Chapter 3

Numerical Methods

In this chapter we describe the theoretical model and the numerical methods used for our two-dimensional model. We first describe the theoretical model and an overview of the spectral methods used to solve the fluid plasma equations, followed by description of the theoretical model in spectral domain. We then discuss the time integration methods for the Ordinary Differential Equations ODEs represented in spectral domain. Last, We consider how the charging model is normalized and the charge equilibrium is initially set in the simulation.

3.1 Theoretical model

In this section, we describe the main features of our physical model used for studying low frequency ion waves in dusty plasmas. The model considers the two dimensional plane perpendicular to the background magnetic field $\vec{B}$. Many plasma phenomena observed in real experiments can be explained by a rather simple model used in fluid dynamics. The fluid model neglects the identity of individual particles and only the motion of fluid elements as a whole is taken into account. The advantage of this approach is that it leads to equations in three spatial dimensions and time rather than the seven-dimensional phase space used in Vlasov theory. In the fluid approximation, we consider the plasma to be composed of two or more interpenetrating fluids, one for each species.

The plasma electrons are treated as a massless fluid whose density $n_{\rm e}$ self-consistently varies due to the dust charging. The electron continuity equation is given by

$$\frac{\partial n_{\rm e}}{\partial t} + \nabla \cdot (n_{\rm e}\vec{v}_{\rm e}) = \left.\frac{dn_{\rm e}}{dt}\right|_{\rm charging} + q_{\rm s}, \tag{3.1}$$

where $dn_{\rm e}/dt|_{\rm charging}$ is the rate of change of the electron density due to electron charging currents,

$$\left.\frac{dn_{\rm e}}{dt}\right|_{\rm charging} = -\frac{1}{q_{\rm e}}\left[\frac{d\rho_{\rm de}}{dt}\right],$$

$q_{\rm s}$ represents a constant production rate of electrons due to some external plasma source, and $\rho_{\rm de}$ is the dust charge density due to electron charging current collection. We consider applications in which the electrons may either be unmagnetized or strongly magnetized in a magnetic field $\vec{B}$. The electron momentum equation describing unmagnetized electrons is given by

$$\frac{\partial \vec{v}_{\rm e}}{\partial t} + (\vec{v}_{\rm e}\cdot\nabla)\vec{v}_{\rm e} = -\left(\frac{q_{\rm e}}{m_{\rm e}}\right)\vec{E} - \gamma\left(\frac{T_{\rm e}}{m_{\rm e}}\right)\frac{1}{n_{\rm e}}\nabla n_{\rm e}, \tag{3.2}$$

where $q_{\rm e}$, $m_{\rm e}$, and $T_{\rm e}$ are the electron charge, mass, and temperature. For cold, massless, and strongly magnetized electrons, the electron momentum equation reduces to the following equation for the electron velocity

$$\vec{v}_{\rm e} = \frac{\vec{E}\ \times\ \vec{B}}{B^2}. \tag{3.3}$$

To obtain equation (3.3), we can use the equation of motion in presence of electric field $\vec{E}$ as following

$$m_{\rm e}\frac{d\vec{v}_{\rm e}}{dt} = q_{\rm e}\left(\vec{E} + \vec{v}_{\rm e}\ \times\ \vec{B}\right). \tag{3.4}$$

We may omit the $m_{\rm e}\frac{d\vec{v}_{\rm e}}{dt}$ term in equation (3.4), since we assume the electrons are massless. Then equation (3.4) becomes

$$\vec{E} + \vec{v}_{\rm e}\ \times\ \vec{B} = 0. \tag{3.5}$$

The equation (3.3) is obtained by taking the cross product with $\vec{B}$ and noting $\vec{v}_{\rm e}\cdot\vec{B} = 0$.

The ions are also treated as a fluid whose density $n_{\rm i}$ is self-consistently reduced due to the dust charging. The ion continuity equation is

$$\frac{\partial n_{\rm i}}{\partial t}\ +\ \nabla\cdot(n_{\rm i}\vec{v}_{\rm i})\ =\ \left.\frac{dn_{\rm i}}{dt}\right|_{\rm charging} + q_{\rm s},, \tag{3.6}$$

where $dn_{\mathrm{i}}/dt|_{\mathrm{charging}}$ is the rate of ion density variation due to ion charging currents,

$$\left.\frac{dn_{\mathrm{i}}}{dt}\right|_{\mathrm{charging}} = -\frac{1}{q_{\mathrm{i}}}\left[\frac{d\rho_{\mathrm{di}}}{dt}\right],$$

again q_{s} is a constant production rate of ions, and ρ_{di} is the dust charge density due to ion charging current collection. Note that equations (3.1) and (3.6) include the ionization sources since there would be a reduction of plasma density over times otherwise. The momentum equation for the unmagnetized ion velocity $\vec{v}_{\mathrm{i}}$ is

$$\frac{\partial \vec{v}_{\mathrm{i}}}{\partial t} + (\vec{v}_{\mathrm{i}} \cdot \nabla)\vec{v}_{\mathrm{i}} = \left(\frac{q_{\mathrm{i}}}{m_{\mathrm{i}}}\right)\vec{E} - \gamma\left(\frac{T_{\mathrm{i}}}{m_{\mathrm{i}}}\right)\frac{1}{n_{\mathrm{i}}}\nabla n_{\mathrm{i}}, \qquad (3.7)$$

where q_{i}, m_{i}, and T_{i} are the ion charge, mass, and temperature and $\gamma = (2 + D)/D$ is the ratio of specific heats. Here, D is the number of dimensions [*Chen*, 1984].

The dust is treated with the Particle-In-Cell (PIC) method. The dust position $\vec{x}_{\mathrm{j}}$ and velocity $\vec{v}_{\mathrm{j}}$ are advanced as follows

$$\frac{d\vec{v}_{\mathrm{j}}}{dt} = \frac{Q_{\mathrm{j}}(t)}{m_{\mathrm{j}}}\vec{E}, \qquad (3.8)$$

$$\frac{d\vec{x}_{\mathrm{j}}}{dt} = \vec{v}_{\mathrm{j}}, \qquad (3.9)$$

where m_{j} is the mass and $Q_{\mathrm{j}}(t)$ is the time dependent charge for the j^{th} dust grain. Note that dust motion dynamics are included in this model. The standard dust charging model is used [*Jana et al.*, 1993]. For the j^{th} dust grain this becomes

$$\frac{dQ_{\mathrm{j}}}{dt} = I_{\mathrm{e}j} + I_{\mathrm{i}j}, \tag{3.10}$$

where $I_{\mathrm{e}j}$, $I_{\mathrm{i}j}$ are electron and ion currents collected by the dust grains. The electron and ion currents on the j^{th} dust grain are given by

$$I_{\mathrm{e}j} = \pi a^2 \left(\frac{8}{\pi}\right)^{1/2} q_{\mathrm{e}} n_{\mathrm{e}} v_{\mathrm{te}} \exp\left[\frac{e\phi_{\mathrm{fj}}}{kT_{\mathrm{e}}}\right], \tag{3.11}$$

$$I_{\mathrm{i}j} = \pi a^2 \left(\frac{8}{\pi}\right)^{1/2} q_{\mathrm{i}} n_{\mathrm{i}} v_{\mathrm{ti}} \left[1 - \frac{e\phi_{\mathrm{fj}}}{kT_{\mathrm{i}}}\right], \tag{3.12}$$

where a is the grain radius, $n_{\mathrm{e,i}}$ are electron and ion densities at the dust grain location, $v_{\mathrm{te,i}}$ are the electron and ion thermal velocity, $T_{\mathrm{e,i}}$ are the electron and ion temperatures, and ϕ_{fj} is the floating potential on the dust grain given by

$$\phi_{\mathrm{fj}} = \frac{Q_{\mathrm{j}}(t)}{C} = \frac{Q_{\mathrm{j}}(t)}{4\pi\epsilon_0 a},$$

where C is the grain capacitance. Since for the case of interest, the electron gyroradius is assumed larger than the dust grain size, the standard dust charging model, which does not include magnetic field effects, is valid [*Jana et al.*, 1995]. It should be noted that the model here represents the simplest model for dust charging and it has been extensively used in the past to study waves and instabilities in dusty plasmas. More sophisticated models exist and currently charging is a topic of considerable interest in dusty plasma physics [*Venturini*, 1998; *Angelis and Forlani*, 1998; *Cui and Goree*, 1994; *Watanabe et al.*, 1996]. It has recently been shown that the standard model does not provide the most accurate description of dust charging in the regime $d \leq \lambda_{\mathrm{D}}$ [*Angelis and Forlani*, 1998]. This is the regime in which the collective effects discussed here occur. However, we believe the standard model will provide a reasonable description for the physical processes investigated in this study. As more accurate charging models, which may include discrete charging effects [*Cui and Goree*, 1994; *Watanabe et al.*, 1996], become established, they will be incorporated in future investigations. Because of the general nature of the numerical model described in the following section, this is straightforward.

