Computational simulations of dusty plasma

by

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requirements for the degree of

Bachelors of Science
in
Physics

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Hey there reader,

First off, thank you SO MUCH for taking the time to read this!

Whether or not you're coming from a science background, you'll be able to help make this draft the best version of itself (in fact, those of you who are non-scientists end up providing some of the most useful insights!).

I'm looking to tell a story. That means, putting the details aside, that there's a macro-structure, a flow, an organization that has to be followed in order to effectively deliver this narrative. Keep in mind that conceptually I had to start somewhere– if you're curious, feel free to look things up (or to reach out)!

This is a rough draft, and there will undoubtedly be issues with grammar and, hopefully to a lesser extent, consistency of voice. The big questions for me are: "Does this thesis tell a story?" and "Does that story make sense?".

To help answer those questions, below are some of the things I'm looking for feedback on:

* Flow/organization (thesis as a whole)

* Flow/organization (chapter level)

* Flow/organization (section level)

* Use of jargon (over/under)

* Effectiveness of voice style used

* Should Chapters 1 and 4 be one chapter??

* Am I missing anything?

Read as much or as little as you'd like.

Thanks again,
Isa

Author's to-do list

* Add: Tables (experimental parameters and simulation parameters)

* Add: References

* Expand: Theory (CH2)

* Consider: Summaries

* Add: Links to git

* Add: To appendix - teaching tool?

* Add: To results - more graphs?

* Review: equations (ALL)

* Consider: would the sections make sense w/o the equations?

* Formatting: vectors in bold, plz

Abstract

From astronomy to industry, dust's ubiquitous presence in plasma (so called "complex" or "dusty" plasma) makes it an interesting object of study for a number of different fields. In some cases, it plays a critical role in the progression of certain processes, such as the formation of complex molecules in interstellar clouds. In laboratory environments, it can play a more troublesome role– hindering, for instance, the efficiency of integrated circuits which are the foundation of our modern technological capabilities. Advances in computing power have enabled the utilization of simulations as a tool for exploring the transport of dust particles in these low-pressure radio-frequency discharges. In this work, results of a Particle-in-Cell (PIC) simulation used to study charging of individual dust particles immersed in a collisionless electron-ion plasma is presented.

For those in search of a gentle introduction to computational plasma physics.
To those without whom this thesis would not exist.

Mil gracias.

Contents

List of Figures

Chapter 1

Background

Everything
Turns,
Rotates,
Spins...
Pulsates,
Resonates,
And
Repeats.

Suzy Kassem

As much as 99.999% of the matter in the observable universe is made up of plasma– an ionized or partially-ionized gas composed of electrons, ions, and neutral atoms– and much of it is laden with dust particulates with sizes ranging from submicron- to millimeters. This additional component in an otherwise typical plasma increases the complexity of the system, and is thus referred to as a "complex" or a "dusty" plasma.

Naturally-occurring complex plasma can be found in the interstellar medium, where it plays an important role in the formation of molecular hydrogen (Garscadden et al. 1994); it is embedded in protoplanetary disks, planetary rings, and in the tails of comets, and can even be observed as noctilucent clouds in the Earth's mesosphere.

In terrestrial environments, dusty plasma can be found everywhere from rocket exhaust to fusion devices, microelectronic fabrication and, of course, those created in the laboratory for scientific study. In industry, it can be regarded as technologically valuable for its applications in the medical field, where it can be used to treat wounds (Lacci et al., 2010); in microelectronics, where plasma processing has been

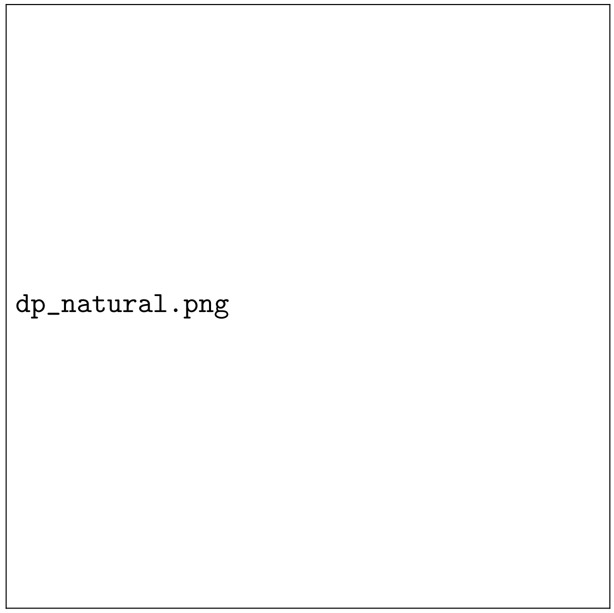

Figure 1.1: Examples of dusty plasma: a) on Earth, noctilucent clouds are high-altitude clouds consisting of charged ice particles; b) in space, the Cassini mission confirmed the presence of spokes in Saturn's rings caused by interactions of charged particles; c) human-made, rocket exhaust.

responsible for innovation and growth; and in aerospace, where ion drives are being developed as a way to break the tyranny of the rocket equation– thereby making long-term space travel practical.

Computational explorations of physical systems are unique in that they fill the space between theoretical and experimental worlds. Working with pen and paper (or pen and whiteboard) starts to break down as your system's complexity increases; on the other hand, some experiments are impractical due to lack of resources or (as in the case of fields such as astronomy) are impossible. Numerical techniques help pick up the slack and inform our knowledge and directions to take.

