Contents

Chapter 1

Theoretical Background

1.1 Plasma

This section presents a short overview of basic plasma theory, it can serve as a quick reminder for those already familiar with the subject, and necessary background to understand the numerical simulations in this work. For a more thorough introduction the books *Plasma Physics* (Fitzpatrick, 2014), *Introduction to Plasma Physics* (Goldston and Rutherford, 1995), *Waves and Oscillations in Plasmas* (Pécseli, 2012) or the classic *Introduction to Plasma Physics and Controlled Fusion* (Chen, 1984) can be consulted.

Plasma is the fourth, lesser known, state of matter. It is similar to a gas in that the particles are free to move, but it has the key distinction that a part of its constituent particles are electrically charged.

> *”A plasma is a quasineutral gas of charged and neutral particles which exhibits collective behaviour.”*
>
> **Francis F. Chen**

The charge causes the particles to be subject to the Lorentz force, which changes the behaviour of the gas. The plasma state is a typical state of matter and appears in various environments, i.e. the sun, and other stars, the upper parts of Earth’s atmosphere, and has many industrial applications as plasma cutters , argon light tubes, fusion.

A greater understanding of the mechanism governing a plasma’s behaviour can help us predict spaceweather, improve design of spacecraft and instruments affacted by plasma.

Figure 1.1: Plasmas occurs both in the hot and dense condiotions in necessary for fusion, as well as in the cold and sparse interstellar environment.

1.1.1 Plasma Parameters

Temperature

A modern view of temperature comes from kinetic theory developed by Maxwell and Boltzmann (Swendsen, 2006). We will not go through it here but a treatment is available in Goldston and Rutherford (1995). Temperature is then related to the average kinetic energy of a particle. For an ideal monoatomic gas the kinetic energy is then

$$\bar{E}_k = \frac{1}{2} m v_{th}^2 = \frac{3}{2} kT \tag{1.1}$$

Here we have introduced $v_{th} \equiv \sqrt{kT/m}$ as the thermal velocity, i.e. the average velocity of a particle considering only 1 dimension. It should be mentioned that the fraction in front of the temperature is dependent on the degrees of freedom of the particle. A monoatomic particle can only move in three directions, but a diatomic particle can also vibrate and spin.

In high energy plasma physics it is also costumary to drop the Boltzmann factor, k, in eq. (1.1), and express temperature directly in electronvolt, eV. Electronvolt is defined as the energy it takes to move an elementary charge through a potential difference of 1 V, and corresponds to approximately 11600K. For the space and atmospheric plasmas, we are mostly dealing with here, the temperatures are generally low, so we will use the Kelvin scale for temperature.

If the particles in a plasma collide often compared to the characteristic timescales of energy and particle changes, the particle velocity distribution can be approximated by a Maxwellian distribution. It is only then that the concept of temperature is valid (Goldston and Rutherford, 1995).

Electron Plasma Frequency

A rather important frequency in plasma physics is the electron plasma frequency (Chen, 1984),

$$\omega_{pe} \equiv \sqrt{\frac{ne^2}{\epsilon_0 m_e}} \tag{1.2}$$

This frequency, ω_{pe}, is dependent on the number density, n, the fundamental charge, e, the vacuum permittivity, ϵ_0, and the electron mass, m_e. It can be thought of as a typical electrostatic oscillatory frequency. Consider an electrically neutral 1D slab, which is then disturbed, from its neutrality, by an infinitesimal charge density on one side.

$$\sigma = en\delta x \tag{1.3}$$

It will have an equal and opposite charge density on the other side. The slab will then have an electric field due to the charge density, caused by Gauss' Law.

$$\frac{\partial E_x}{\partial x} = -\frac{\sigma}{\epsilon_0} \qquad \rightarrow \qquad E_x = \frac{-en\delta x}{\epsilon_0} \tag{1.4}$$

Inserting this field as the only force in Newtons law for a single particle yields

$$m\frac{\partial \delta x}{\partial t} = eE_x = -m\omega_{pe}^2 \delta x \tag{1.5}$$

The particle will then oscillate around its equilibrium position with the electron plasma frequency. The same phenomen often happens in plasma as it tries to go back to its equilibrium and is called plasma oscillations, or Langmuir oscillations, see section 1.5 for a treatment of plasma oscillations.

An otherwise useful timescale is the reciprocal of the plasma frequency, the plasma period

$$\tau_p \equiv 2\pi/\omega_{pe} \tag{1.6}$$

Some researchers prefer to define the τ_p, without the 2π prefactor, as that makes some concepts neater.