Poisson's equation is used to calculate the electrostatic potential ϕ. It is given by

$$\epsilon_0 \nabla^2 \phi = -(q_{\mathrm{e}} n_{\mathrm{e}} + q_{\mathrm{i}} n_{\mathrm{i}} + Q_{\mathrm{d}} n_{\mathrm{d}}). \tag{3.13}$$

where $Q_{\mathrm{d}} n_{\mathrm{d}}$ denotes the dust charge density and $Q_{\mathrm{d}} n_{\mathrm{d}} \equiv \rho_{\mathrm{d}} = \rho_{\mathrm{de}} + \rho_{\mathrm{di}}$. The electric field is calculated from $\vec{E} = -\nabla \phi$.

3.2 Spectral methods

3.2.1 Spectral methods using Fourier series

Spectral methods, in general, are based on representing the solution to a Partial Differential Equation PDE as a truncated series of a smooth function of the dependent variable. Consider a spatially dependent function u. This function can be expanded in terms of an infinite sequence of orthogonal functions ϕ_{k} so that $u = \sum_{k=-\infty}^{\infty} u_{\mathrm{k}}\phi_{\mathrm{k}}$. The most famillIar approximate solution in solving problems with periodic functions is the Fourier series. In one dimension, this corresponds to the set of functions $\phi_{\mathrm{k}} = e^{ikx}$ which is an orthogonal system over the interval $(0, 2\pi)$. Any physical process can be described either in spatial domain or spectral domain. To go back and forth between these two domains, we can introduce the one-dimensional Fourier Transform equation of u:

$$\bar{u}_{\mathrm{k}} = \frac{1}{2\pi}\int_0^{2\pi} u(x)e^{-ikx}dx \qquad k = 0, \pm 1, \pm 2, \cdots. \tag{3.14}$$

where $\bar{u}_{\mathrm{k}}$ is the continuous Fourier transform of u. In computer applications, we have to use the descretized version of the Fourier transform. A common situation is to have a function sampled at evenly spaced, discrete time intervals, Δx. For any sampling interval Δx, the Nyquist critical wavenumber is defined by

$$k_{\mathrm{c}} = \frac{1}{2\Delta x} \tag{3.15}$$

This lead to an important theorem for discrete sampling known as the sampling theorem: If a continuous function $u(x)$, sampled at an interval Δx, is bandwidth limited to wavenumbers smaller in megnitude than k_{c}, then the function $u(x)$ is completely determined by its samples u_{n}. The function $u(x)$ is defined by

$$u(x) = \Delta x \sum_{n=-\infty}^{\infty} u_{\mathrm{n}} \frac{\sin[2\pi k_{\mathrm{c}}(x - n\Delta x)}{\pi(x - n\Delta x)} \tag{3.16}$$

The sampling theorem is significant because it allows for the entire information content of a signal to be reproduced provided it is sampled at s sufficient rate. Suppose we have an even function of N consecutive samples

$$u_{\mathrm{j}} \equiv u(x_{\mathrm{j}}), \quad x_{\mathrm{j}} \equiv j\Delta x, \quad x = 0, 1, 2, ...N - 1 \tag{3.17}$$

assuming uniform sampling. The set of points x_{j} is referred to as nodes or grid points. Here $2\pi/N$ is the sampling interval. The discrete Fourier coefficients of a complex-valued function u with respect to these points are

$$u_{\mathrm{k}} = \frac{1}{N}\sum_{\mathrm{j=0}}^{\mathrm{N-1}} U_{\mathrm{j}} e^{-ikx_{\mathrm{j}}} \qquad k = \frac{-N}{2}, ..., \frac{N}{2} - 1 \tag{3.18}$$

where $U_{\mathrm{j}} = u(x_{\mathrm{j}})$. The inverse Fourier coefficients are

$$U_{\mathrm{j}} = \sum_{\mathrm{k=-N/2}}^{\mathrm{N/2-1}} u_{\mathrm{k}} e^{ikx_{\mathrm{j}}} \qquad j = 0, ..., N - 1. \tag{3.19}$$

The Discrete Fourier Transform DFT maps N complex numbers U_{j} into N complex numbers u_{k}. It is easy to see that as the number of input data increases, the output data frequency spectrum becomes closer to the continuous spectrum.

Similiar to the one-dimensional case, we define the two-dimensional DFT coefficients as following:

$$u_{\mathrm{k_x,k_y}} = \frac{1}{N_1}\frac{1}{N_2}\sum_{\mathrm{j_x=0}}^{\mathrm{N_1-1}}\sum_{\mathrm{j_y=0}}^{\mathrm{N_2-1}} U_{\mathrm{j_x,j_y}} \exp(-ik_{\mathrm{x}}x_{\mathrm{j_x}})\exp(-ik_{\mathrm{y}}y_{\mathrm{j_y}}) \tag{3.20}$$

where $k_{\mathrm{x}} = \frac{-N_1}{2}, ..., \frac{N_1}{2} - 1$ and $k_{\mathrm{y}} = \frac{-N_2}{2}, ..., \frac{N_2}{2} - 1$ are the corresponding wavenumbers. The inverse Fourier coefficients are

$$U_{\mathrm{x_j,y_j}} = \sum_{\mathrm{k_x=-N_1/2}}^{\mathrm{N_1/2-1}}\sum_{\mathrm{k_y=-N_2/2}}^{\mathrm{N_2/2-1}} u_{\mathrm{k_x,k_y}} \exp(ik_{\mathrm{x}}x_{\mathrm{j_x}})\exp(ik_{\mathrm{y}}y_{\mathrm{j_y}}) \tag{3.21}$$

defined at discrete grid points x_{j} ,y_{j} where $j_{\mathrm{x}} = 0, ..., N_1 - 1$ and $j_{\mathrm{y}} = 0, ..., N_2 - 1$, respectively.

We can now apply the general Fourier spectral method to the set of fluid equations we need to solve in two-dimensions. Note that using spectral method in space reduces the a PDE into an ODE. As is well known, when spectral methods are used, products in real space give rise to convolution sums in Fourier space; derivation in real space domain is equivalent to multiplication by the algebraic factor $i\mathbf{k}$ in the Fourier domain. Furthermore, Laplacian(∇^2) corresponds to $-k^2$ in transform space. These operations will be considered.

3.2.2 Differentiation

Differentiation using spectral methods, such as computing the gradient of density n depends upon in which space it is performed. Taking derivative in the Fourier transform space consists of simply multiplying each Fourier coefficients with the imaginary unit times the corresponding wavenumber. This could be expressed analytically by

$$\mathcal{F}\left\{\frac{du}{d\mathbf{x}}\right\} = i\mathbf{k}u_{\mathbf{k}} \tag{3.22}$$

in two-dimensional space or higher, where F represents the Fourier Transform operation and $\mathbf{k}$ is the Fourier wavenumber. This is the true spectral derivative which we refer to as the Fourier Galerkin derivative.

Differentiation in physical space is based upon the values of the function to be differentiated at the collocation points. Discrete Fourier coefficients are found for these values and are multiplied by $i\mathbf{k}$. The results are consequently transformed back into the physical space. The values of the approximate derivative at the grid points make up the Fourier collocation (pseudospectral) derivative.

Computationally, the evaluation of collocation derivative and Galerkin derivative is comparably equal. The operation count is $O(N \log_2 N)$ in one-dimension. However, since we plan to have all the calculations done in Fourier space, it is just as easy to perform all differentiations using the Fourier Galerkin method. Furthermore, phase errors are avoided if spectral Galerkin method is used to compute derivatives.