In the remainder of this work, we will look at some of the theory behind plasma and dust plasma, modeling techniques, motivating fields of interest, and how an electrostatic particle-in-cell algorithm was used to explore behaviors of plasma in the presence of dust.

Chapter 2

Characteristics of dusty plasma

> Physics depends on a universe
> infinitely centered on an equals sign.
>
> Mark Z. Danielenski

2.1 Primer: What is a plasma?

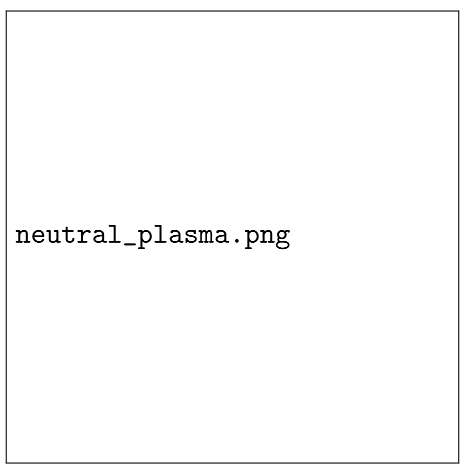

Figure 2.1: A quasi-neutral plasma contains roughly equal amounts of ions, or positively charged particles, and electrons, or negatively charged particles. From some distance away, the charges cancel each other out and is considered to be neutral. In this plasma we can pick out a single charge, Q, and use it as a way to understand how this plasma behaves.

In its simplest definition, a plasma is gas that has become so energetic that most or all of its constituent atoms are ionized (a process by which electrons are stripped from its parent atom). Looking at it another way, a plasma can be considered to be a "soup" of electrons and ions along with some neutral atoms. Taking it a step further, there are three conditions that need to be satisfied before you can call a plasma a plasma, but before we go into what they are, we need to first define important time and length scales. To do this, we will first consider a very simple plasma containing an equal number of ions and electrons (a condition called quasineutrality).

If we pick out one of the charges in this system, let's call Q our test particle, and look at the potential (recall that electric potential is the work per unit of charge needed to move that charge from one point to another) [FIG], we get the graph shown in [FIG]. This differs from the distribution for an isolated charged particles in free space (shown as dashed lines in FIG)– this is the Coulomb potential which drops off as the inverse of the distance. Our test particle embedded in the plasma, on the other hand, has a potential which at first drops off as the Coulomb potential, but for larger distances drops off more sharply.

shielding_graph.png

Figure 2.2: The solid line is the way the electric potential of a single (isolated) charge drops off over a given distance. The drop-off behavior of our Q embedded in an ambient plasma is shown in the dashed line. This is due to an effect called shielding. [ISA, lets make this one a two-parter figure. LEFT: Top: isolated particle, Bottom: reuse above figure. RIGHT: Graphs]

The potential function of an isolated point charge can be treated as a sphere of charge.

$$\phi = \frac{q}{4\pi\epsilon_0 r} \tag{2.1}$$

Compare this to the potential of our test charged embedded in the plasma,

$$\phi = \frac{q_T e^{-r/\lambda_D}}{4\pi\epsilon_0 r}. \tag{2.2}$$

where q_t is the charge, r is the distance, and λ_d is the Debye length.

As can be seen in both EQ and FIG, at points larger than the Debye length the potential approaches zero. It is at this point that the test charge has been "screened" or "shielded" from other charges in the plasma.

In a quasineutral plasma in which the ions are treated as immobile compared to the electrons, the Debye length is defined as,

$$\lambda_D = \sqrt{\frac{\epsilon T_e}{n_e q_e}}. \tag{2.3}$$

This quantity influences an important time scale– the plasma frequency, with the relation shown in [EQ 2.3].

Armed with the plasma frequency and Debye length, we can now talk about the three criteria for a plasma:

- Quasineutrality ($\lambda_d \ll L$)
- Collective effects dominate ($N\lambda_d^3 \gg 1$)
- Neutral collisions are negligible ($\omega\tau \gg 1$)

For an electrostatic plasma, that is a plasma in which no magnetic fields (external or self-generated) are present, three of the most important time and length scales to consider are plasma frequency, Debye length, and skin depth (there is a fourth parameter, the Larmour frequency, necessary to describe magnetic plasma which we will not consider here).

The frequency of plasma oscillations is given by the following,

$$\omega_p = \sqrt{\frac{4\pi n_s Z^2 e^2}{m_s}}, \tag{2.4}$$

where s is the species (electron, ion, or dust).

The Debye length is related to this frequency by,

$$\lambda_D = \frac{v_{ts}}{\omega_p}. \tag{2.5}$$

Here, v_{ts} is the typical velocity of a given species as determined by its Maxwell-Boltzmann distribution.

The depth at which plasma radiation can penetrate is called the plasma skin depth and is given by,

$$\lambda_{skin} = \frac{c}{\omega_p}. \tag{2.6}$$

A more comprehensive look at plasma physics can be found in the works of Chen (1964).

