh and kept at a potential of +500 V, repels any ions transmitted through the grounded mesh towards that plate. This plate is referred to as the repeller plate (RP). The tail collector is kept at a slightly positive potential of ∼100 V to prevent ions from going upwards.

The extraction of ions from a plasma is not straight-forward, as the applied electric field cannot penetrate the whole block of plasma. Ions from only a thin layer of the plasma facing the electric field are influenced by the external field [237, 238]. The depth of this layer depends on the plasma density and the strength of the applied electrostatic field (for the case of RF field, it will depend on the frequency, too). For $n = 7.6\times10^9$ cm^{-3} and mesh potential of -1.5 kV, the penetration depth is ∼4 mm. Ions from this layer of plasma are accelerated towards the mesh with an average kinetic energy of ∼1.5 keV. After crossing the mesh, the ions face a decelerating electric field as the collector plate is at a higher potential relative to the mesh. The ions finally lands on the collector plate with an average kinetic energy equal to the potential of the collector plate (∼500 eV) [212].

The region between the mesh and the collector plate, because of its decelerating electric field, sends back a fraction of the ions towards the interaction region through the mesh setting up an oscillation of ions across the mesh. This results in an increase of ion loss onto the mesh structure due to multiple pass-throughs across it. Another effect of the defocusing field is the loss of ions in the gaps towards the upper and the lower sides of the region.

The plasma expands on its own because of an effect called the ambipolar diffusion [235]. For the aforesaid density of plasma, the plasma would take several hundred microseconds to fully diffuse. In the presence of an extracting electric field, however, a sheath of ions form in the plasma facing the external field and ions are extracted from this layer following the

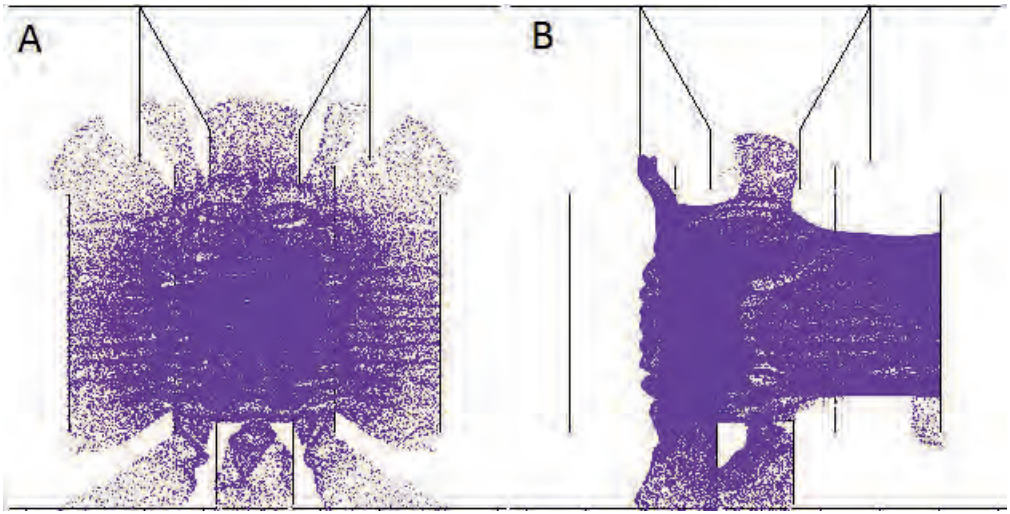

Figure 20.2: Ions' locations after 7 microseconds of plasma generation: (A) in absence of any external field, (B) in presence of the external electric field.

Child-Langmuir law [237, 238]:

$$J_{CL} = \frac{4}{9}\varepsilon_0\sqrt{\frac{2e}{m_i}}\frac{V^{3/2}}{d^2} \tag{20.8}$$

where V and d are respectively the potential drop and the distance between the plasma sheath and the mesh; m_i is the mass of the ions and J_{CL} is the ion current density (in A/m^2). This equation holds, as long as the current is in the space-charge limited region. For the density and geometry under consideration, the Child-Langmuir current comes out to be ~3 mA.

Figure 20.2 shows the evolution of the plasma ions computed using an in-house 2D PIC code. The locations of the ions after 7 microseconds from the generation of the plasma are shown with coloured dots for two different cases: with and without the external electric field. Without any external electric field, the plasma undergoes ambipolar diffusion in all directions. But in presence of the electric field, set up by the applied voltages, Child-Langmuir current, directed from the ion sheath of the plasma towards the negative mesh, dominates over the (isotropic) ambipolar diffusion current as explained above. It is to be noted that, under the influence of the applied electric field, extraction of ions and electrons occur (to different electrodes) simultaneously in similar time-scales (a few microseconds). Had there been no collective behaviour, electrons would have reached the repeller plate in just a few nanoseconds under the applied field. The extraction process completes in about 30 microseconds in presence of the applied field, whereas it continues for several hundred microseconds for the evolution driven by ambipolar diffusion. For the particular case study, the collection efficiency at CP is ~50% with an extraction potential of -1.5 kV.

20.5 Sources of Error

Energy is not conserved exactly in the PIC method of simulation the way momentum is. In PIC, potentials are calculated at the nodes of the spatial grid for a group of particles per cell. There can be infinite number of combinations of particle locations inside the cell for

which the potential values at the nodes are the same. This causes finite grid instability and results in lack of exact energy conservation [231, 232, 239]. This may lead to simulation artefacts and wrong diagnosis. Therefore, satisfying the stability conditions is not enough and one has to monitor the energy evolution for any required correction to time-step and grid spacing to achieve reasonably sufficient conservation of energy. Another error, specific to this case study, arises from the fact that the plasma evolves in all 3 dimensions, and the losses of particles in electrodes/components in the third dimension cannot be taken into account as the simulation code is 2D. This may result in ∼5% error in collection efficiency and it depends on the geometry and voltage parameters along the third dimension. On the other hand, a 3D code with spatial parameters ranging from λ_D ∼30 micron to L_x, L_y, L_z ∼20 cm will require about $3x10^{11}$ cells in the spatial grid for evaluating potential, which is extremely computation-intensive, let alone the fact that it has to run for about 10,000 time-steps to cover the entire plasma evolution.

20.6 Summary

The fundamentals behind the Particle-In-Cell (PIC) technique have been discussed and a test case of plasma expansion in a parallel plate-like field configuration has been simulated. The logic behind the choice of initial parameters for setting up a plasma simulation has been explained and the factors influencing the process of plasma evolution have been described. PIC is the method of choice for simulating transient plasma although it is computationally intensive and time-consuming. New hybrid methods are emerging where electrons are considered to be fluid and ions as particles, thereby eliminating the need for electron-level time-steps, but they are very application specific and they work under stringent input criteria.

Frequently Asked Questions

Q1. What is a super-particle? What is the need for considering a super-particle?

Q2. How is the time-scale and length-scale of a PIC simulation decided?

Q3. What is the difference between a transient plasma and a steady-state plasma?

Q4. Can the self-expansion process of plasma be used for ion collection instead of applying an external electric field?

Q5. Why cannot an electric field penetrate a plasma?

Q6. What is the basis of formation of an ion sheath in plasma under an external field?

Q7. What is the difference in time-scales for collection of ions and electrons under an external electric field?

Q8. What are the primary sources of error in the PIC method and how can those be minimised?