The Laplacian (∇^2) follows directly from derivative operation since $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ in two-dimensions. The Laplacian operator in the Fourier space becomes a multiplication of each Fourier coefficients with $-k^2$, where $k^2 = k_{\mathrm{x}}^2 + k_{\mathrm{y}}^2$ in two-dimensions.

In performing derivatives and Laplacian on a computation discrete grid, $\mathbf{k}$ and k^2 are actually replaced by k and K^2, respectively, where

$$k = k_{\mathrm{x}}\left[\frac{\sin(k_{\mathrm{x}}\Delta x)}{k_{\mathrm{x}}\Delta x}\right]\hat{\mathbf{k}}_{\mathrm{x}} + k_{\mathrm{y}}\left[\frac{\sin(k_{\mathrm{y}}\Delta y)}{k_{\mathrm{y}}\Delta y}\right]\hat{\mathbf{k}}_{\mathrm{y}} \tag{3.23}$$

and

$$K^2 = k_{\mathrm{x}}^2 \left[\frac{\sin \frac{k_{\mathrm{x}}\Delta x}{2}}{\frac{k_{\mathrm{x}}\Delta x}{2}} \right]^2 + k_{\mathrm{y}}^2 \left[\frac{\sin \frac{k_{\mathrm{y}}\Delta y}{2}}{\frac{k_{\mathrm{y}}\Delta y}{2}} \right]^2 \tag{3.24}$$

in two dimensions. This discreteness effect can be explained by considering the derivative operator and the Laplacian operator (in one-dimension for simplicity) as

$$\frac{du}{dx} \longrightarrow \frac{u^{n+1} - u^{n-1}}{2\Delta x} \tag{3.25}$$

$$\frac{d^2u}{dx^2} \longrightarrow \frac{u^{n+1} - 2u^n + u^{n-1}}{(\Delta x)^2} \tag{3.26}$$

obtained by finite differencing. Then substituting (3.18) into the Fourier transform of (3.25) and (3.26) and specializing them for the two-dimensional case, we obtain the results in (3.23) and (3.24). k and K^2 approach teh continuous result $\mathbf{k}$ and k^2, respectively, as the grid becomes finer, $\mathbf{k}\Delta x \rightarrow 0$.

3.2.3 Convolution

Nonlinear terms such as the ones found in (3.1) and (3.6) need a careful treatment by the spectral method. This is due to the property of the Fourier transform which states products in real space give rise to convolution in Fourier space. Thus, we need a specific method that can evaluate Fourier-space convolution effectively and accurately.

Consider the evaluation of the one-dimensional convolutional sum

$$\hat{w}_{\mathrm{k}} = \sum_{\mathrm{p+q=k}} \hat{u}_{\mathrm{p}} \hat{v}_{\mathrm{q}} \tag{3.27}$$

where

$$u(x) = \sum_{p=-\infty}^{\infty} \hat{u}_{\mathrm{p}} e^{ipx} \tag{3.28}$$

$$v(x) = \sum_{q=-\infty}^{\infty} \hat{v}_{\mathrm{q}} e^{iqx} \tag{3.29}$$

$$\hat{w}_{\mathrm{k}} = \frac{1}{2\pi} \int_0^{2\pi} w(x) e^{ikx} dx. \tag{3.30}$$

When u, v, and w are approximated by their respective truncated Fourier series of degree $N/2$, (3.27) becomes

$$\hat{w}_{\mathrm{k}} = \sum_{\mathrm{p+q=k}} \hat{u}_{\mathrm{p}} \hat{v}_{\mathrm{q}} \qquad |p|, |q| \ \leq \ \frac{N}{2}, \tag{3.31}$$

where u_{p} and v_{q} are generally complex, and p, q, k denote the Fourier mode numbers. Direct summation of (3.31) takes $O(N^2)$ operations in one-dimension, compared to only $O(N)$ operations if we were to use a finite difference algorithm for the nonlinear terms. If we use FFT, the number of operations is improved somewhat to $O(N \log_2 N)$ as we have seen earlier. However, the number of operations still gets large very fast as we go to higher dimensions and larger N. The convolution using Fourier Galerkin is not very efficient. The feature that makes direct evaluation of (3.31) inefficient is their nonlocality: w_{k} depends on u_{p} and v_{q} for $\max(k - N/2, -N/2) < p < \min(k + N/2, N/2)$.

This nonlocality can be avoided by using suitable discrete Fourier transforms to express w_{k} as local product of Fourier-transformed fields. The approach is to use inverse DFT given in (3.19) to transform u_{p} and v_{q} to U_{j} and V_{j} in physical space. U_{j} and V_{j} are defined at exactly N points of $x_{\mathrm{j}} = 2\pi/N$ for $j = 0, ..., N-1$. We can define W_{j} as the local product $U_{\mathrm{j}} V_{\mathrm{j}}$ of the transform fields, and then use the DFT to return to the Fourier space. The overall convolution sequence can be summarized by

$$u_{\mathrm{k}}, v_{\mathrm{k}} \xrightarrow{IFFT} U_{\mathrm{j}}, V_{\mathrm{j}} \xrightarrow{\times} W_{\mathrm{j}} \xrightarrow{FFT} \hat{w}_{\mathrm{k}}. \tag{3.32}$$

We find that

$$\begin{aligned} \hat{w}_{\mathrm{k}} &= \frac{1}{N} \sum_{\mathrm{j}=0}^{N-1} U_{\mathrm{j}} V_{\mathrm{j}} e^{-ikx_{\mathrm{j}}} \\ &= \frac{1}{N} \sum_{\mathrm{j}=0}^{N-1} \sum_{|p| \leq N/2} u_{\mathrm{p}} e^{-ipx_{\mathrm{j}}} \sum_{|q| \leq N/2} v_{\mathrm{q}} e^{-iqx_{\mathrm{j}}} \\ &= \sum_{|p|,|q| \leq N/2} u_{\mathrm{p}} v_{\mathrm{q}} \frac{1}{N} \sum_{\mathrm{j}=0}^{N-1} e^{-i(p+q-k)x_{\mathrm{j}}}, \end{aligned} \tag{3.33}$$

where $\hat{w}_{\mathrm{k}}$ is the aliased convolution sum. Using the discrete transform orthogonality relation

$$\sum_{\mathrm{j}=0}^{N-1} e^{-i(k-p)x_{\mathrm{j}}} = \begin{cases} N & \text{if } k \equiv p (\mathrm{mod}\ N) \\ 0 & \text{otherwise}, \end{cases} \tag{3.34}$$

Equation (3.33) can be rewritten as

$$\begin{aligned} \hat{w}_{\mathrm{k}} &= \sum_{\mathrm{p+q=k}} u_{\mathrm{p}} v_{\mathrm{q}} + \sum_{\mathrm{p+q=k\pm N}} u_{\mathrm{p}} v_{\mathrm{q}} \\ &= w_{\mathrm{k}} + \sum_{\mathrm{p+q=k\pm N}} u_{\mathrm{p}} v_{\mathrm{q}}, \end{aligned} \tag{3.35}$$

where $w_{\rm k}$ is the convolution term given in (3.31). The second term on teh right-hand side of (3.35) originates from the property that $\exp[i(k \pm N)x_{\rm j}] = \exp[ikx_{\rm j}]$ for all integral j, k such that the discrete grid points $x_{\rm j}$ cannot distinguish the wave vector k and its alias $k \pm N, k \pm 2N$, etc. For any $k < N/2$, there always exists a nonzero aliasing error. Equation (3.35) is applicable only for one-dimensional case. Derivation for higher dimension cases, although is much more involved, is similar to that of the one-dimensional case. In three dimensions, in addition to the singly-aliased term on the right-hand side of (3.35), there are two other singly-aliased contributions, three doubly-aliased terms and one triply-aliased contribution. Aliasing errors usually, but not always, lead to numerical instabilities; they, however, always lead to inaccuracies, especially for high k modes.

In order to eliminate the aliasing terms, we used phase shifting method.

