Particle in Cell Simulations and Correlation Heating

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The Particle-in-Cell (PIC) method, a cornerstone of plasma modeling, is widely employed for its ability to simulate kinetic phenomena within device-scale domains. This capability stems from the representation of numerous physical particles by computational macroparticles. Our work investigates correlation heating in PIC simulations, focusing initially on the feasibility of employing the PIC method to observe physical phenomena pertinent to atmospheric pressure discharges, such as disorder-induced heating (DIH). Subsequently, we explore artificial correlation heating (ACH) and its implications as a constraint on the applicability of PIC simulations.

In the first part of this work, molecular dynamics simulations are used to test when the PIC method applies to atmospheric pressure plasmas. It is found that PIC applies only when the plasma density and macroparticle weight are sufficiently small because of two effects associated with correlation heating. The first is the physical effect of DIH. This occurs if the plasma density is large enough that a species (typically ions) is strongly correlated in the sense that the Coulomb coupling parameter exceeds one $\Gamma_{ii} > 1$. In this situation, DIH causes ions to rapidly heat following ionization [1]. PIC is not well suited to capture DIH because doing so requires using a macroparticle weight of one and a grid that well resolves the physical interparticle spacing. These criteria render PIC intractable for macroscale domains. Furthermore, it is shown that simulations in reduced dimensions exacerbate these issues.

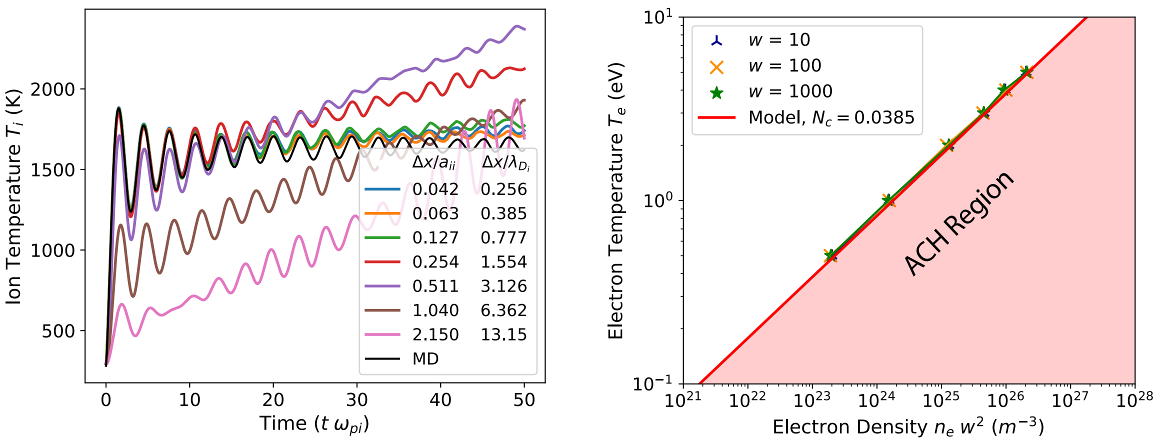

Fig. 1: (a) Evolution of the ion temperature for an ion density of $n_i = 2.5\times10^{24}$ m^{-3} and initial room temperature obtained from MD and using the PIC method for different grid spacing and unity macroparticle weight. (b) Limiting curve for ACH region from the the developed and numerical results from 3D-PIC simulations with different macroparticle weights.

The second part of this work is focused on a numerical error due to artificial correlation heating. ACH is like DIH in that it is caused by the Coulomb repulsion between particles, but differs in that it is a numerical effect caused by a macroparticle weight larger than one. Like DIH, it is associated with strong correlations. However, the macroparticle coupling strength is found to scale as $\Gamma^w = \Gamma w^{2/3}$, where Γ is the physical coupling strength and w is the macroparticle weight. So even if the physical coupling strength of a species is small, a sufficiently large macroparticle weight can cause the macroparticles to be strongly coupled and therefore heat due to ACH. We introduce a new constraint to PIC simulations necessary to avoid ACH. This requires that the macroparticle coupling strength be smaller than one $\Gamma^w < 1$. If this condition is violated, the finite macroparticle weight artificially enhances the coupling strength and causes the plasma to heat until the macroparticle coupling strength is near unity, depending on the grid resolution. A comprehensive model of ACH is developed that incorporates density, temperature, macroparticle weight, and grid resolution. It is then tested using PIC simulations, delineating the boundaries of the method's applicability and offering a predictive framework for ACH. Moreover, the research explores a runaway heating process induced by ACH in the presence of ionization, which can lead to numerical instability. A critical conclusion of this study is that the onset of ACH imposes more stringent constraints on the macroparticle weight and average number of macroparticles per cell than those typically employed in standard PIC simulations, thereby establishing a new limitation to the method's applicability.

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