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Numerical Vlasov-Maxwell Modelling of Space Plasma

BY

BENGT ELIASSON

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Abstract

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The Vlasov equation describes the evolution of the distribution function of particles in phase space $(\mathbf{x},\mathbf{v})$, where the particles interact with long-range forces, but where short-range "collisional" forces are neglected. A space plasma consists of low-mass electrically charged particles, and therefore the most important long-range forces acting in the plasma are the Lorentz forces created by electromagnetic fields.

What makes the numerical solution of the Vlasov equation a challenging task is that the fully three-dimensional problem leads to a partial differential equation in the six-dimensional phase space, plus time, making it hard even to store a discretised solution in a computer's memory. Solutions to the Vlasov equation have also a tendency of becoming oscillatory in velocity space, due to free streaming terms (ballistic particles), in which steep gradients are created and problems of calculating the v (velocity) derivative of the function accurately increase with time.

In the present thesis, the numerical treatment is limited to one- and two-dimensional systems, leading to solutions in two- and four-dimensional phase space, respectively, plus time. The numerical method developed is based on the technique of Fourier transforming the Vlasov equation in velocity space and then solving the resulting equation, in which the small-scale information in velocity space is removed through outgoing wave boundary conditions in the Fourier transformed velocity space. The Maxwell equations are rewritten in a form which conserves the divergences of the electric and magnetic fields, by means of the Lorentz potentials. The resulting equations are solved numerically by high order methods, reducing the need for numerical over-sampling of the problem.

The algorithm has been implemented in Fortran 90, and the code for solving the one-dimensional Vlasov equation has been parallelised by the method of domain decomposition, and has been implemented using the Message Passing Interface (MPI) method. The code has been used to investigate linear and non-linear interaction between electromagnetic fields, plasma waves, and particles.

Key words: Vlasov equation, Maxwell equation, Fourier method, outflow boundary, domain decomposition.

Bengt Eliasson, Department of Information Technology, Scientific Computing, Uppsala University, Box 337, SE-751 05 Uppsala, Sweden

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List of papers

The present thesis is based on the papers below, which are referred to by Roman numerals.

I B. Eliasson. Outflow boundary conditions for the Fourier transformed one-dimensional Vlasov-Poisson system. *J. Sci. Comput.*, 16(1):1–28, 2001.*

II B. Eliasson. Outflow boundary conditions for the Fourier transformed two-dimensional Vlasov equation. *J. Comput. Phys.*, 181:98–125, 2002.**

III J. Bergman and B. Eliasson. Linear wave dispersion laws in unmagnetised relativistic plasma: Analytical and numerical results. *Phys. Plasmas*, 8(5):1482–1492, 2001.***

IV B. Eliasson. Numerical Modelling of the Two-Dimensional Vlasov-Maxwell System. *IT Scientific Report 2002-028*, ISSN 1404-3203, Department of Information Technology, Uppsala University, November 2002. Downloadable from Web site http://www.it.uu.se/research/reports/

V B. Eliasson. Domain Decomposition of the Padé Scheme and Pseudo-Spectral Method, Used in Vlasov Simulations. *IT Scientific Report 2002-029*, ISSN 1404-3203, Department of Information Technology, Uppsala University, November 2002. Downloadable from Web site http://www.it.uu.se/research/reports/

In Paper III, the contribution from the present author is mainly the numerical treatment.

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Contents

CHAPTER 1

Introduction

Space plasma research is a relatively new discipline, going back in time some eighty years. Before the "space age" opened up with the advent of artificial satellites, space was assumed to be essentially a vacuum, whose content of matter was limited to the high energy particles that constitute the cosmic radiation. The discovery of the Earth's ionosphere came from early radio wave observations and the recognition that only a reflecting layer composed of electrons and ions could explain the characteristics of the observations [10].

The Earth's ionosphere [10] begins at an altitude below 100 km and extends to an altitude of about 1000 km. The gas of the ionosphere is composed mainly of neutral and ionised atoms and molecules formed by the elements oxygen and nitrogen. The ionisation comes about by the radiation from the Sun and by the impact of energetic particles. The degree of ionisation is of the order 10^{-2} to 10^{-4}, hence the ionosphere is a partially ionised *plasma* [14].