Aliasing removal by grid and phase shifting

We first define the phase shifted discrete transform

$$\tilde{U}_{\rm j} = \sum_{\rm k=-N/2}^{N/2-1} u_{\rm k} e^{ik(x_{\rm j}+\Delta)} \tag{3.36}$$

$$\tilde{V}_{\rm j} = \sum_{\rm k=-N/2}^{N/2-1} v_{\rm k} e^{ik(x_{\rm j}+\Delta)} \tag{3.37}$$

which are just the transform on a grid shifted by the factor Δ in physical space. We then compute the local product of $\tilde{U}_{\rm j}\tilde{V}_{\rm j}$ and inverse transform it back to the Fourier space. The result of the convolution of the shifted grid is

$$\tilde{w}_{\rm k} = \frac{1}{N} \sum_{\rm j=0}^{N-1} \tilde{U}_{\rm j}\tilde{V}_{\rm j} e^{ik(x_{\rm j}+\Delta)} \tag{3.38}$$

while the result for the unshifted grid is given in (3.33).

3.2.4 The Gibbs phenomenon

In a spectral analysis, the Gibbs phenomenon frequently arises. The Gibbs phenomenon occurs with a truncated or a discrete Fourier series in the neighborhood of a point of discontinuity. Frequently, when taking approximations around the discontinuity, oscillations, indicating a gibbs phenomenon, will occur; thus possibly making the numerical results suspect. In our simulation, we will defining our simulation box to be a grid. Thus, if our simulation contains gradients which are too steep for the grid to resolve, then the solution will appear to have a discontinuity. This can result in such oscillations.

There are two ways to deal with Gibbs phonomena arising from ateep gradients. The most obvious way is to increase the spatial resolution of the grid. This, however, is not practical due to memery and speed constraints. The way is to numerically compensate for the Gibbs phenomenon. One way of doing this is by adding an artifical diffusion constant. This acts as a "smoothing" process by attenuating the higher order Fourier coefficients. However, if the diffusion constant is too high then the approximation will be excessively smeared. Therefore the diffusion constant must be tuned so that no important structures are lost, but the effects of the Gibbs phenomenon are minimized. Unfortunately, in our case, the optimum balance still results in some artifacts due to Gibbs phenomenon. The resulting oscillations adds some structures, but does not effect the overall accuracy of the simulation. The structure resulting from the Gibbs phenomenon, however, needs to be recognized as such and consequently ignored.

3.3 Theoretical model in the spectral domain

We now describe the numerical model in two-dimensions (x,y). First, we consider the electron continuity equation (3.1) and electron momentum equation (3.2) in unmagnetized plasmas. The two-dimensional electron continuity equation is

$$\frac{\partial n_{\mathrm{e}}}{\partial t} + \left(\frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y}\right) \cdot n_{\mathrm{e}}(v_{\mathrm{ex}}\hat{x} + v_{\mathrm{ey}}\hat{y}) = \left.\frac{dn_{\mathrm{e}}}{dt}\right|_{\mathrm{charging}} + q_{\mathrm{s}}.$$

Simplifying, this becomes

$$\frac{\partial n_{\mathrm{e}}}{\partial t} + v_{\mathrm{ex}}\frac{\partial n_{\mathrm{e}}}{\partial x} + n_{\mathrm{e}}\frac{\partial v_{\mathrm{ex}}}{\partial x} + v_{\mathrm{ey}}\frac{\partial n_{\mathrm{e}}}{\partial y} + n_{\mathrm{e}}\frac{\partial v_{\mathrm{ey}}}{\partial y} = \left.\frac{dn_{\mathrm{e}}}{dt}\right|_{\mathrm{charging}} + q_{\mathrm{s}}. \tag{3.39}$$

Since

$$\vec{E} = -\nabla\phi = -\left(\frac{\partial \phi}{\partial x}\hat{x} + \frac{\partial \phi}{\partial y}\hat{y}\right)$$

the electron momentum equations can be written as

$$\frac{\partial v_{\mathrm{ex}}}{\partial t} + v_{\mathrm{ex}}\frac{\partial v_{\mathrm{ex}}}{\partial x} + v_{\mathrm{ey}}\frac{\partial v_{\mathrm{ex}}}{\partial y} = -\left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}}\right)\frac{\partial \phi}{\partial x} - \gamma\left(\frac{T_{\mathrm{e}}}{m_{\mathrm{e}}}\right)\frac{1}{n_{\mathrm{e}}}\frac{\partial n_{\mathrm{e}}}{\partial x} \tag{3.40}$$

and

$$\frac{\partial v_{\mathrm{ey}}}{\partial t} + v_{\mathrm{ex}}\frac{\partial v_{\mathrm{ey}}}{\partial x} + v_{\mathrm{ey}}\frac{\partial v_{\mathrm{ey}}}{\partial y} = -\left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}}\right)\frac{\partial \phi}{\partial y} - \gamma\left(\frac{T_{\mathrm{e}}}{m_{\mathrm{e}}}\right)\frac{1}{n_{\mathrm{e}}}\frac{\partial n_{\mathrm{e}}}{\partial y}. \tag{3.41}$$

For strongly magnetized electrons, the left side of equation (3.1) will be simplified by using a vector identity as follows

$$\nabla \cdot (n_{\mathrm{e}}\vec{v}_{\mathrm{e}}) = \vec{v}_{\mathrm{e}} \cdot \nabla n_{\mathrm{e}} + n_{\mathrm{e}}\nabla \cdot \vec{v}_{\mathrm{e}}.$$

Next $\nabla \cdot \vec{v}_\mathrm{e} = 0$ since $\vec{v}_\mathrm{e} = \frac{\vec{E} \times \vec{B}}{B^2} = \frac{-\nabla\phi \times \vec{B}}{B^2}$. Therefore, $\nabla \cdot (n_\mathrm{e}\vec{v}_\mathrm{e}) = \vec{v}_\mathrm{e} \cdot \nabla n_\mathrm{e}$ in equation (3.1). The conversion into two-dimensions is as follows. The electron velocity can be written as

$$\vec{v}_\mathrm{e} = v_\mathrm{ex}\hat{x} + v_\mathrm{ey}\hat{y} = \frac{E_\mathrm{y}}{B_\mathrm{z}}\hat{x} - \frac{E_\mathrm{x}}{B_\mathrm{z}}\hat{y}.$$

Noting that

$$\vec{v}_\mathrm{e} \cdot \nabla n_\mathrm{e} = v_\mathrm{ex}\frac{\partial n_\mathrm{e}}{\partial x} + v_\mathrm{ey}\frac{\partial n_\mathrm{e}}{\partial y}$$

equation (3.1) becomes

$$\frac{\partial n_\mathrm{e}}{\partial t} + v_\mathrm{ex}\frac{\partial n_\mathrm{e}}{\partial x} + v_\mathrm{ey}\frac{\partial n_\mathrm{e}}{\partial y} = \left.\frac{dn_\mathrm{e}}{dt}\right|_\mathrm{charging} + q_\mathrm{s}. \tag{3.42}$$

For the ions, we can use the same continuity and momentum equations in magnetized and unmagnetized plasmas because the ion plasma is not affected by the background magnetic field due to relatively heavy mass. The two-dimensional ion continuity equation is

$$\frac{\partial n_\mathrm{i}}{\partial t} + \left(\frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y}\right) \cdot n_\mathrm{i}(v_\mathrm{ix}\hat{x} + v_\mathrm{iy}\hat{y}) = \left.\frac{dn_\mathrm{i}}{dt}\right|_\mathrm{charging} + q_\mathrm{s}.$$

Simplifying, this becomes

$$\frac{\partial n_{\mathrm{i}}}{\partial t} + v_{\mathrm{ix}}\frac{\partial n_{\mathrm{i}}}{\partial x} + n_{\mathrm{i}}\frac{\partial v_{\mathrm{ix}}}{\partial x} + v_{\mathrm{iy}}\frac{\partial n_{\mathrm{i}}}{\partial y} + n_{\mathrm{i}}\frac{\partial v_{\mathrm{iy}}}{\partial y} = \left.\frac{dn_{\mathrm{i}}}{dt}\right|_{\mathrm{charging}} + q_{\mathrm{s}}. \tag{3.43}$$