Debye Shielding

Debye shielding length is the distance at which the electric influence from a particle is shielded out by the surrounding plasma. Consider a charged particle immersed in a plasma bath. The plasma is in a thermodynamical equilibrium, i.e. there is no significant temperature gradients. We artificially place a positively charged ion into the plasma. This ion will then attract electrons and repel positive ions. There will be a tendency for there to be more negativily charged particles, and less positive, near the ion, which in effect will work as an electric shield around the ion. The distance away from a particle, where its field is reduced by a factor $1/e$, called the Debye Shielding Length, λ_D.

$$\lambda_D \equiv \sqrt{\frac{\epsilon_0 k T_e}{n_e e^2}} \tag{1.7}$$

The above definition is often used, (Pécseli, 2012), neglecting the ion influence since they often have a much lower temperature. The shielding length is dependent on the ratio between temperature, T_e, and electron density, n_e. In a varmer plasma the particles will move quickly and efficiently shield any charges, so the λ_D becomes smaller. While In cases where we also need to account for ions, a more complete definition can be used

$$\lambda_D \equiv \sqrt{\frac{\epsilon_0 k T_e}{n_e e^2 (1 + Z\frac{T_e}{T_i})}} \tag{1.8}$$

Due to the earlier argument, and the statistical approach used when deriving it (Goldston and Rutherford, 1995), there must be a significant amount particles close to the ion to shield it out.

It should be noted that the shielding length is related (Fitzpatrick, 2014) to the plasma period and the thermal velocity through

$$\lambda_D \omega_{pe} = v_{th} \tag{1.9}$$

Quasineutrality

The assumption of quasi-neutrality is a crucial approximation for collective phenomen in plasma physics. By quasi-neutrality we assume that the electron density is equal to the ion density, $n_e \approx n_i$. This is often called the *"plasma approximation"* (Chen, 1984). This approximation is usually valid on length scales much larger than the shielding length. If we had a case where a large volume of plasma lost a significant amount of charge, a large electric field would accompany the density imbalance. This electric field would quickly correct the imbalance, and quasineutrality would be regained.

Plasma Classification

For a plasma description to be applicable the system we consider must have a typical length scale, L, and time scale, τ, larger than the Debye length and plasma period respectively.

$$\frac{\lambda_D}{L} \ll 1 \qquad\qquad \frac{\tau_p}{\tau} \ll 1$$

A plasma treatment aims to describe the collective behaviour of many particles. If the length scale is smaller than the λ_D the charges from individual particles are not effectively shielded out and the trajectories of each particle should be considered. On a shorter timescale than the τ_{pe} the plasma oscillation is can be averaged out and needs treatment.

1.2 Single Particle Motion

To better understand the collective motion of plasma it is useful to consider the motions of the single particles that the plasma consists of. By at first treating only one particle we can ignore the electromagnetic influence from the other particles which greatly simplifies the situation. The Lorentz force, eq. (1.10), governs the dynamics of a charged particle in a plasma, provided that other forces, e.g. gravity, are neglible. The Lorentz force is due to charged particles in the electric field, **E**, and charged particles moving across the magnetic field **B**

$$\mathbf{F} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) \tag{1.10}$$

To simplify matters we will only consider particles in static electric and magnetic fields, as that is often a valid approximation on the time and spatial scales of interest.

1.2.1 Gyration

Let us consider a situation with a single moving particle in a static and isotropic external magnetic field, a similar set up as in Baumjohann and Treumann (1997). Newtons Second law together with eq. (1.10) then gives

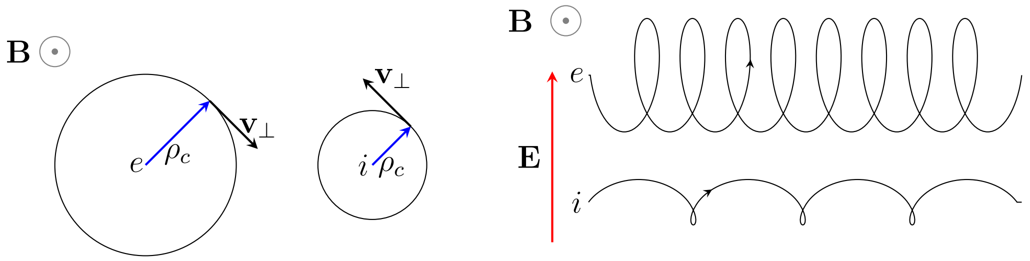
$$m\frac{\partial \mathbf{v}}{\partial t} = q\mathbf{v} \times \mathbf{B} \tag{1.11}$$

We should note that the velocity component parallel to the magnetic field, is not affected by the field and will remain constant, $\frac{\partial \mathbf{v}_\parallel}{\partial t} = 0$. The cross product of two parallel vectors is always zero, so $\mathbf{v}_\parallel \times \mathbf{B} = 0$. Using these two notions we can write the equation only in terms of the perpendicular, with respect to **B**, velocity.

$$m\frac{\partial \mathbf{v}_\perp}{\partial t} = q\mathbf{v}_\perp \times \mathbf{B} \tag{1.12}$$

Then we perform a temporal derivative.

$$\frac{\partial^2 \mathbf{v}_\perp}{\partial t^2} = \frac{q}{m}\frac{\partial \mathbf{v}_\perp}{\partial t} \times \mathbf{B} \tag{1.13}$$



(a) The trajectories of an electron, left, and a positive ion, right, is shown The particles trajectory is a gyration around the magnetic field lines.

(b) Here we can see a particle experiencing the E-cross-B drift. The motion consists of a gyration as well a constant drift along the x-axis.