2.2 Conditions for a dusty (complex) plasma

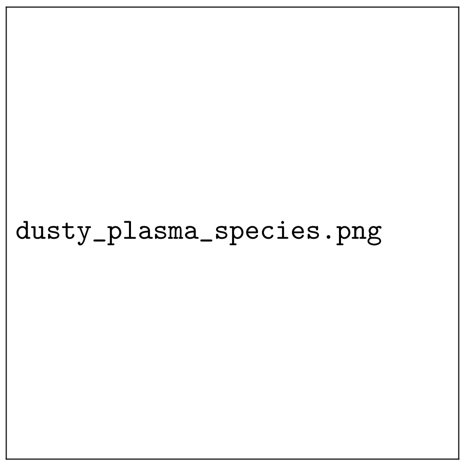

Figure 2.3: Components of a dusty plasma. Left to right: electron (e), ion (i), neutral atom (n), and dust particle (d).

The loose definition of complex plasma is the presence of dust particles in a normal plasma (Fig.1), however it is important to distinguish between simply having dust *in* plasma and having a *dusty plasma*. This distinction is dependent on the ordering of three characteristic length scales: the dust radius r_d, intergrain distance a, and the Debye length λ_D (Shukla et al., 2002). Debye shielding will be discussed in more detail in the next subsection.

$$r_d \ll \lambda_D < a \tag{2.7}$$

$$r_d \ll a < \lambda_D \tag{2.8}$$

Put another way, if the distance between dust particles is smaller than the Debye length (2), the dust participates in the collective behavior of the system; conversely, if the interparticle distance is larger than the Debye length (1), you can regard it as having a collection of isolated screened grains. Furthermore, if the distance between dust particles is much smaller than the Debye length ($a \ll \lambda_D$), then we can treat the dust grains as if they were massive charged particles (Shukla et al., 2002).

2.3 Debye shielding

Figure 2.4: Debye shielding of dust particles. A positively charged sheath with length λ_D results from the attraction of ions to the negatively charged dust particles that are separated by a distance a. This sheath shields the particles from 'seeing' the electric field generated by neighboring particles.

Figure 2 illustrates the concept of Debye shielding in a dusty plasma. If we regard a dust particle as a ball of charge, we expect that it would attract particles of opposite charge (i.e, negative electrons if the dust has a net positive charge, or ions if the dust has net negative charge). This attraction creates a cloud surrounding the dust particle, called a sheath, which shields the electric field of our dust particle from the rest of the plasma. In a complex plasma, however, dust particles are not perfectly shielded due to the velocity distribution of ions and electrons in the sheath.

2.4 Forces on dust particles

The basic governing equation describing the dynamics of a charged grain of dust with a mass m_d and velocity v_d is shown below.

$$M_d \frac{dv_d}{dt} = \vec{F}_E + \vec{F}F_G + \vec{F}_T + \vec{F}_D + \vec{F}_P, \tag{2.9}$$

where F_E is the electromagnetic force, F_G is the gravitational force, F_T is the thermophoretic force associated with a temperature gradient in the plasma, F_D is the drag force, and F_P is the radiation pressure force. The electromagnetic force is a combination of the Coulomb force and the Lorentz force, where E is the associated electric field, and B is the associated magnetic field.

$$\vec{F}_E = \vec{F}_C + \vec{F}_L = q_d \left(\vec{E} + \vec{v} \times \vec{B} \right). \tag{2.10}$$

For an electrostatic plasma, we would leave out the Lorentz force term.

2.5 Charging mechanisms

There are three basic processes by which dust particles immersed in an ambient plasma become charged:

- Interactions between dust and neutral particles
- Interactions between dust and energetic charged particles
- Interactions between dust and energetic charged particles

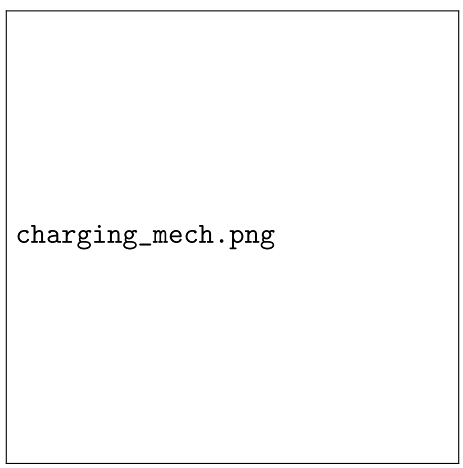

Figure 2.5: Left: Absorption of electrons incident to the dust particle's surface cause the dust to obtain a net negative charge. Right: An example of secondary emission as a result of highly energetic photons striking the dust particle (photoemission).

Don't be fooled, however! These elementary processes are actually quite complex and are difficult to understand, especially when trying to consider the different processes at one time as well as when looking at collections of dust particles. We will instead focus on the case of an isolated dust particle of finite size (i.e. several Debye lengths in diameter).

A dust particle placed in a plasma acts as a probe that will collect the primary species in that plasma. Absorption of the ions present will cause a dust particle to become positively charged. However, in laboratory plasmas it is often the case for dust particles to acquire a negative surface charge. This is because the thermal velocity of electrons is much greater than that of ions, thus the electrons will tend to reach the dust first.