Generally, a planet's ionosphere is a plasma which envelops the planet, forming an interface between the planet's atmosphere (if it exists) and space. A plasma has some properties different from those of an ordinary neutral gas. Firstly, since the plasma is ionised, it cannot be fully described by the equations of neutral fluid dynamics. Secondly, collisions between particles are relatively rare in a dilute plasma, and therefore the system may be far from statistical equilibrium. Hence, it is necessary to use models which take the non-equilibrium distribution of particles in velocity space into account.

The studies of the Earth's ionosphere were made possible by the development of equipment for remote sensing, and by the space programme with the associated development of instruments for balloons, sounding rockets, and satellites, which made *in situ* measurements possible. Most of the early research was aimed at explaining the various layers in the ionosphere and their variability with local time, latitude, season, etc. As time passed by, the emphasis of ionospheric research shifted toward understanding the dynamics and plasma physics of ionospheric phenomena. Following this line toward basic research, researchers about twenty years ago began to use the ionosphere as a test bed for fundamental non-linear plasma physics experiments, where the plasma was perturbed by the injection of electromagnetic waves [19, 12]. By these controlled experiments, dynamic and often non-linear processes could be studied and compared with theoretical predictions, much the same as in a ground-based laboratory.

The development of computers and numerical methods has made it possible to test mathematical models of plasma physics, sometimes in a more controlled manner than in physical experiments which are often disturbed by unwanted interference from radio transmitters and other electrical equipment. Numerical simulations make it easier to measure and visualise physical quantities, without having to consider the design and operation of invasive sensing equipment as in a physical experiment. By performing the relatively inexpensive numerical experiments, one can test the mathematical models and predict more carefully which physical experiments should be undertaken.

The thesis is organised as follows: In Chapter 2, the one-dimensional Vlasov equation is introduced together with a discussion about the basic properties of the equation, and about the numerical difficulties which may arise, illustrated with numerical examples. Chapter 3 contains summaries of the Papers, and some conclusions and future perspectives are discussed in Chapter 4. In Paper I, well-posed boundary conditions for the one-dimensional Vlasov equation are developed, and in Paper II the theory is generalised to the two-dimensional Vlasov equation for magnetised plasma. Paper III is devoted to linear dispersion laws for waves in relativistic Vlasov plasma. In Paper IV, the full Vlasov-Maxwell system with mobile electrons and ions is discussed; electrostatic and electromagnetic waves in two dimensions are investigated numerically, and the results are compared with theory. Paper V is devoted to the numerical algorithms developed for solving the Vlasov equation on parallel computers, together with numerical tests of efficiency.

CHAPTER 2

Properties of the Vlasov equation

2.1 Introduction

In the present chapter, certain properties of the Vlasov equation, important for its numerical solution, are discussed. For simplicity, the discussion is mostly restricted to the one-dimensional Vlasov equation, but most of the properties are quite general and carry over to higher dimensions.

2.2 The incompressible flow of particles in phase space

A well-known property of the Vlasov equation is that an initially smooth solution to the equation may become increasingly oscillatory in phase space (x, v) due to *kinetic effects* as time increases, making the numerical solution of the Vlasov equation a challenging task. Kinetic effects are phenomena depending on the non-equilibrium, non-Maxwellian distribution in velocity space.

In order to explore the reason for this behaviour of the solution, we study the one-dimensional Vlasov-Poisson system

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \frac{eE}{m_e}\frac{\partial f}{\partial v} = 0 \tag{2.1}$$

$$\frac{\partial E}{\partial x} = \frac{e}{\varepsilon_0}\left[n_0 - \int_{-\infty}^{\infty} f(x,v,t)\,\mathrm{d}v\right] \tag{2.2}$$

describing the evolution of the distribution function for electrons having the mass m_e and electric charge $-e$ in a self-consistent electric field E. (The second equation is Maxwell's equation for the divergence of the electric field.) The Vlasov equation (2.1) is a hyperbolic equation, for which the initial conditions are transported unchanged along the characteristic curves (trajectories) in (x, v, t) space, given by

$$\dot{x}(t) = v(t) \tag{2.3}$$

$$\dot{v}(t) = -\frac{e}{m_\mathrm{e}} E(x(t), t) \tag{2.4}$$

where the dots in the left hand sides denote total time derivatives, $\mathrm{d}/\mathrm{d}t$. The partial differential equation (2.1) is thus described by the pair of ordinary differential equations (2.3–2.4), together with the equation

$$\dot{f}(x(t), v(t), t) = 0 \tag{2.5}$$

which says that f is constant along the characteristic curves. After some time, regions with initially large function values may be located next to regions with initially small function values, giving the large gradients.