The ion momentum equations can be written as

$$\frac{\partial v_{\mathrm{ix}}}{\partial t} + v_{\mathrm{ix}}\frac{\partial v_{\mathrm{ix}}}{\partial x} + v_{\mathrm{iy}}\frac{\partial v_{\mathrm{ix}}}{\partial y} = -\left(\frac{q_{\mathrm{i}}}{m_{\mathrm{i}}}\right)\frac{\partial \phi}{\partial x} - \gamma\left(\frac{T_{\mathrm{i}}}{m_{\mathrm{i}}}\right)\frac{1}{n_{\mathrm{i}}}\frac{\partial n_{\mathrm{i}}}{\partial x} \tag{3.44}$$

and

$$\frac{\partial v_{\mathrm{iy}}}{\partial t} + v_{\mathrm{ix}}\frac{\partial v_{\mathrm{iy}}}{\partial x} + v_{\mathrm{iy}}\frac{\partial v_{\mathrm{iy}}}{\partial y} = -\left(\frac{q_{\mathrm{i}}}{m_{\mathrm{i}}}\right)\frac{\partial \phi}{\partial y} - \gamma\left(\frac{T_{\mathrm{i}}}{m_{\mathrm{i}}}\right)\frac{1}{n_{\mathrm{i}}}\frac{\partial n_{\mathrm{i}}}{\partial y}. \tag{3.45}$$

The theoretical model for the electrons and ions is represented in the spectral domain as follows. The subscript k denotes that the quantity is in the spectral domain, $\otimes$ denotes Fourier convolution, $k_{\mathrm{x,y}}$ are the Fourier wavenumbers in x and y, and $k^2 = k_{\mathrm{x}}^2 + k_{\mathrm{y}}^2$ where k_{x} and k_{y} are given by [*Orszag*, 1971]

$$k_{\mathrm{x}} = \kappa_{\mathrm{x}}\frac{\sin(\kappa_{\mathrm{x}}\Delta x)}{\kappa_{\mathrm{x}}\Delta x}, \tag{3.46}$$

$$k_{\mathrm{y}} = \kappa_{\mathrm{y}}\frac{\sin(\kappa_{\mathrm{y}}\Delta y)}{\kappa_{\mathrm{y}}\Delta y}, \tag{3.47}$$

where $\kappa_{\mathrm{x}} = 2\pi n_{\mathrm{x}}/L_{\mathrm{x}}$ and $\kappa_{\mathrm{y}} = 2\pi n_{\mathrm{y}}/L_{\mathrm{y}}$. Here n_{x} and n_{y} are the mode numbers in the x and y direction. The finite difference terms, k_{x} and k_{y}, are introduced to represent derivatives and Laplacians on the discrete grid and approach the actual differential equation results as the grid becomes finer, $\kappa_{\mathrm{x}}\Delta x, \kappa_{\mathrm{y}}\Delta y \rightarrow 0$.

Taking the spatial Fourier transformation of the unmagnetized electron equations (3.39), (3.40) and (3.41) in spectral domain are

$$\frac{dn_{\mathrm{ek}}}{dt} + v_{\mathrm{ex}} \otimes ik_{\mathrm{x}} n_{\mathrm{ek}} + n_{\mathrm{e}} \otimes ik_{\mathrm{x}} v_{\mathrm{exk}} + v_{\mathrm{ey}} \otimes ik_{\mathrm{y}} n_{\mathrm{ek}} + n_{\mathrm{e}} \otimes ik_{y} v_{\mathrm{eyk}} = \left.\frac{dn_{\mathrm{ek}}}{dt}\right|_{\mathrm{charging}} + q_{\mathrm{sk}}, \quad (3.48)$$

$$\frac{dv_{\mathrm{exk}}}{dt} + v_{\mathrm{exk}} \otimes ik_{\mathrm{x}} v_{\mathrm{exk}} + v_{\mathrm{eyk}} \otimes ik_{\mathrm{y}} v_{\mathrm{exk}} = -\left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}}\right) ik_{\mathrm{x}} \phi_{\mathrm{k}} - \gamma \left(\frac{T_{\mathrm{e}}}{m_{\mathrm{e}}}\right) \left(\frac{1}{n_{\mathrm{e}}}\right)_{\mathrm{k}} \otimes ik_{\mathrm{x}} n_{\mathrm{k}}, \quad (3.49)$$

and

$$\frac{dv_{\mathrm{eyk}}}{dt} + v_{\mathrm{exk}} \otimes ik_{\mathrm{x}} v_{\mathrm{eyk}} + v_{\mathrm{eyk}} \otimes ik_{\mathrm{y}} v_{\mathrm{eyk}} = -\left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}}\right) ik_{\mathrm{y}} \phi_{\mathrm{k}} - \gamma \left(\frac{T_{\mathrm{e}}}{m_{\mathrm{e}}}\right) \left(\frac{1}{n_{\mathrm{e}}}\right)_{\mathrm{k}} \otimes ik_{\mathrm{y}} n_{\mathrm{k}}. \quad (3.50)$$

For strongly magnetized electrons, the equation (3.42) becomes

$$\frac{dn_{\mathrm{ek}}}{dt} + v_{\mathrm{exk}} \otimes ik_{\mathrm{x}} n_{\mathrm{exk}} + v_{\mathrm{eyk}} \otimes ik_{\mathrm{y}} n_{\mathrm{eyk}} = \left.\frac{dn_{\mathrm{ek}}}{dt}\right|_{\mathrm{charging}} + q_{\mathrm{sk}}. \quad (3.51)$$

The ion equations (3.43), (3.44) and (3.45) in spectral domain are

$$\frac{dn_{\rm ik}}{dt} + v_{\rm ix} \otimes ik_{\rm x} n_{\rm ik} + n_{\rm i} \otimes ik_{\rm x} v_{\rm ixk} + v_{\rm iy} \otimes ik_{\rm y} n_{\rm ik} + n_{\rm i} \otimes ik_{y} v_{\rm iyk} = \left.\frac{dn_{\rm ik}}{dt}\right|_{\rm charging} + q_{\rm sk}, \quad (3.52)$$

$$\frac{dv_{\rm ixk}}{dt} + v_{\rm ixk} \otimes ik_{\rm x} v_{\rm ixk} + v_{\rm iyk} \otimes ik_{\rm y} v_{\rm ixk} = -\left(\frac{q_{\rm i}}{m_{\rm i}}\right) ik_{\rm x}\phi_{\rm k} - \gamma\left(\frac{T_{\rm i}}{m_{\rm i}}\right)\left(\frac{1}{n_{\rm i}}\right)_{\rm k} \otimes ik_{\rm x} n_{\rm k}, \quad (3.53)$$

and

$$\frac{dv_{\rm iyk}}{dt} + v_{\rm ixk} \otimes ik_{\rm x} v_{\rm iyk} + v_{\rm iyk} \otimes ik_{\rm y} v_{\rm iyk} = -\left(\frac{q_{\rm i}}{m_{\rm i}}\right) ik_{\rm y}\phi_{\rm k} - \gamma\left(\frac{T_{\rm i}}{m_{\rm i}}\right)\left(\frac{1}{n_{\rm i}}\right)_{\rm k} \otimes ik_{\rm y} n_{\rm k}. \quad (3.54)$$

We note that upon Fourier transforming, we have reduced the PDEs into ODEs which are easy to time integrate. Poisson's equation becomes

$$\epsilon_0 k^2 \phi_{\rm k} = (q_{\rm e} n_{\rm ek} + q_{\rm i} n_{\rm ik} + \rho_{\rm dk}) \quad (3.55)$$

3.4 Time integration methods

Although the spectral or pseudospectral method is used for spatial discretization, for time integration this is not necessarily the best method. In our case, finite difference methods are used for the time integration.

In this section, we will discuss the methods used to solve the temporal dependence of our theoretical model. We chose a predictor-corrector method [*Shampine*, 1994] which is most appropriate for our simulation.

Predictor-corrector methods

A Predictor-corrector method is a combination of an explicit predictor formula and an implicit corrector formula. Predictor-corrector methods store the solution along the way, and use those results to extrapolate the solution one step advanced. They then correct the extrapolation using derivative information at the new point. Predictor-corrector methods have good stability properties and are best for smooth functions. Consider the following ODE

$$\frac{dn}{dt} = f(n,t) \tag{3.56}$$

where $f(n,t)$ is represented in the spectral domain. The predictor-corrector method is as follows

$$step1 : n^{\dagger} = n^t + \ dt \cdot f(n^t, t) \tag{3.57}$$

$$step2 : f(n^*, t + \frac{dt}{2}) = \frac{1}{2}(f(n^t, t) + f(n^{\dagger}, t + dt)) \tag{3.58}$$

$$step3 : n^{t+dt} = n^t + \ dt \cdot f(n^*, t + \frac{dt}{2}) \tag{3.59}$$

where $n^{\dagger}$ is the estimate of n^{t+dt} and dt is the time step.