Then we insert eq. (1.12) into the equation and use the vector relation $a \times b \times c = b(a \cdot b) - c(a \cdot b)$.

$$\frac{\partial^2 \omega_\perp}{\partial t^2} + \left(\frac{qB}{m}\right)^2 \omega_\perp = 0 \tag{1.14}$$

In the last equation we also changed the term describing the rotational motion to $\omega_\perp$, which will from now on signify gyrational motion. This differential equation corresponds to a gyration around the magnetic field lines with the gyration frequency, $\omega_c = \frac{qB}{m}$, as the frequency. The particles are free to move parallel to the magnetic field lines causing a spiralling motion along the magnetic field lines, as illustrated in fig. 1.2a. This spiral effect is often an important part of why there are often field-aligned currents, such as 'Birkeland Currents' (Cummings and Dessler, 1967), transporting plasma along magnetic field lines.

1.2.2 E-cross-B Drift

A drift called E-cross-B drift can appear when a particle is moving within static and isotrop electric and magnetic fields. The equation of motion, neglecting all forces except the electromagnetic, is then

$$m\frac{\partial v}{\partial t} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{1.15}$$

In plasma physics it is often a good strategy to decompose quantities into parallel and perpendicular, with respect to $\mathbf{B}$, quantities. We start by seperating the velocity into $\mathbf{v} = \mathbf{v}_\parallel + \mathbf{v}_\perp$ and the electric field into $\mathbf{E} = \mathbf{E}_\parallel + \mathbf{E}_\perp$. Inserting this and using that $\mathbf{v}_\parallel \times \mathbf{B} = 0$ again the equation becomes

$$m\frac{\partial}{\partial t}\left(\mathbf{v}_\parallel + \mathbf{v}_\perp\right) = q\left(\mathbf{E}_\perp + \mathbf{E}_\parallel + (\mathbf{v}_\perp) \times \mathbf{B}\right) \tag{1.16}$$

The parallel motion consist of an acceleration caused by the parallel part of the electric field and is given by

$$m\frac{\partial \mathbf{v}_{\parallel}}{\partial t} = q\mathbf{E}_{\parallel} \tag{1.17}$$

The remaining part of the equation describes the perpendicular motion.

$$m\frac{\partial \mathbf{v}_{\perp}}{\partial t} = q\left(\mathbf{E}_{\perp} + (\mathbf{v}_{\perp}) \times \mathbf{B}\right) \tag{1.18}$$

Now we assume there is a time-invariant drift $\mathbf{v}_D$, i.e. not dependent on time, and then we seperate the perpendicular motion into a drift and gyration, $\mathbf{v} = \mathbf{v}_{\parallel} + \boldsymbol{\omega}_{\perp} + \mathbf{v}_D$.

$$m\frac{\partial}{\partial t}\left(\boldsymbol{\omega}_{\perp} + \mathbf{v}_D\right) = q\left(\mathbf{E}_{\perp} + (\boldsymbol{\omega}_{\perp} + \mathbf{v}_D) \times \mathbf{B}\right) \tag{1.19}$$

From section 1.2.1 we know that the gyration part is given by

$$m\frac{\partial \omega_{\perp}}{\partial t} = q\omega_{\perp} \times \mathbf{B} \tag{1.20}$$

Taking this out of the equation we have

$$\frac{\partial \mathbf{v}_D}{\partial t} = \frac{q}{m}\left(\mathbf{E}_{\perp} + \mathbf{v}_D \times \mathbf{B}\right) \tag{1.21}$$

Then we use the previous assumption that the drift velocity is constant, cross the equation with $\mathbf{B}$ and simplify, see Goldston and Rutherford (1995), to arrive at

$$\mathbf{v}_D = \frac{\mathbf{E} \times \mathbf{B}}{B^2} \tag{1.22}$$

As we can see the E-cross-B drift is independent of particle charge and mass, which means both the ions and electrons will be drifting in the same direction and speed, fig. 1.2b.

This is just an example, and there are many other important concepts found in considering single particles, that we will not go into here, see Fitzpatrick (2014), or a different introductionary plasma physics book. Other examples that could be useful include gradient-B drift, curvature drift, polarization drift and magnetic mirroring.

1.3 Kinetic Theory

Here we will shortly introduce kinetic theory in relation to plasma physics. Let $\mathcal{F}_s$ be the exact phase-space density of a particle species, it contains all the positions, velocities for all the particles at all times. By integrating over all velocities and multiplying with the charge for all species we obtain the charge density, ρ_c.

$$\rho_c = \sum_s e_s \int \mathcal{F}_s(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{v}$$

Likewise we find the current density, $\mathbf{j}$.

$$\mathbf{j} = \sum_s e_s \int \mathbf{v}\mathcal{F}_s(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{v}$$

Then its seems we can derive all plasma interaction from considering the conservation of the phase-space density, coupled with Maxwells equations. The phase-space conservation is given by what is known as Vlasovs equation eq. (1.23) (Pécseli, 2012)).

$$\frac{\partial \mathcal{F}}{\partial t} + \mathbf{v} \cdot \nabla \mathcal{F}_s + \frac{e_s}{m_s}\left(\mathbf{E} + v \times \mathbf{B}\right) \cdot \nabla_v \mathcal{F}_s = 0 \tag{1.23}$$

where ∇_v is the velocity grad-operator. Unfortunately this expression, combined with Maxwells equations, is only solvable for special simple geometries.