The equations for the characteristic curves can be identified as the Newton equations of motion for a single electron with mass m_e and charge $-e$, moving in an electric field E. Due to the form of Eqs. (2.3–2.4), the phase space divergence of the velocity field $(\dot{x}, \dot{v})$ is zero,

$$\frac{\partial}{\partial x}(\dot{x}) + \frac{\partial}{\partial v}(\dot{v}) = \frac{\partial}{\partial x}(v) + \frac{\partial}{\partial v}\left(-\frac{eE(x,t)}{m_\mathrm{e}}\right) = 0 \tag{2.6}$$

hence the Vlasov equation describes an incompressible flow in phase space (x, v). Therefore large gradients are not created by *shocks*, as they are in other non-linear hyperbolic equations (e.g., the Burger's equation), but by *shearing* of the solution.

Most numerical schemes used for solving the Vlasov equation are based on the solution of the equations for the characteristic curves (2.3–2.5), instead of direct solutions of the Vlasov equation (2.1). In that manner the need to calculate the derivatives in (2.1) is avoided, and the problem can be turned into an interpolation problem [4], less sensitive to sharp gradients in (x, v) space.

2.3 The Vlasov equation and thermalisation

A non-linear problem which has been investigated numerically by many authors (see e.g. [1, 4, 3] and references therein) is the Vlasov equation (2.1) with the initial condition

$$f(x, v, 0) = [1 + A\cos(kx)]\, f_0(v) \tag{2.7}$$

with a *Maxwellian distribution* in velocity v space,

$$f_0(v) = \frac{n_0}{v_\mathrm{th,e}} (2\pi)^{-1/2} \exp(-v^2/2v_\mathrm{th,e}^2) \tag{2.8}$$