3.5 Time integration of the theoretical model

The predictor-corrector method is applied to our model for the time integration after performing spatial Fourier transforms on the continuity and momentum equations for the plasma electrons and ions.

3.5.1 Predictor step

The predictor step equations for the spectral domain electron density n_{ek}, and the x and y components of the electron velocity, v_{exk} and v_{eyk} for the unmagnetized case are as follows

$$\begin{aligned} n^{\dagger}_{\mathrm{ek}} = n^{t}_{\mathrm{ek}} - dt \cdot \Big(& v^{t}_{\mathrm{exk}} \otimes ik_{\mathrm{x}} n^{t}_{\mathrm{ek}} + n^{t}_{\mathrm{ek}} \otimes ik_{\mathrm{x}} v^{t}_{\mathrm{exk}} + v^{t}_{\mathrm{eyk}} \otimes ik_{y} n^{t}_{\mathrm{ek}} \\ & + n^{t}_{\mathrm{ek}} \otimes ik_{\mathrm{y}} v^{t}_{\mathrm{eyk}} + D^{*}_{\mathrm{e}} k^{2} n^{t}_{\mathrm{ek}} \Big) + dt \cdot \frac{1}{q_{\mathrm{e}}} \left[\frac{d\rho_{\mathrm{dek}}}{dt} \right]^{t} + q_{\mathrm{sk}}, \end{aligned} \tag{3.60}$$

$$\begin{aligned} v^{\dagger}_{\mathrm{exk}} = v^{t}_{\mathrm{exk}} - dt \cdot \Bigg(& v^{t}_{\mathrm{exk}} \otimes ik_{\mathrm{x}} v^{t}_{\mathrm{exxk}} + v^{t}_{\mathrm{eyk}} \otimes ik_{\mathrm{y}} v^{t}_{\mathrm{exyk}} - \left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}} \right) E^{t}_{\mathrm{xk}} \\ & - \gamma \left(\frac{T_{\mathrm{e}}}{m_{\mathrm{e}}} \right) \left(\frac{1}{n_{\mathrm{e}}} \right)^{t}_{\mathrm{k}} \otimes ik_{\mathrm{y}} n_{\mathrm{exk}} + \mu^{*}_{\mathrm{e}} k^{2} v^{t}_{\mathrm{exk}} \Bigg), \end{aligned} \tag{3.61}$$

and

$$\begin{aligned} v^{\dagger}_{\mathrm{eyk}} = v^{t}_{\mathrm{eyk}} - dt \cdot \Bigg(& v^{t}_{\mathrm{exk}} \otimes ik_{\mathrm{x}} v^{t}_{\mathrm{eyxk}} + v^{t}_{\mathrm{iyk}} \otimes ik_{\mathrm{y}} v^{t}_{\mathrm{eyyk}} - \left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}} \right) E^{t}_{\mathrm{yk}} \\ & - \gamma \left(\frac{T_{\mathrm{e}}}{m_{\mathrm{i}}} \right) \left(\frac{1}{n_{\mathrm{e}}} \right)^{t}_{\mathrm{k}} \otimes ik_{\mathrm{y}} n^{t}_{\mathrm{eyk}} + \mu^{*}_{\mathrm{e}} k^{2} v^{t}_{\mathrm{eyk}} \Bigg). \end{aligned} \tag{3.62}$$

For the case of the strongly magnetized electrons,

$$n^{\dagger}_{\mathrm{ek}} = n^{t}_{\mathrm{ek}} - dt \cdot \left(v^{t}_{\mathrm{exk}} \otimes ik_{\mathrm{x}} n^{t}_{\mathrm{exk}} + v^{t}_{\mathrm{eyk}} \otimes ik_{\mathrm{y}} n^{t}_{\mathrm{eyk}} + D^{*}_{\mathrm{e}} k^{2} n^{t}_{\mathrm{ek}} \right) +$$

$$dt \cdot \frac{1}{q_{\rm e}} \left[\frac{d\rho_{\rm dek}}{dt} \right]^t + q_{\rm sk}. \tag{3.63}$$

Note that $v_{\rm exk} = \frac{E_{\rm yk}}{B}$ and $v_{\rm eyk} = -\frac{E_{\rm xk}}{B}$.
The ion equations in the spectral domain are

$$n_{\rm ik}^{\dagger} = n_{\rm ik}^t - dt \cdot \Big(v_{\rm ixk}^t \otimes ik_{\rm x} n_{\rm ik}^t + n_{\rm ik}^t \otimes ik_{\rm x} v_{\rm ixk}^t + v_{\rm iyk}^t \otimes ik_y n_{\rm ik}^t$$
$$+ n_{\rm ik}^t \otimes ik_{\rm y} v_{\rm iyk}^t + D_{\rm i}^* k^2 n_{\rm ik}^t \Big) + dt \cdot \frac{1}{q_{\rm i}} \left[\frac{d\rho_{\rm dik}}{dt} \right]^t, \tag{3.64}$$

$$v_{\rm ixk}^{\dagger} = v_{\rm ixk}^t - dt \cdot \left(v_{\rm ixk}^t \otimes ik_{\rm x} v_{\rm ixxk}^t + v_{\rm iyk}^t \otimes ik_{\rm y} v_{\rm ixyk}^t - \left(\frac{q_{\rm i}}{m_{\rm i}} \right) E_{\rm xk}^t \right.$$
$$\left. - \gamma \left(\frac{T_{\rm i}}{m_{\rm i}} \right) \left(\frac{1}{n_{\rm i}} \right)_{\rm k}^t \otimes ik_{\rm y} n_{\rm ixk} + \mu_{\rm i}^* k^2 v_{\rm ixk}^t \right), \tag{3.65}$$

and

$$v_{\rm iyk}^{\dagger} = v_{\rm iyk}^t - dt \cdot \left(v_{\rm ixk}^t \otimes ik_{\rm x} v_{\rm iyxk}^t + v_{\rm iyk}^t \otimes ik_{\rm y} v_{\rm iyyk}^t - \left(\frac{q_{\rm i}}{m_{\rm i}} \right) E_{\rm yk}^t \right.$$
$$\left. - \gamma \left(\frac{T_{\rm i}}{m_{\rm i}} \right) \left(\frac{1}{n_{\rm i}} \right)_{\rm k}^t \otimes ik_{\rm y} n_{\rm iyk}^t + \mu_{\rm i}^* k^2 v_{\rm iyk}^t \right), \tag{3.66}$$

where $v_{\rm ixxk}$ and $v_{\rm ixyk}$ denote x and y derivatives of $v_{\rm ix}$ in the spectral domain and $v_{\rm iyxk}$ and $v_{\rm iyyk}$ denote x and y derivatives of $v_{\rm iy}$ in the spectral domain. Note that $d\rho_{\rm de}/dt$ and $d\rho_{\rm di}/dt$ are calculated by linear PIC weighting the dust grain currents to the grid points. Fast Fourier Transforms FFTs are applied to our numerical simulation. A real-valued initial density is specified which is transformed into the Fourier space since all computations are done in the Fourier spectral domain. The convolutions are evaluated using the pseudospectral method [*Orszag*, 1971]. Aliasing is minimized by grid shifting and truncation of Fourier modes that lie outside .94K where $K = 2\pi n_{\rm x,y}/2L_{\rm x,y}$ is the maximum wavenumber [*Patterson and Orszag*, 1971]. The numerical diffusion $D^*_{\rm e,i}$ and viscosity $\mu^*_{\rm i}$ coefficients are chosen to provide numerical stability.

The predictor step for the dust charging model is

$$Z^\dagger_j = Z^t_j + dt \cdot \left(\frac{1}{q_{\rm e}} I_{{\rm e}j}(n^t_{\rm e}, Z^t_j) + \frac{1}{q_{\rm i}} I_{{\rm i}j}(n^t_{\rm i}, Z^t_j) \right), \tag{3.67}$$

where the subscript j denotes the j^{th} dust grain and $Z_{\rm j} = Q_{\rm j}/e$. The electron and ion current on the j^{th} dust grain depend on the electron and ion densities and dust charge. Linear weighting is used to calculate $n^t_{\rm e}$ and $n^t_{\rm i}$ at the simulation particle position. The PIC time advance for the dust grain position and velocity are given by

$$v_j^{t+\frac{dt}{2}} = v_j^{t-\frac{dt}{2}} + dt \cdot \frac{eZ^t_{\rm j}}{m_{\rm j}} E^t \tag{3.68}$$

and

$$x_j^{t+dt} = x^t_j + dt \cdot v_{\rm j}^{t+\frac{dt}{2}}, \tag{3.69}$$

where $x_{\rm j}$ and $v_{\rm j}$ are the position and velocity of the j^{th} dust grain.