The charge of a dust grain is described by the following equation,

$$\frac{dq_d}{dt} = \sum_s I_s(q), \tag{2.11}$$

Where I is the current and s is the particle species. For an electron-ion plasma, [EQ] becomes,

$$\frac{dq_d}{dt} = I_e + I_i. \tag{2.12}$$

At equilibrium,

$$\frac{dq_d}{dt} = \sum_s I_s = 0, \tag{2.13}$$

and with no net current flow, the dust particle is left with a surface potential (which, again, tends to be negative for laboratory dusty plasmas). A [TABLE] can be found listing the typical surface potentials for the most commonly used plasma sources.

$$I_s = \sum_s \int q_s f_s \sigma_s(v, q) v d\vec{v}, \tag{2.14}$$

where $v \equiv |\vec{v}|$ is the absolute value of the speed of the particles, and σ_s is the charge-collection cross-section (Vladimirov, 1997) given as

$$\sigma_s = \pi a^2 \left(1 - \frac{2q_s q_d}{a m_s v^2}\right) \quad \text{if} \quad \frac{2q_s q}{a m_s v^2} < 1, \tag{2.15}$$

and

$$\sigma_s = 0 \quad \text{if} \quad \frac{2q_s q_d}{a m_s v^2} \geq 1. \tag{2.16}$$

A negatively charged dust particle can become positively charged through secondary electron emissions resulting from surface impacts with energetic electrons and ions [FIG], or through the process of photoemission, in which an energetic ultraviolet photon (found both in space and industry environments) incident on the dust's surface emits electrons [FIG].

(FIG) illustrates the concept of Debye shielding in a dusty plasma. If we regard a dust particle as a sphere of charge, we expect that it would attract particles of opposite charge (i.e, negative electrons if the dust has a net positive charge, or ions if the dust has net negative charge). This attraction creates a cloud surrounding the dust particle, called a sheath, which shields the electric field of our dust particle from the rest of the plasma. In a complex plasma, however, dust particles are not perfectly shielded due to the velocity distribution of ions and electrons in the sheath.

Another important consequence is the interplay of charges that allows particles to cluster/grow and create grains/larger particles.

Chapter 3

Plasma modeling

> There is no need to ask the question, *"Is the model true?"*...The only question of interest is *"Is the model illuminating and useful?"*.
>
> *George Box*

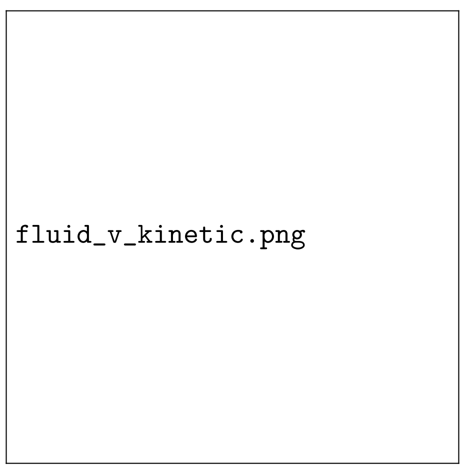

Figure 3.1: LEFT: Fluid models tend to dominate fields such as astrophysics and astronomy. Pictured: Simulation of a supernova explosion (REF). RIGHT: Kinetic models are often used for low-temperature, low-pressure plasmas such as those typically used in (WHICH) industry. Pictured: (NOT SURE, BUT WILL NEED SOMETHING AND A REF)

Plasmas are dynamic, nonlinear, and can often be unstable. As such, numerical modeling is essential for filling the gaps in our knowledge and is a critical tool for informing experimental diagnosis and experimental design (Bell, 1998). To be able to *fully* describe a problem in three dimensions, you really need six: three in position space, and three in velocity space. The goal, as is also the case for the theoretical and experimental branches of plasma physics, is to be able to get at the *essence* of plasma. The challenge is to be able to leave out just enough details while maintaining the integrity of the information you later want to retrieve. Surprisingly, you can leave out a lot! A spatial dimension or two, for instance. This is because plasma is a collective phenomena. Going back to the condition we laid out in SECTION 2.1, we are interested in plasma systems that are much longer than the Debye length ($\lambda_D \ll L$).

For a plasma that has magnetic fields (internal and/or applied) and for whose particles you can ignore quantum effects, we can fully describe it using Maxwell's equations.

$$\nabla \cdot \vec{E} = -\frac{\rho}{\epsilon_0}, \tag{3.1}$$

$$\nabla \times \vec{E} = -\frac{\partial B}{\partial t}, \tag{3.2}$$

$$\nabla \cdot \vec{B} = 0, \tag{3.3}$$

$$\nabla \times \vec{B} = \mu_0 \left(J + \epsilon_0 \frac{\partial \vec{E}}{\partial t} \right). \tag{3.4}$$

Plasma simulations can be split into two categories: fluid and kinetic [FIG 3.1]. A kinetic description is the more physically realistic of the two, as it focuses on the effects of motion of charged particles within a plasma (Callen, 2003). It is this type of model that dominates the literature [REFS]. Particle-in-cell (PIC) and cloud-in-cell (CIC) simulation methods are some of the more common examples of kinetic simulations. At the most basic level, PIC and CIC rely on a field solver and particle mover to add up behaviors and effects on an individual-particle level. While the physics here is more accurate, it suffers from computational limitations. [ELABORATE ON THOSE LIMITATIONS, AND MENTION THAT TRICKS CAN BE USED TO GET AROUND THESE. IT'S THE more sensible/practical method FOR A REASON]

PIC simulations are often supplemented by a Monte Carlo Collisions (MCC) module, which is a way of taking interparticle interactions into account. [EXPAND]

[ADD VLASLOV EQ?]