1.4 Fluid Description

This section aims to provide an overview of the derivation of the fluid equations from a Kinetic Theory perspective. First the Vlasov equation is introduced, then it is explained how the fluid equations can be obtained by taking different order moments of the Vlasov equation. This can help understand the limitations of the fluid model of plasma. Lastly a few different approximations to make the fluid equations closable.

1.4.1 Velocity Moments

To investigate plasma as a fluid we have to make certain fluid approximations. The plasma is then characterized by local parameters describing particle density, kinetic temperature, flow velocity and so on. These parameters refer to a small volume of plasma, in contrast with the discussions earlier section 1.2. The time evolution is then governed by the fluid equation, but unfortunately the resulting equations are generally less tractable than the usual hydrodynamical equations.

The usual quantity known as the momemt is given by mass times velocity, here we will introduce a more general form of moment where the usual moment is the first order moment. This will help understand how the fluid equations result from averaging over different moments of the general transport equation. The zeroth, first and second order moment is respectively given by

$$\Phi^0(\mathbf{v}) = m \tag{1.24a}$$

$$\Phi^1(\mathbf{v}) = m\mathbf{v} \tag{1.24b}$$

$$\Phi^2(\mathbf{v}) = m\mathbf{v}\mathbf{v} \tag{1.24c}$$

By integrating the moment functions and the distribution function $\mathcal{F}$, over the velocity space we can retrieve different quantities.

Integrating the zeroth order moment gives the density, if we divide by the mass.

$$n = \frac{1}{m}\int m\mathcal{F}\mathrm{d}\mathbf{v} \tag{1.25}$$

Integrating over the first order moment gives the momentum, if we divide by density.

$$m\mathbf{v} = \int m\mathbf{v}\mathcal{F}\mathrm{d}\mathbf{v} \tag{1.26}$$

We can in fact find the mean of any order moment by integrating the distribution function over $\mathcal{F}$.

$$\langle \Phi^n(\mathbf{v})\rangle = \frac{1}{n}\int \Phi^n\mathcal{F}\mathrm{d}\mathbf{v} \tag{1.27}$$

1.4.2 Transport Equation

By multiplying the a momentum function, Φ, with the Vlasov equation, eq. (1.23), we obtain the general momentum transport equation (Shu, 2010).

$$\frac{\partial n\,\langle \Phi^n(\mathbf{v})\rangle}{\partial t} + \nabla\cdot(\langle \Phi^n(\mathbf{v})\mathbf{v}\rangle) = \frac{n}{m}\,\langle \mathbf{F}_L\cdot\nabla_v\Phi^n(\mathbf{v})\rangle \tag{1.28}$$

This then becomes a conservation equation for the average macroscopic quantity $\langle\Phi\rangle$. By using this equation and inserting in the zeroth, first and second order moment we obtain the fluid equations, eqs. (1.29a) to (1.29c). We refer you to Fitzpatrick (2014) to see a derivation of the fluid equations.

1.4.3 Fluid Equations

The generalized fluid equations is given in eqs. (1.29a) to (1.29c), where the three equations describe the conservation of mass, momentum and energy respectively. The collision term is negleted. We refer you to the earlier mentioned Fitzpatrick (2014), although some notation differ, for the rather involved derivation to obtain them.

$$\left(\frac{\partial}{\partial t} + \mathbf{u}_s \cdot \nabla\right) n_s + n_s \nabla \cdot \mathbf{u}_s = 0 \tag{1.29a}$$

$$m_s n_s \left(\frac{\partial}{\partial t} + \mathbf{u}_s \cdot \nabla\right) \mathbf{u}_s = -\nabla p_s - \nabla \cdot \pi + n_s \mathbf{f}_s \tag{1.29b}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u_s} \cdot \nabla\right) p_s = -\frac{5}{3} p_s \nabla \cdot \mathbf{u}_s - \frac{2}{3} \pi_s : \nabla \mathbf{u_s} - \frac{2}{3} \nabla \cdot \mathbf{q}_s \tag{1.29c}$$

The first equation, eq. (1.29a), is the continuity equation, it states that the total mass in a volume should be preserved. $\mathbf{u}_s$ is the flow velocity and n_s is the number density, i.e. number of particles in a volume. The divergence terms signifies change due to the compressability of the fluid and can in many cases be set to 0. The total derivative, i.e. $\left(\frac{\partial}{\partial t} + \mathbf{u}_s \cdot \nabla\right)$ accounts for change in density in a volume taking into account substance exiting and entering. The momentum equation eq. (1.29b) shows that the fluid momentum change, left hand side, is due to pressure gradients, ∇p_s, visceous forces, $\nabla \cdot \pi$ and external forces, $n_s \mathbf{f}_s$, per unit volume. Lastly we have the energy equation, in its pressure form, which shows that changes to thermal energy, $p = nkT$, is caused by compression, $p_s \nabla \cdot \mathbf{u}_s$, visceous effects $\pi_s : \nabla \mathbf{u_s}$ and heat transport $\frac{2}{3} \nabla \cdot \mathbf{q}_s$. The fluid equations is in general not closeable and adding higher order moments always introduces more unknowns. Due to this one generally uses different closing schemes, some of which is described in the next section, to make them tractable.