Once the electron, ion, and dust charge densities are calculated, the electrostatic potential ϕ and the electric field $\mathbf{E} = -\nabla\phi$ $(= ik_{\rm x}\phi_{\rm k}\hat{\mathbf{x}} + ik_{\rm y}\phi_{\rm k}\hat{\mathbf{y}}$ in the spectral domain) are calculated from Poisson's equation. Poisson's equation in the spectral domain is

$$\phi_{\mathrm{k}}^{\dagger} = \frac{1}{\epsilon_0 k^2}(q_{\mathrm{e}} n_{\mathrm{ek}}^{\dagger} + q_{\mathrm{i}} n_{\mathrm{ik}}^{\dagger} + \rho_{\mathrm{dk}}^{\dagger}). \tag{3.70}$$

Linear PIC weighting is also used to calculate $\rho_{\mathrm{dk}}^{\dagger}$ on the simulation grid.

3.5.2 Corrector step

Next all relevant quantities are averaged to calculate their values at $t + \frac{dt}{2}$. The corrector step equations for unmagnetized electrons are as follows

$$\begin{aligned} n_{ek}^{t+dt} = n_{ek}^{t} - dt \cdot \Big(& v_{\mathrm{exk}}^{t+\frac{dt}{2}} \otimes ik_x n_{\mathrm{ek}}^{t+\frac{dt}{2}} + n_{\mathrm{ek}}^{t+\frac{dt}{2}} \otimes ik_x v_{\mathrm{exk}}^{t+\frac{dt}{2}} + v_{\mathrm{eyk}}^{t+\frac{dt}{2}} \otimes ik_y n_{\mathrm{ek}}^{t+\frac{dt}{2}} \\ & + n_{\mathrm{e}}^{t+\frac{dt}{2}} \otimes ik_y v_{\mathrm{eyk}}^{t+\frac{dt}{2}} + D_{\mathrm{e}}^{*} k^2 n_{\mathrm{ek}}^{t+\frac{dt}{2}} \Big) + dt \cdot \frac{1}{q_{\mathrm{e}}} \left[\frac{d\rho_{\mathrm{dek}}}{dt} \right]^{t+\frac{dt}{2}} + q_{\mathrm{sk}}, \end{aligned} \tag{3.71}$$

$$\begin{aligned} v_{\mathrm{exk}}^{t+dt} = v_{\mathrm{exk}}^{t} - dt \cdot \Big(& v_{\mathrm{exk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{x}} v_{\mathrm{ixxk}}^{t+\frac{dt}{2}} + v_{\mathrm{eyk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} v_{\mathrm{ixyk}}^{t+\frac{dt}{2}} - \left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}}\right) E_{\mathrm{xk}}^{t+\frac{dt}{2}} \\ & - \gamma \left(\frac{T_{\mathrm{e}}}{m_{\mathrm{e}}}\right) \left(\frac{1}{n_{\mathrm{e}}}\right)_{\mathrm{k}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} n_{\mathrm{exk}}^{t+\frac{dt}{2}} + \mu_{\mathrm{e}}^{*} k^2 v_{\mathrm{exk}}^{t+\frac{dt}{2}} \Big), \end{aligned} \tag{3.72}$$

and

$$\begin{aligned} v_{\mathrm{eyk}}^{t+dt} = v_{\mathrm{eyk}}^{t} - dt \cdot \Big(& v_{\mathrm{exk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{x}} v_{\mathrm{eyxk}}^{t+\frac{dt}{2}} + v_{\mathrm{eyk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} v_{\mathrm{eyyk}}^{t+\frac{dt}{2}} - \left(\frac{q_{\mathrm{e}}}{m_{\mathrm{e}}}\right) E_{\mathrm{yk}}^{t+\frac{dt}{2}} \\ & - \gamma \left(\frac{T_{\mathrm{e}}}{m_{\mathrm{e}}}\right) \left(\frac{1}{n_{\mathrm{e}}}\right)_{k}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} n_{\mathrm{eyk}}^{t+\frac{dt}{2}} + \mu_{\mathrm{e}}^{*} k^2 v_{\mathrm{iyk}}^{t+\frac{dt}{2}} \Big). \end{aligned} \tag{3.73}$$

For the case of magnetized electrons this becomes

$$n_{\mathrm{ek}}^{t+dt} = n_{\mathrm{ek}}^{t} - dt \cdot \left(v_{\mathrm{exk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{x}} n_{\mathrm{exk}}^{t+\frac{dt}{2}} + v_{\mathrm{eyk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} n_{\mathrm{eyk}}^{t+\frac{dt}{2}} + D_{\mathrm{e}}^{*} k^2 n_{\mathrm{ek}}^{t+\frac{dt}{2}} \right)$$

$$+dt \cdot \frac{1}{q_{\mathrm{e}}} \left[\frac{d\rho_{\mathrm{dek}}}{dt} \right]^{t+\frac{dt}{2}} + q_{\mathrm{sk}}. \tag{3.74}$$

The ion equations are as follows

$$n_{ik}^{t+dt} = n_{ik}^{t} - dt \cdot \left(v_{\mathrm{ixk}}^{t+\frac{dt}{2}} \otimes ik_x n_{\mathrm{ik}}^{t+\frac{dt}{2}} + n_{\mathrm{ik}}^{t+\frac{dt}{2}} \otimes ik_x v_{\mathrm{ixk}}^{t+\frac{dt}{2}} + v_{\mathrm{iyk}}^{t+\frac{dt}{2}} \otimes ik_y n_{\mathrm{ik}}^{t+\frac{dt}{2}} \right.$$
$$\left. + n_{\mathrm{i}}^{t+\frac{dt}{2}} \otimes ik_y v_{\mathrm{iyk}}^{t+\frac{dt}{2}} + D_{\mathrm{i}}^{*} k^2 n_{\mathrm{ik}}^{t+\frac{dt}{2}} \right) + dt \cdot \frac{1}{q_{\mathrm{i}}} \left[\frac{d\rho_{\mathrm{dik}}}{dt} \right]^{t+\frac{dt}{2}} + q_{\mathrm{sk}}, \tag{3.75}$$

$$v_{\mathrm{ixk}}^{t+dt} = v_{\mathrm{ixk}}^{t} - dt \cdot \left(v_{\mathrm{ixk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{x}} v_{\mathrm{ixxk}}^{t+\frac{dt}{2}} + v_{\mathrm{iyk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} v_{\mathrm{ixyk}}^{t+\frac{dt}{2}} - \left(\frac{q_{\mathrm{i}}}{m_{\mathrm{i}}} \right) E_{\mathrm{xk}}^{t+\frac{dt}{2}} \right.$$
$$\left. -\gamma \left(\frac{T_{\mathrm{i}}}{m_{\mathrm{i}}} \right) \left(\frac{1}{n_{\mathrm{i}}} \right)_{\mathrm{k}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} n_{\mathrm{ixk}}^{t+\frac{dt}{2}} + \mu_{\mathrm{i}}^{*} k^2 v_{\mathrm{ixk}}^{t+\frac{dt}{2}} \right), \tag{3.76}$$

and

$$v_{\mathrm{iyk}}^{t+dt} = v_{\mathrm{iyk}}^{t} - dt \cdot \left(v_{\mathrm{ixk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{x}} v_{\mathrm{iyxk}}^{t+\frac{dt}{2}} + v_{\mathrm{iyk}}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} v_{\mathrm{iyyk}}^{t+\frac{dt}{2}} - \left(\frac{q_{\mathrm{i}}}{m_{\mathrm{i}}} \right) E_{\mathrm{yk}}^{t+\frac{dt}{2}} \right.$$
$$\left. -\gamma \left(\frac{T_{\mathrm{i}}}{m_{\mathrm{i}}} \right) \left(\frac{1}{n_{\mathrm{i}}} \right)_{k}^{t+\frac{dt}{2}} \otimes ik_{\mathrm{y}} n_{\mathrm{iyk}}^{t+\frac{dt}{2}} + \mu_{\mathrm{i}}^{*} k^2 v_{\mathrm{iyk}}^{t+\frac{dt}{2}} \right). \tag{3.77}$$

for the electron and ion continuity and momentum equations. The dust charging model corrector step is

$$Z_j^{t+dt} = Z_j^{t} + dt \cdot \left(\frac{1}{q_{\mathrm{e}}} I_{\mathrm{e}j} \left(n_{\mathrm{e}}^{t+\frac{dt}{2}}, Z_j^{t+\frac{dt}{2}} \right) + \frac{1}{q_{\mathrm{i}}} I_{\mathrm{i}j} \left(n_{\mathrm{i}}^{t+\frac{dt}{2}}, Z_j^{t+\frac{dt}{2}} \right) \right). \tag{3.78}$$