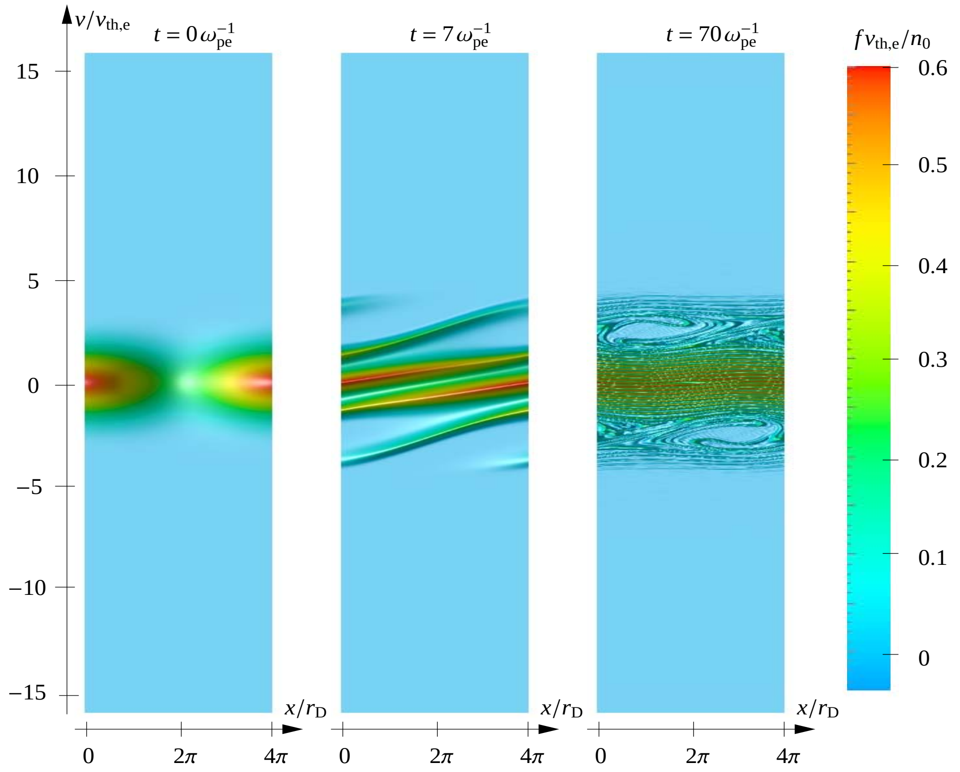

Figure 2.1: The distribution function $f(x,v,t)$ at different times t.

Here, we choose the initial amplitude and wave number to be $A = 0.5$ and $k = 0.5\,r_{\mathrm{D}}^{-1}$, respectively. The phase plot of the initial condition is displayed in the left-hand panel of Fig. 2.1, for $t = 0\,\omega_{\mathrm{pe}}^{-1}$. As can be seen in the middle panel of Fig. 2.1, the solution at $t = 7\,\omega_{\mathrm{pe}}^{-1}$ has formed filaments with large gradients in v space. At $t = 70\,\omega_{\mathrm{pe}}^{-1}$, these filaments have become much denser, and two vortex-like structures, known as Bernstein-Green-Kruskal (BGK) waves [16], have been created; see the right-hand panel of Fig. 2.1 and a closeup of the BGK waves in the left-hand panel of Fig. 2.3. The upper vortex, for positive speeds v, moves to the right and the lower vortex, for negative speeds v, moves to the left as time t increases. Clearly, the smooth initial condition is later converted into an oscillatory solution with steep gradients, first in v space and later also in x space due to the BGK modes. The increasingly oscillatory structure of the Vlasov equation is a problem when one wants to solve the equation numerically; especially the v derivative in Eq. (2.1) becomes difficult to perform numerically, often with a catastrophic increase of truncation errors if a difference scheme is used. The solution eventually

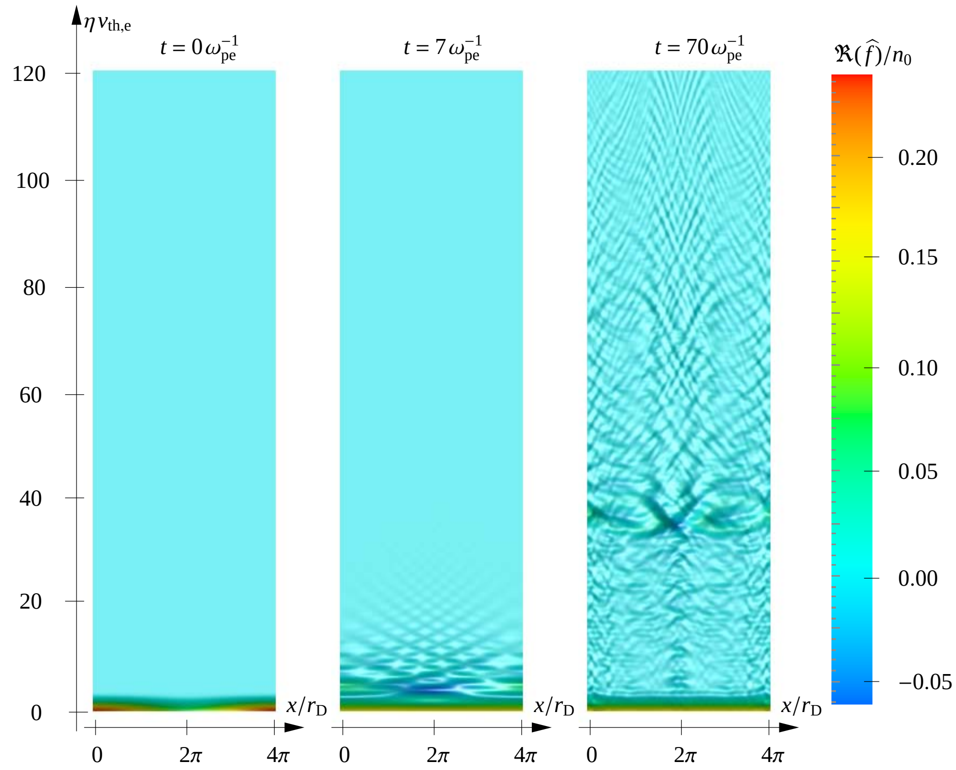

Figure 2.2: The real part of the Fourier transformed distribution function $\widehat{f}(x,\eta,t)$ at different times t.