1.4.4 Plasma States

Plasma can be classified according to which approximations and simplifications that are valid for them. Here we will go through a few of them.

Local Thermodynamic Equilibrium

A plasma is said to be in a *local thermodynamic equalibrium* (LTE) if the phase-space distribution is locally Maxwellian. This means the variations in temperature is slow enough that we can consider it to flow no heat. We can also ignore the viscosity due to there being little local variations to the momentum flow.

$$\mathcal{F}_m = \frac{n}{(2\pi)^{3/2} v_t^3} \exp\left\{ -\frac{(v-u)^2}{2v_t^2} \right\} \tag{1.30}$$

Since the viscosity tensor, π, and the heat flux tensor, $\mathbf{q}$ contains odd integrals over the distribution, see Fitzpatrick (2014), they dissappear.

Cold Plasma

In what we consider a cold plasma the pressure, p, and viscosity, π, is set to zero. This can be useful if the velocities of interest far exceed the thermal velocities. (ADD MORE)

Isothermal

An isothermal plasma is one where we assume an infinite heat conductivity, this means the temperatures is constant in all space and time. This can be used to describe macroscopic plasma. (ADD MORE)

1.5 Plasma Oscillations

Plasma oscillations, also called Langmuir oscillations, is the basic resulting oscillation that happens as a plasma tries to right disturbances to its equilibrium. We will use this to show how the fluid equations can be closed for a simple system using assumptions. This is also very suited to test simulations, as we do later in **??**.

Here we will consider an one specie plasma fluid consisting of electrons under local thermal equilibrium, LTE. The electron density, n_0 and pressure p_0 is initally homogenous. The fluid has a vanishing flow, $\mathbf{u}_0 = 0$, and the electric field $\mathbf{E}_0 = 0$. See Pécseli (2012) for a more thorough overview.

A small perturbation of the electron density will cause the electric field to try to restore the equilibrium. When the electrons reach the equilibrium position they will have a kinetic energy and will overshoot.This will cause a new perturbation away from the equilibrium.

Under the LTE conditions the fluid equations simplify to

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{u}_e) = 0 \tag{1.31a}$$

$$m_e n_e \left(\frac{\partial}{\partial t} + \mathbf{u}_e \cdot \nabla \right) \mathbf{u}_e = e n_e \nabla \phi - \nabla p_e \tag{1.31b}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u}_e \cdot \nabla \right) p_e + \frac{5}{3} p_e \nabla \cdot \mathbf{u}_e = 0 \tag{1.31c}$$

Since this set of equations have more unknowns than equations so we need additional information to close the set. Here we can use the Poisson equation to close it.

$$\epsilon_0 \nabla^2 \phi = e\left(n_e - n_0\right) \tag{1.32}$$

Now we let a small perturbation, denoted by a tilde, happen to the equilibrium. Since we are free to choose an inertial reference frame, we select one co-moving with the plasma so the inital fluid velocity is $\mathbf{u}_0 = 0$. We also select the reference potential so the initial potential, ϕ_0, is 0.

$$\text{Perturbation} \rightarrow \begin{cases} n_e = n_0 + \tilde{n}_e \\ p_e = p_0 + \tilde{p}_e \\ \mathbf{u}_e = \tilde{\mathbf{u}}_e \\ \phi = \tilde{\phi} \end{cases}$$

Since the pertubation is small, we can say that any part that contains second order terms of perturbation of a quantity will be much smaller than the value of the quantity, $q \gg \tilde{q}\tilde{q}$. So even though we may miss some processes by doing this we can drop the second order perturbation terms. This process is called linearization.

Inserting the perturbation and linearizing the equations we get:

$$\frac{\partial \tilde{n}_e}{\partial t} + \nabla \cdot \left(n_0 \tilde{\mathbf{u}}_e\right) = 0 \tag{1.33a}$$

$$m_e \frac{\partial \tilde{\mathbf{u}}_e}{\partial t} = e\nabla\tilde{\phi} - \frac{\nabla \tilde{p}_e}{n_0} \tag{1.33b}$$

$$\frac{\partial \tilde{p}}{\partial t} + \frac{5}{3} p_0 \nabla \cdot \tilde{\mathbf{u}}_e = 0 \tag{1.33c}$$

$$\epsilon_0 \nabla^2 \tilde{\phi} = e\tilde{n}_e \tag{1.33d}$$

Then we combine the continuity and energy equations, eq. (1.33a) and eq. (1.33c).

$$\frac{\partial}{\partial t}\left(\frac{\tilde{p}_e}{p_0} + \frac{5}{3}\frac{\tilde{n}_e}{n_0}\right) = 0 \tag{1.34}$$

The perturbed pressure and density is proportional, $\nabla \tilde{p}_e = \left(5p_0/3n_0\right)\nabla\tilde{n}_e$. Assuming plane wave solutions along the x-axis, the differential operators become $\nabla \rightarrow ik$ and $\frac{\partial}{\partial t} \rightarrow -i\omega$, we can solve for the dispersion relation.

$$\epsilon(\omega, k) = 1 + \frac{5}{3}\lambda_{se}^2 k^2 - \frac{\omega^2}{\omega_{pe}^2} \tag{1.35}$$

Here we have subsituted in the electron debye length λ_D and the plasma frequency ω_p.