In contrast, fluid simulations reduce the computational complexity by focusing on macroscopic behaviors (e.g. density) of charged particles. This dispenses with phase space information, collapsing a 6d problem into a 3d velocity space. The payoff is the to simulate large systems for long periods of time (Bell, 1998).

[HYBRID BIT] This reduction in complexity also results in the loss of some of the physics which can be recovered through a hybrid approach.

Chapter 4

Motivation

Fascinating.

Mr. Spock

4.1 Dusty plasma in space

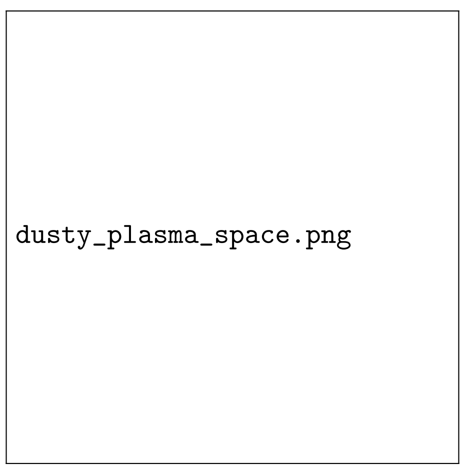

Figure 4.1: Dusty plasma in LEFT: interstellar environment (REF) RIGHT: microgravity (REF)

Interest in dusty plasma as an astrophysical phenomena dates back to the 1980s. Examples in our solar system include cometary tails and Saturn's rings, which consits of charged ice and rock (NOT THE RIGHT WORD) particles. The 1980 flyby of Saturn by Voyager 2 was the first time dynamic behavior was observed in Saturns rings. Termed "spokes", it's believed that these interactions are the result of the interplay between charges and electric fields, a belief that was followed up by the Cassini mission in 2006.

Leaving our galactic neighborhood, we find that nebula, interstellar clouds of dust and ionized gases, are also full of complex organic molecules which may help give us clues to the origin of life.

4.2 Dusty plasma in fusion devices

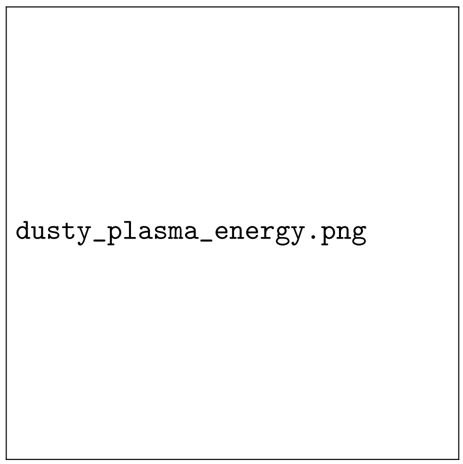

Figure 4.2: Dusty particles in thermonuclear fusion devices (REF).

From inertial confinment devices to the high-energy thermonuclear fusion chambers these alternative forms of energy have the potential to help alleviate humankind's dependence on fossil fuels. These technologies, perpetually a decade or two on the horizon, harness plasma as their secret weapon. In the case of thermonuclear fusion, tokamak reactors generate plasmas with energies in the [MILLIONS? eV]– that's [SOME ANALOGY HERE]! These hot dense plasmas, while contained using magenetic fields, are still energetic enough to interact with the chamber walls. This not only compromises structual integrity, but the debris from those interactions end up entering the plasma at a rate of [WHATS THE RATE?] [REF].

In ICF devices, I'm not sure what to say but the plasma characteristics are different and the dust forms in these ways.

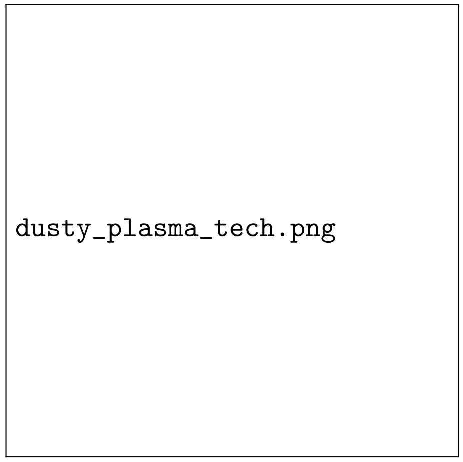

Figure 4.3: Dusty plasma in semiconductor processing devices (REF).

4.3 Plasma sources in semiconductor processing

Capacitavely Coupled Plasmas are the most frequently used in the creation/development of the semiconductor wafers that are found in all of our electronic devices. [FIG] The plasma sources in these processing technologies are typically [THESE GASES], but CF3 (a fluorocarbon) tends to result in a self-generated contamination process. Somehow, clumps start to form, and somehow these larger pieces make their way to the surface of these wafers. This creates a layer of contamination that needs to be remove, thereby adding a step in the manufacturing process.

Chapter 5

Description of the model

There is no problem more difficult
to solve than that created by
ourselves.