Poisson's equation is

$$\phi_{\mathrm{k}}^{t+dt} = \frac{1}{\epsilon_0 k^2}\left(q_{\mathrm{e}} n_{\mathrm{ek}}^{t+dt} + q_{\mathrm{i}} n_{\mathrm{ik}}^{t+dt} + \rho_{\mathrm{d}}^{t+dt}\right). \tag{3.79}$$

3.6 Simulation initialization

3.6.1 Normalized dust charging equation

To normalize the dust charging equation (3.10) appropriately for the simulation, we note that two parameters, the charging rate ω_{chg} and the normalized equilibrium charge Z_{eq}, control the dust charging. Assuming $T_{\mathrm{e}} = T_{\mathrm{i}}$, from equations (3.11) and (3.12) the dust charging equation can be rewritten in a normalized form as

$$\frac{dZ}{dt} = \omega_{\mathrm{chg}}\left(\exp\left(\phi_{\mathrm{f0}}\frac{\mathrm{Z}}{\mathrm{Z_{eq}}}\right) - \frac{\mathrm{n_i}}{\mathrm{n_e}}\left(\frac{\mathrm{m_e}}{\mathrm{m_i}}\right)^{1/2}\left(1 - \phi_{\mathrm{f0}}\frac{\mathrm{Z}}{\mathrm{Z_{eq}}}\right)\right) \tag{3.80}$$

where $\omega_{\mathrm{chg}} = \pi a^2 \left(\frac{8}{\pi}\right)^{1/2} n_{\mathrm{e}} v_{\mathrm{te}}$, Z is the number charges on the dust grain, and ϕ_{f0} is the equilibrium floating potential. For an electron-ion plasma ($\frac{m_{\mathrm{i}}}{m_{\mathrm{e}}} = 1836$), note that $\phi_{\mathrm{f0}} =$ -2.51 when $n_{\mathrm{e}} = n_{\mathrm{i}}$. In the simulation the equilibrium floating potential ϕ_{f0} is calculated to satisfy the charge equilibrium which will be discussed in the next section. From the above we see that when $Z = Z_{\mathrm{eq}}$ then $dZ/dt = 0$ and the system stays at the equilibrium charge value. It is convenient to write ω_{chg} in terms of some natural frequency of interest. In our case, the waves and instabilities we want to study have a rate on the order of ω_{pi}, the ion plasma frequency. So we write

$$\omega_{\mathrm{chg}} = \alpha\omega_{\mathrm{pi}} \tag{3.81}$$

where α is the ratio of charging rate to ion plasma frequency. In the simulation code ω_{pi} is typically normalized to 1 so the charging rate is α. The normalized equation is easily extended for $T_{\mathrm{e}} \neq T_{\mathrm{i}}$ and a dispersion of dust masses.

3.6.2 Charge equilibrium and neutrality

For the charge equilibrium, the simulation must start with the same electron and ion currents on the dust grains as follows

$$I_{\mathrm{e}} + I_{\mathrm{i}} = 0. \tag{3.82}$$

From (3.9) and (3.10), equation (3.82) can be described by

$$v_{\mathrm{e}} n_{\mathrm{e}} e^{x} - v_{\mathrm{i}} n_{\mathrm{i}} (1 - x) = 0 \tag{3.83}$$

where $x = e\phi_{\mathrm{f}}/kT$. By assuming $T_{\mathrm{e}} = T_{\mathrm{i}}$ equation (3.83) can be rewritten as

$$\sqrt{\frac{m_{\mathrm{i}}}{m_{\mathrm{e}}}} \frac{n_{\mathrm{e}}}{n_{\mathrm{i}}} e^{x} - 1 + x = 0. \tag{3.84}$$

The solution to equation (3.84) at equilibrium charge determines ϕ_{f0}, i.e. $x = \phi_{\mathrm{f0}}$. Finally, equation (3.82) can be expressed in general as

$$\sqrt{\frac{m_{\mathrm{i}}}{m_{\mathrm{e}}}}\frac{n_{\mathrm{e}}}{n_{\mathrm{i}}}e^{\phi_{\mathrm{f0}}\frac{Z_{\mathrm{d}}}{Z_{\mathrm{eq}}}} - 1 + \phi_{\mathrm{f0}}\frac{Z_{\mathrm{d}}}{Z_{\mathrm{eq}}} = 0, \tag{3.85}$$

where Z_{d} is the dust charge. For the charge neutrality, we can describe the relation of densities for each species as follows

$$n_{\mathrm{e}}(x,y) - n_{\mathrm{i}}(x,y) + Z_{\mathrm{d}}(x,y)n_{\mathrm{d}}(x,y) = 0, \tag{3.86}$$

where $\rho_{\mathrm{d}}(x,y) = -eZ_{\mathrm{d}}(x,y)n_{\mathrm{d}}(x,y)$ is the dust charge density, $n_{\mathrm{d}}(x,y)$ is the dust number density, and $Z_{\mathrm{d}}(x,y)$ is the dust charge as stated before. Equation (3.86) can be rewritten as

$$n_{\mathrm{e}}(x,y) = n_{\mathrm{i}}(x,y) - Z_{\mathrm{d}}(x,y)n_{\mathrm{d}}(x,y). \tag{3.87}$$

Note that $n_{\mathrm{d}}(x,y)$ is known from the initial loading. Using equations (3.85) and (3.87), we get an equilibrium charge equation

$$\sqrt{\frac{m_{\mathrm{i}}}{m_{\mathrm{e}}}}\frac{n_{\mathrm{i}}(x,y) - Z_{\mathrm{d}}(x,y)n_{\mathrm{d}}(x,y)}{n_{\mathrm{i}}(x,y)}e^{\phi_{\mathrm{f0}}\frac{Z_{\mathrm{d}}}{z_{\mathrm{eq}}}} - \left(1 - \phi_{\mathrm{f0}}\frac{Z_{\mathrm{d}}(x,y)}{z_{\mathrm{eq}}}\right) = 0 \tag{3.88}$$

From equation (3.88) knowing $n_{\rm i}(x,y)$, $n_{\rm d}(x,y)$, and $Z_{\rm eq}$ the initial $Z_{\rm d}(x,y)$ can be determined for equilibrium.

3.6.3 Calculation of production rate $q_{\rm s}$

In general, ionization sources may be relevant depending on the model applications. For simplicity here, we consider the electron and ion production rates to be equal and to maintain constant equilibrium background electron and ion densities during dust charging. We define $q_{\rm s}$ as the electron and ion production rate which is given by

$$q_{\rm s} = \left.\frac{dn_{\rm i}}{dt}\right|_{\rm ionization} = \left.\frac{dn_{\rm e}}{dt}\right|_{\rm ionization} = \frac{1}{e}\frac{d\rho_{\rm e}}{dt} = \frac{1}{e}\frac{d\rho_{\rm de}}{dt} \cong n_{\rm d0}\frac{dZ_{\rm de}}{dt}, \tag{3.89}$$

where $d\rho_{\rm e}/dt$ is the change in electron charge density due to dust charging, $d\rho_{\rm de}/dt$ is the change in dust charge density due to dust charging with electrons, $n_{\rm d0}$ is the number of dust particles per cell, and $dZ_{\rm de}/dt = I_{\rm e0}$ is the normalized simulation electron current to the dust grain. Therefore, the electron and ion production rate is simplified to be

$$q_{\rm s} \cong n_{\rm d0} I_{\rm e0}. \tag{3.90}$$