1.6 Magnetohydrodynamics

In a plasma there are usually several types of species, then it follows that each specie needs its own set of fluid equations. Magnetohydrodynamics, (MDH), is an attempt to simplify this situation by combining it into one electrically conducting fluid. Conventional MHD assumes local thermodynamical equilibrium, negligable electron inertia and quasi-neutrality (Goldston and Rutherford, 1995). This simplifies Maxwell's equations to

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} \tag{1.36a}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{1.36b}$$

$$\nabla \cdot \mathbf{B} = \nabla \cdot \mathbf{E} = 0 \tag{1.36c}$$

The MHD fluid can be considered a neutral fluid with a current running through it (Hockney and Eastwood, 1988). The current is described by the conductivity σ and the bulk velocity $\mathbf{v}$ and is given as

$$\mathbf{j} = \sigma\left(\right) \tag{1.37}$$

With the condition that the condictivity is high and a finite current eq. (1.36b) becomes

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}) \tag{1.38}$$

Then it remains to close the MHD equations by continuity and momentum conservation, where rho is the mass density and p is the scalar pressure.

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \mathbf{v}) \tag{1.39a}$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\nabla p + \mathbf{j} \times \mathbf{B} \tag{1.39b}$$

1.7 Numerical Simulations

While mathematical analysis of plasma is helpful to improve our understanding of the physics, many situations doesn't fall neatly into convenient assumptions or is untractable. Then we have experiments and computer simulations to further help us understand. All of these methods work in symbiosis and is interdependent on each other. Numerical simluations can be thought of as cheap easily repetable experiments, but it also has the advantage of being applied to situations that no experiment can reproduce. Modelling generally needs to be validated against against experiments and has a foundation built upon theory. As the computational resources have improved more sophisticated simulations have been possible.

Plasma simulations vary from fluid descriptions, as MHD codes, to kinetic descriptions, as Particle-in-Cell and Vlasov codes, with hybrid codes inbetween as well. This thesis focuses on the development of a Particle-in-Cell code, but here we will give a brief overview of other modelling approaches as well.

MHD

Magnetohydrodynamical codes solve the one-fluid equations, given in section 1.6, with various approaches and has similarities to Computational Fluid Dynamics. For the fluid equations to be a good approximations the dynamics needs to happen at much larger scales than the Debye Shielding Length. This approach has been widely used in large scale plasma simulations such as astrophysics, (Hawley and Stone, 1995) and space physics (Watanabe and Sato, 1990).

Particle-in-Cell

Particle-in-Cell models the particles directly, this has the advantage that few approximations are done, but computational increases fast with more particles.

Vlasov

Vlasov codes takes the kinetic description as the starting point and is often used in plasma laser modelling (Bertrand et al., 1990). It has an advantage over PiC in low density zones, where there is often too few particles for PiC.

(Add more on MHD, PiC an Vlasov, uninspired now)

1.8 Collisions: MCC-Null Model

First we will go through the Monte Carlo Collisional model and then show how the Null-Collision scheme can reduce the amount of arithmetic operations. To avoid spending computational time on the neutral particles we consider them as background species. We assume for simplicity that the neutral particles are uniformly distributed, with a normal velocity distribution.

Particle species s has N type of collisions with a target species. Each particle has kinetic energy

$$\varepsilon_i = \frac{1}{2} m_s \left(v_x + v_y + v_z\right) \tag{1.40}$$

The collisional cross section σ_j for each type of collision is dependent on the kinetic energy of the particle and the total cross section is given by adding together all the types of collisions.

```
for Each particle do
  if $r \le P_{Null}$ then
                                        $r$  $\le \nu_0(\varepsilon_i)/\nu'$                                   Type 0
    $\nu_0(\varepsilon_i)/\nu' \le$  $r$  $\le (\nu_0(\varepsilon_i) + \nu_1(\varepsilon_i))/\nu'$   Type 1
                                        $\vdots$
    $\sum_j(\nu_j(\varepsilon_i))/\nu' \le$  r                                                            Type Null
```

Table 1.1: Algorithm to select a particle collisions (Need to be improved)

$$\sigma_T(\varepsilon_i) = \sum_j^N \sigma_j(\varepsilon_i) \tag{1.41}$$

The probability that a particle has a collision with a target species, in one timestep, is be dependent on the collisional cross section, distance travelled, $\Delta r_i = v_i \Delta t$, and the density of the target specie, $n_t(\mathbf{r_i})$ by the following relation.

$$P_i = 1 - \exp\{-v_i \Delta t \sigma_T(\varepsilon_i) n_t(\mathbf{r_i}\} \tag{1.42}$$

In a Monte Carlo model we say that a collision has taken place for a particle if a random number $r = [0, 1]$, is smaller than P_i. To compute P_i for each particle, we need to find ε_i, all the cross sections σ_j, and the density $n_t(\mathbf{r_i}$. This demands many floating point operations for each particle, so we will use a Null-Collisional model to only compute the collisional probability for a subset of the particles. We compute a maximal collisional frequency

$$\nu' = \max(v_i \Delta t \sigma_T(\varepsilon_i)) \max(n_t(n_t)) \tag{1.43}$$

and consider if it was a dummy or one of the proper collisions, if r is smaller than the resulting constant $P_{Null} = 1 - \exp\{\nu'\}$.