becomes so oscillatory that it is impossible to represent on a fixed numerical grid due to the sampling (Nyqvist) theorem, which says that more than two sampling points per "wavelength" are needed to represent the solution.

The BGK modes are interesting in their own right and are worth a short discussion. One vortex is formed at the velocity between $v = 2\,v_{\mathrm{th,e}}$ and $v = 3\,v_{\mathrm{th,e}}$, and a second vortex at the same negative velocities; see Fig. 2.3. The physical explanation for the formation of the vortices is that particles (electrons) are trapped in the potential wells of the electrostatic waves. The trapping of particles can occur if the particles travel approximately the same velocity as phase velocity of the wave. For the given initial conditions, two propagating waves are created, one travelling to the right and one travelling to the left. Linear waves with the wave number $k = 0.5\,r_{\mathrm{D}}^{-1}$ have the real frequency $\omega_{\mathrm{R}} = 1.42\,\omega_{\mathrm{pe}}$, which gives the phase velocity of these waves as $v_{\mathrm{ph}} = \omega_{\mathrm{R}}/k = 2.84\,v_{\mathrm{th,e}}$ (calculated with the WHAMP [15] algorithm; see [7]). Particles with approximately this velocity are trapped, oscillating in the potential wells of the wave, and these oscillating groups of particles form the vortex-like structures in phase space. The BGK waves are very long-lived structures, and it is not clear if they are damped or undamped after a long time; two seemingly contradictory results (one theoretical and one numerical) are given by [9, 13].

It is well-known that a gas, where the velocity distribution is initially different from a Maxwellian, will thermalise to a Maxwellian as a result of collisions. The Vlasov equation is, however, a collision-less model which conserves entropy. This formally prevents a thermalisation of the Vlasov equation by diffusion, since that would increase the entropy of the solution. Even so, it seems that collective electromagnetic interactions can have the same effects as collisions [16], in which ordered motion is destroyed and a thermal velocity distribution is established, often with plateau-like structures in velocity space [3]. Again, since the Vlasov equation conserves entropy, it cannot thermalise *point-wise*, but only in *average* where the highest frequency components in (x,v) space are neglected.

This process is illustrated in Fig. 2.1. The distribution function at $t = 0\,\omega_{\rm pe}^{-1}$ in Fig. 2.1 is a Maxwellian. At $t = 7\,\omega_{\rm pe}^{-1}$, the distribution has become strongly non-Maxwellian, with the filaments in velocity space. At $t = 70\,\omega_{\rm pe}^{-1}$, however, the distribution has in a sense begun to thermalise, because the velocity distribution is becoming more and more unordered, except for the two BGK modes; this suggests that one could remove the information about the highest frequencies in velocity space without destroying the general behaviour of the solution. It is therefore natural to study the the Fourier transform in velocity space of the solution.

By employing the Fourier transform pair

$$f(x,v,t) = \int_{-\infty}^{\infty} \widehat{f}(x,\eta,t)\mathrm{e}^{-\mathrm{i}\eta v}\,\mathrm{d}\eta \tag{2.9}$$

$$\widehat{f}(x,\eta,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x,v,t)e^{\mathrm{i}\eta v}\,\mathrm{d}v \tag{2.10}$$

the system (2.1–2.2) is transformed into a new set of equations

$$\frac{\partial \widehat{f}}{\partial t} - \mathrm{i}\frac{\partial^2 \widehat{f}}{\partial x \partial \eta} + \mathrm{i}\frac{eE}{m}\eta \widehat{f} = 0 \tag{2.11}$$