Felix Alba-Juez

5.1 Governing Equations

For an electrostatic plasma, a plasma for which no external magnetic fields are imposed and currents are sufficiently slow such that self-generated magnetic fields can be ignored, we need only concern ourselves with the electric potential and electric fields. These are given to us through [EQ 2.1], where the electric field is given as,

$$\vec{E} = -\nabla\phi. \tag{5.1}$$

This turns [EQ 3.1] into Poisson's equation,

$$\nabla^2\phi = -\frac{\rho}{\epsilon_0} \tag{5.2}$$

We can then pair these equations with a recasting of Newton's second law of motion (F = ma) to move the particles.

$$\frac{d\vec{v}}{dt} = \frac{q}{m}\vec{E}, \tag{5.3}$$

$$\frac{d\vec{x}}{dt} = \vec{v}. \tag{5.4}$$

[NEEDS BIT ON BOLTZMANN RELATION FOR IONS]

5.2 Particle in Cell Method

plasma_on_grid.png

Figure 5.1: 1d vs 2d plasma on a grid. In 1-dimension, charges are infinite sheets while in 2-dimensions each macrocharge encompasses a grid cell.

pic_algorithm.png

Figure 5.2: A flow chart laying out the Particle-in-Cell algorithm.

As illustrated in [FIG 5.2], the general outline of a PIC code proceeds as follows (1) $\vec{x}_{particle} \rightarrow$ (2) $\rho_{grid} \rightarrow$ (3) $\phi_{grid} \rightarrow$ (4) $\vec{E}_{grid} \rightarrow$ (5) $\vec{F}_{particle}$. This is looped until a steady state is reached.

Steps (1) to (2) and (4) to (5) are achieved using a weighting scheme, while the others require a recasting of the equations to a finite-difference form. The use of a spatial grid in 2-dimensions leads to finite-sized square particles, and while they are fairly symmetric, this can lead to some unwanted effects due to the fact that the forces on the particles will depend on their position within the cell in addition to the distance to other particles.

A comprehensive look at plasma simulations can be found in the seminal work Birdsall and Langdon (2005). In the sections that follow, we will take a brief look at the individual components outlined in [FIG].

5.2.1 Weighting (charge deposition)

Figure 5.3: Area weighting used to deposit charge.

Once we've set up our spatial domain, the first thing we need to do is distribute our charged particles. There are several ways to go about this, but one of the common schemes is to use what's called a first order weighting scheme [FIG], (also called area weighting or linear interpolation). This is given by the following,

$$w_1 = \frac{(\Delta x - x)(\Delta y - y)}{\Delta x \Delta y}, \tag{5.5}$$

$$w_2 = \frac{x(\Delta y - y)}{\Delta x \Delta y}, \tag{5.6}$$

$$w_3 = \frac{(\Delta x - x)y}{\Delta x \Delta y}, \tag{5.7}$$

$$w_4 = \frac{xy}{\Delta x \Delta y}. \tag{5.8}$$

Here, Δx and Δy are fractional directions in the x and y directions respectively and $\Delta x \Delta y$ is the cell volume. At the boundaries of our domain, we have to account for the fact that only half of the grid cells are contributing (REF).

Once the charge has been distributed, the charge density, ρ, is then computed by dividing the total charge by the volume of each grid cell.

5.2.2 Solving for Φ

Once we have the charge density in hand, we can plug that into the right hand of [EQ 3.2] and put it into a finite-difference form using central differencing (also called a five-point difference),

$$\frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{\Delta x^2} + \frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}}{\Delta y^2} = -\frac{\rho_{i,j}}{\epsilon_0}. \tag{5.9}$$

5.2.3 Field solvers

With the potential calculated, we can put that into [EQ 5.1] and use a two-point difference to calculate the electric field at those points,

$$\vec{E}_x = \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\Delta x}, \tag{5.10}$$

and

$$\vec{E}_y = \frac{\phi_{i,j+1} - \phi_{i,j-1}}{2\Delta y}. \tag{5.11}$$

5.2.4 Add/Move Particles

Using the force (EQ 5.3), we then advance our particles one time step Δt. To do this, the leapfrog method is commonly employed [FIG 5.4] by taking EQ. 5.3 and 5.4 and replacing them with a finite difference,

$$\frac{v_{new} - v_{old}}{\Delta t} = \frac{q}{m}\vec{E} = \vec{F}_{old}, \tag{5.12}$$

and

$$\frac{x_{new} - x_{old}}{\Delta t} = v_{new}. \tag{5.13}$$

This requires the velocity to be pushed back to a negative half time step using the force calculated at $t = 0$, and for resulting calculations (i.e. the electric field) to be adjusted in such a way that they appear at the same time.

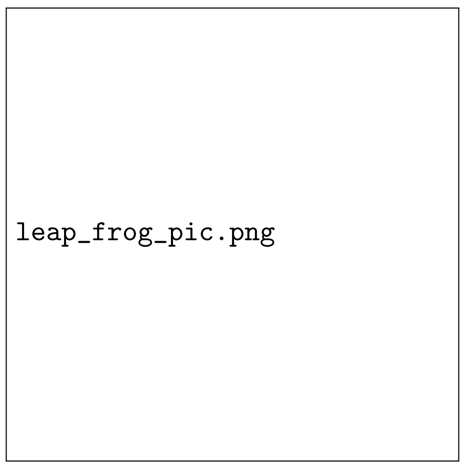

Figure 5.4: An illustration of the leap-frog method. We time-center the force while advancing the particle's velocity, and likewise time-center the velocity while advancing a particle's position.