The maximum collisional frequency may need to be recomputed each timestep due to the density of the target specie, n_t, changing. The algorithm for each particle is then.

Appendix A

Further Development

Here is a list of what possible improvements and extensions that we hope is eventually developed in our PinC program. Our aim was to develop a solid, basic and easy to use parallel PiC program, that is suited to further development. Our hope is that this project eventually develops into a full scale open source PiC program.

- Objects
- Adaptive mesh
- Realtime plasma vizualizations (ala Atomify)
- Full Electromagnetic PiC
- Compatibility with FEM (dolphin) as a solver
- Hybrid, add on possibility of fluid-species and molecular dynamics
- Spectral Solvers (Wish that was available for testing of other solvers)
- Variable Ghost Layers
- Various stencils, interpolation and discretizations of different orders

Appendix B

Notation

B.1 Notation

While the notation is described in the main text at its first instance, we have also included this small note on the notation used to make it easier to look up. Notation that are only used in locally in smaller sections are not included here.

In the PinC project we have decided to try to keep different indexes tied different objects to help avoid confusion and increase readability. Since the i index is reserved for incrementing particles, the spatial x, y, z-indexes are j, k, l instead of the more usual i, j, k. So to make the transition between this document and the code easier we have also used the j, k, l indexes to denote the spatial area. This is the convention used by Birdsall and Langdon, (cite plasma physics via simulation).

Subscripts are usually used to denote spatial index, and a superscripts are usually reserved for temporal cases. So $\Phi^n_{j,k,l}$ means the potential at the timestep n and position j, k, l. When plasma theory is involved the subscript can also signify the particle species.

Φ	Electric Potential
ρ	Charge Density
ω_{pe}	Electron Plasma Frequency
ω_{ce}	Electron Cycletron Frequency
T_e	Electron Kinetic Temperature
$\mathbf{E}$	Electric Field
$\mathbf{B}$	Magnetic Field
$\mathbf{r}$	Position
m	Mass
T	Kinetic Temperature

Appendix C

Unittests

C.1 Unittests

Unittests are small tests that is used to check that the single pieces of the code work as they should. This serves a dual purpose in developing a software project. When a part of the code is developed it serves as a framework to create a standardized test of the piece of code that can easily be repeated. It also helps when developing the higher level algorithms, in that the unittests ensures that the problem lies in the higher level algorithm and not in the lower level pieces it uses. When implementing wider changes, for example datastructures, the unittests can help making sure that the changes are not causing any unintended bugs. For information of how to use the unittests see the documentation, **documentation**

C.1.1 Prolongation and Restriction

The prolongation and restriction operators with the earlier proposed stencils will average out the grid points when applied. So the idea here is to set up a system with a constant charge density, $\rho(\mathbf{r}) = C$, and then apply a restriction. After performing the restriction we can check that the grid points values are preserved. Then we can do the same with the prolongation. While this does not completely verify that the operators work as wanted, it gives an indication that we have not lost any grid points and the total mass of the charge density should be conserved.

C.1.2 Finite difference

The finite difference operators is tested by setting up a test field based on a polynomial on which the operator should give an exact answer for. For example if we have a quantity $f(x) = 3x$, then a first order finite difference scheme will give $\hat{\nabla} f(x) = 3$.

C.1.3 Multigrid and Grid structure

We want the basic grid to be available through a grid datastructure and the stack of grids stored in the multigrid structure. To ensure that this will still work through changes in the the structs there is a simple unittest that uses a grid struct to set up a field, then it is changed in the multigrid struct. Then it confirms that the values in the grid struct is also changed.

C.1.4 Edge Operations

In the communication between the subdomains, as well as in the treatment of boundary conditions, there is a group of functions dealing with slice operations. These are tested by putting assigning each subdomain different constant values, then different slice operations is performed.

Appendix D

Examples

D.1 Ex: 3 level V cycle, steps necessary

(This should probably be cut.)