Chapter 6

Simulation results

> Physicists like to think that all you have to do is say, these are the conditions, now what happens next?
>
> *Richard Feynman*

6.1 1D PIC Results

[TABLE: SIMULATION PARAMETERS (NX, NY, DT, N...)]

Building computational environments is a modular process. As such, it's critical to test as you go. We'll start with the 1D case which consists simply of electrons moving in a background of ions. To this program, we'll apply a benchmark test: the two-stream instability. This problem, illustrated in [FIG] models two opposing streams of electrons. [FIG] shows the time evolution of this stream, given an initial perturbation, in phase space (position vs velocity instead of the familiar position/velocity vs time).

What do we mean by perturbation? Well consider that a perfectly stationary beam of like charges will be equally spaced from each other in some equilibrium configuration. Disturbing a single particle from its equilibrium position is going to oscillate around that point at some frequency. To disturb *all* of the charged particles in this beam, as is the case in these simulations, we get a sinusoidal response where a particle's position is described as follows,

$$x = x_0 + x_1 cos\left(x_0 \frac{2\pi n}{L}\right), \tag{6.1}$$

Figure 6.1: Top: Two opposing electron streams moving in a background of ions. An instability will develop due to charge bunching as the streams move through each other. Bottom: Evolution of the electron-electron two stream instability in phase space at times a) t=0, b) t = 49, c) = 99, and d) t = 199. The initial velocities are 0.2, the grid has 1000 cells, there are 20000 particles per beam, and the beams have an initial sinusoidal perturbation of mode 2.

Here L is the length of the length of the domain and n is the mode of excitation of the wave.

Allow that initial perturbation to run over time, and adding the second opposing beam in the mix, you get an instability that grows exponentially over time (Landon and Birdsall, 2005). We see this play out in [FIG].

6.2 2D PIC Results

[TABLE: SIMULATION PARAMETERS (NX, NY, DT, V_D...)]

Upon implementing a 2D version of 6.1, a dust particle [some number of micrometers] in diameter with a potential of [some negative number of Volts] was added. In this case, the electrons were treated as a background fluid (VALIDATION?), and we focus instead on the behavior of the flowing ions in the presence of this massive charged particle. [FIG] shows some of the results of these simulations. We are looking here at how the electric potential (REMIND PPL WHAT THAT MEANS) is distributed at any given time. Notice (what are things we'd expect to notice?)

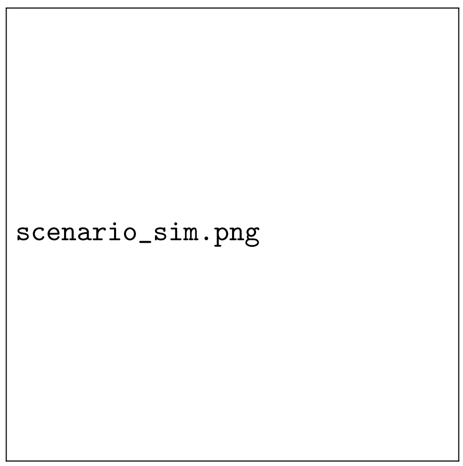

Figure 6.2: A single dust charge in an ambient plasma. Electrons are treated as a background fluid, and ions flow around the particle with a fixed potential.

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Pinhão, N. (2007). pypk-A Python extension module to handle chemical kinetics in plasma physics modeling.

This paper describes a Python library package (plasmakin.py) that was developed to tackle the chemical and physical computations needed for plasma physics modeling. Such a package allows for integration with existing Python modules, such as Scipy and Matplotlib, in a way that enables the efficient development of reliable programs. The paper also contains an example of how the library can be called into a user's program, through the simulation of the passage of an electron swarm through gas.

Ricci, P., Lapenta, G., de Angelis, U., Tsytovich, V. N. (2001). Plasma kinetics in dusty plasmas. Physics of Plasmas, 8(3), 769-776.

Seo, H., Kim, S. B., Song, J., Kim, Y., Soh, H., Kim, Y. C., Jeon, H. (2002). Low temperature remote plasma cleaning of the fluorocarbon and polymerized residues formed during contact hole dry etching. Journal of Vacuum Science Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena, 20(4), 1548-1555.

Shoeb, J., Kushner, M. J. Comparison Of Cleaning And Damage Of Porous Low-k SiCOH In Ar/O2 And He/H2 Plasmas With UV/VUV Fluxes.

Shoeb and Kushner give a succinct overview of the current challenges in semiconductor manufacturing, including one–the buildup of a polymer contaminant–that is the byproduct of a particular solution (the introduction of porous low dielectric constant materials such as silicon dioxide), and is the motivation behind their work. Their approach utilizes numerical modeling via The Hybrid Plasma Experiment Model (HPEM) to characterize and compare the effects of two different types of plasma hybrids (Ar/O2 and He/H2) and their effects on both the polymer residue and underlying low-k surface. It was concluded that the He/H2 was more effective at removing polymer without causing significant damage. Additionally, it was also noted that the interconnectivity of pores played a role, as interconnective pores allow for additional pathways into the materials and thus more opportunities for damage.

Shoeb, J., Wang, M. M., Kushner, M. J. (2012). Damage by radicals and photons during plasma cleaning of porous low-k SiOCH. I. Ar/O2 and He/H2 plasmas. Journal of Vacuum Science Technology A: Vacuum, Surfaces, and Films, 30(4), 041303.

Shukla, P. K., Mamun, A. A. (2002). Introduction to dusty plasma physics. IoP Publishing.

This textbook is a repository of the progress that had been made in dusty plasmas between the 1990's and early 2000's. Chapters 1-3 will be the most useful sections of this textbook, as they cover: 1) the historical background, characteristics, and aspects

of dusty plasmas, 2) dust charging processes, and 3) the dynamics of dust grains. Chapters 2 and 3 in particular will be important for understanding the parameters that need to be taken into account when building a numerical model, such as particle interactions, consequences of charging processes, as well as forces that act on the dust particles.

Somashekhar, A., Ying, H., Smith, P. B., Aldrich, D. B., Nemanich, R. J. (1999). Hydrogen Plasma Removal of Post-RIE Residue for Backend Processing. Journal of The Electrochemical Society, 146(6), 2318-2321.

Appendix A

Sample: Python code

The most current version of the 2D code used in this project can be found on my Github page, https://github.com/space-isa. Included is an annotated notebook created using the Jupyter platform, as well as a .py file that can be downloaded and run. Take it, reproduce it, break it, change it, share it!

Included below is a sample of the main cycle used to run the simulations presented in Chapter 6.

```
start = time.clock()

NP = 0
print("Calculating...")

for count in range(0, iterations):

    q = np.zeros((nx, ny))
    rho = np.zeros((ny, nx))

    for p in range (1, NP):
        fi = (1 + p_pos[p,0]) / (dh)
        i = np.floor(fi)
        hx = fi - i

        fj = (1 + p_pos[p,1]) / (dh)
        j = np.floor(fj)
        hy = fj - j
```

```
    q[i,j] = q[i,j] + (1-hx) * (1-hy)
    q[i+1, j] = q[i+1, j] + hx * (1-hy)
    q[i, j+1] = q[i, j+1] + (1-hx) * hy
    q[i+1, j+1] = q[i+1, j+1] + hx * hy

rho = (sw + q_mp * q) / (dh * dh)

rho[0,:] = 2 * rho[0,:]
rho[-1, :] = 2 * rho[-1, :]
rho[:, 0] = 2 * rho[:, 0]
rho[:, -1] = 2 * rho[:, -1]

rho = rho + (1 * 10 ** 4)
#print(rho)

#potential solver
V = solver_2d(rho, tol, Ti, n0, V_ref, QE)


#E field solver
Ex = np.zeros([nx, ny])
Ey = np.zeros([nx, ny])
E = np.zeros([nx, ny])

#internal nodes
Ex[1:nx-1, :] = V[0:nx-2,:] - V[nx-(nx-2):, :]
Ey[0: ,1:nx-1] = V[:, 0:ny-2] - V[:, 2:ny]

#boundaries
#multiplied by 2 to keep values equivalent to internal nodes
Ex[0,:] = 2* (V[0,:] - V[1,:])
Ex[nx-1, :] = 2 * (V[nx-2,:] - V[nx-1, :])

Ey[:, 0] = 2 * (V[:,0] - V[:,1])
Ey[:,ny-1] = 2 * (V[:, ny-2] - V[:, ny-1])
```

```
Ex = np.floor (Ex / (2 * dx) )
Ey = Ey / (2 * dy)


#generate particles

if NP + np_in >= N:
    np_in = N - NP

#insert particles
#(NOTE: save this for after 2d environment works)

#x position
p_pos[NP:NP+np_in, 1:] = np.random.rand(np_in,1) * dh

#y position
p_pos[NP:NP+np_in, 1:] = np.random.rand(np_in,1) * Ly

#sample Maxwellian in x,y
#add drift velocity in x

p_velo[NP:NP+np_in, 1:] = v_drift + (-1.5 + np.random.rand(np_in,1)
     + np.random.rand(np_in,1) + np.random.rand(np_in, 1)) * vth
p_velo[NP:NP+np_in, 1:] = 0.5 * (-1.5 + np.random.rand(np_in,1)
     + np.random.rand(np_in,1) + np.random.rand(np_in, 1)) * vth

#move particles
p = 1

while p <= NP:

    fi = 1 + p_pos[p,0]/dx
    i = np.floor(fi)
    hx = fi - i

    fj = 1+ p_pos[p,1]/dy
    j = np.floor(fj)
```

```
    hy = fj - j

    E = ([Ex[i, j], Ey[i,j]]) * (1-hx) * (1-hy)
    E = E + ([Ex[i + 1, j], Ey[i + 1, j]]) * hx * (1-hy)
    E = E + ([Ex[i, j + 1], Ey[i + 1, j]]) * (1-hx) * hy
    E = E + ([Ex[i + 1, j + 1], Ey[i + 1, j + 1]]) * hx * hy

    F = QE * E
    a = F/MI

    p_pos[p, :] = p_velo[p, :] + a * dt
    p_velo[p, :] = p_pos[p, :] + p_velo[p, :] * dt

    if p_pos[p,1] < 0:
        p_pos[p,1] = -p_pos[p,1]
        p_velo[p,1] = -p_velo[p,1]

    p = p + 1
    print(p_pos, p_velo)

print("Clocking in at %s seconds"  % (time.clock() - start))
```