① Compute defect on grid 0, the finest grid:

- $\widehat{\phi}_0 = \mathcal{S}(\phi_0, \rho_0)$
- $d_0 = \nabla^2 \widehat{\phi}_0 - \rho_0$
- Restrict defect: $\rho_1 = \mathcal{R} d_0$

② Compute defect on grid 1:

- $\widehat{\phi}_1 = \mathcal{S}(\phi_1^0, \rho_1)$
- $d_1 = \nabla^2 \widehat{\phi}_1 - \rho_1$
- Restrict defect: $\rho_2 = \mathcal{R} d_1$

③ Solve Coarse Grid for correction ω

- $\phi_2 = \mathcal{S}(\phi_2^0, \rho_2)$
- Interpolate as correction:$\omega_1 = \mathcal{I} \phi_2$

④ Add correction on level 1:

- $\widetilde{\phi}_1 = \widehat{\phi}_1 + \omega_1$
- $\phi_1 = \mathcal{S}(\widetilde{\phi}_1, \rho_1)$
- Interpolate correction:$\omega_0 = \mathcal{I} \phi_1$

⑤ Compute solution.

- $\widetilde{\phi}_0 = \widehat{\phi}_0 + \omega_0$
- $\phi_0 = \mathcal{S}(\widetilde{\phi}_0, \rho_0)$

Appendix E

Optional methods

E.1 MG-Methods

E.1.1 FMG

- 'Easy' to implement.
- Theoretically scales $\mathcal{O}(N)$ (**Press1987**), in reality
- FMG and W cycles are usually avoided in massive parallel computers (Chow et al., 2006), as they visit the coarsest grid often, due to:
  - At the coarsest level the computation is fast, communication usually the bottleneck
  - Coarsest grid may couple all the domain, needs global communication
- Options to solve the coarse matrix (Chow et al., 2006)
  - Direct solver: Sequential, if small problem may be done on each processor to avoid communication
  - Iterative method, Gauss-Seidel. Can be parallelized
- Will use G-S with R-B ordering, has good parallel properties

E.2 Other methods worth considering

- MUMPS (MUltifrontal Massive Parallel Solver), tried and compared in **Kacem2012** slower than MG.
  - Solves $Au = \rho$ for a sparse matrix.

Appendix F

Multigrid Libraries

Efficient computation of the poisson equation, or other elliptic equations, is a common problem with many applications, and there exists several predeveloped and optimized libraries to help solve it. These include Parallel Particle Mesh (PPM) (Sbalzarini et al., 2006), Hypre (Falgout and Yang, 2002), Muelu (??), METIS (A fast and high quality multilevel scheme for partitioning irregular graphs — Karypis Lab 2016) and PETCs (manual.pdf 2016) amongst others. There is also PiC libraries that can be used PICARD and VORPAL to mention two.

If we want to have an efficient integration of a multigrid library into our PiC model we need to consider how easy it is to use with our scalar and field structures. To have an effiecient program we need to avoid having the program convert data between our structures and the library structures. Since our PiC implementation uses the same datastructures for the scalar fields in several other parts, than the solution to the poisson equation, we could have an efficiency problem in the interface between our program and the library.

We could also consider that only part of the multigrid algorithm uses building blocks from libraries. The algorithm is now using the conceptually, and programatically easy, GS-RB as smoothers, but if we implement compatibility with a library we could easily use several other types of smoothers which could improve the convergence of the algorithm

F.1 Libraries

F.2 PPM - Parallel Particle Mesh

Parallel Particle Mesh is a library designed for particle based approaches to physical problems, written in Fortran. As a part of the library it includes a structured geometric multigrid solver which follows a similar algorithm to the algorithm we have implemented in our project implemented in both 2 and 3 dimensions. For the 3 dimensional case the laplacian is discretized with a 7-point stencil, then it uses a RB-SOR (Red and Black Succesive Over-Relaxation), which equals GS-RB with the relaxation parameter ω set as 1, as a smoother. The full-weighting scheme is used for restriction and trilinear interpolation for the prolongation, both are described in (Trottenberg et al., 2000). It has implementations for both V and W multigrid cycles. To divide up the domains between the computational nodes it uses the METIS library. The efficiency of the parallel multigrid implementation was tested

F.3 Hypre

Hypre is a library developed for solving sparse linear systems on massive parallel computers. It has support for c and Fortran. Amongst the algorithms included is both structured multigrid as well as element-based algebraic multigrid. The multigrid algorithms scales well on up to 100000 cores, for a detailed overview see Baker et al 2012. (bibtex files started to argue, will fix).

F.4 MueLo - Algebraic Multigrid Solver

MueLo is an algebraic multigrid solver, and is a part of the TRILINOS project and has the advantage that it works in conjunction with the other libraries there. It is written as an object oriented solver in cpp. For a investigation into the scaling properties see Lin et. al. 2014.

F.5 METIS - Graph Partitioning Library

METIS is a library that is used for graph partitioning, and could have been used in our program to partition the grids. The partitionings it produces has been shown to be 10% to 50% faster than the partionionings produces by spectral partitioning algorithms (A fast and high quality multilevel scheme for partitioning irregular graphs — Karypis Lab 2016). It is mostly used for irregular graphs, and we are not sure if it could be easily made to work with the datastructures used throughout the program.

F.6 PETSc - Scientific Toolkit

The PETSc is an extensive toolkit for scientific calculation that is used by a multitude of different numerical applications, including FEniCS. It has a native multigrid option, DMDA, where the grid can be constructed as a cartesian grid. In addition there is large amount of inbuilt smoothers that can be used.

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