$$\frac{\partial E(x,t)}{\partial x} = \frac{e}{\varepsilon_0}\left[n_0 - 2\pi \widehat{f}(x,\eta,t)_{\eta=0}\right] \tag{2.12}$$

for the Fourier transformed distribution function $\widehat{f}(x,\eta,t)$. The initial condition in the Fourier transformed variables is

$$\widehat{f}(x,\eta,0) = [1 + A\cos(k_x x)]\,\widehat{f_0}(\eta) \tag{2.13}$$

with $\widehat{f_0}(\eta) = n_0(2\pi)^{-1}\exp(-\eta^2 v_{\text{th,e}}^2/2)$. The real part of the Fourier transformed solution $\widehat{f}(x,\eta,t)$ is displayed in Fig. 2.2 for the same times as for the solution $f(x,v,t)$ in Fig. 2.1.

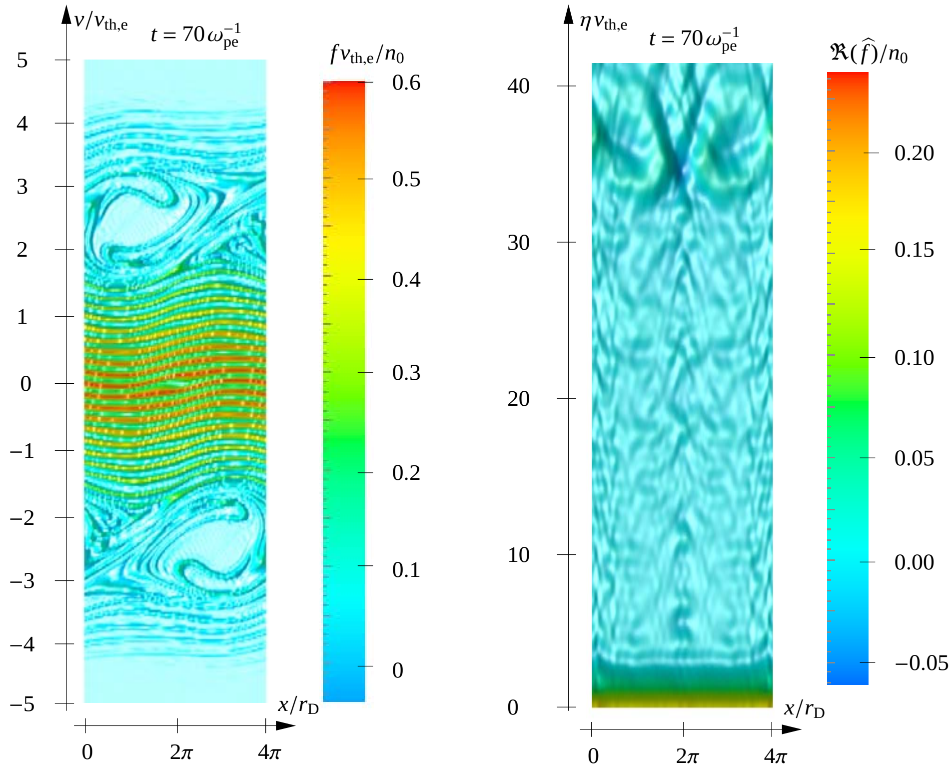

Figure 2.3: A closeup of the distribution function $f(x,v,t)$ and of the real part of the Fourier transformed distribution function $\widehat{f}(x,\eta,t)$ at the time $t = 70\,\omega_{\text{pe}}^{-1}$.

In the calculation of the electric field E, the integral over all velocity space in Eq. (2.2) is transformed into an evaluation in the Fourier transformed velocity space at $\eta = 0$, in Eq. (2.12). This is interesting because the highly oscillatory structures of the solution which can be seen for $t = 70$ in Fig. 2.1 are transformed into wave packets moving away from the origin in η space; see Fig. 2.2 and the closeups in Fig. 2.3. A wave packet can clearly be seen at $\eta \approx 35\,v_{\text{th,e}}^{-1}$ in the right-hand panel of Fig. 2.3; this value of η is the main “frequency” of the solution in velocity space, displayed in the left-hand panel of Fig. 2.3. This wave packet is decoupled from the origin $\eta = 0\,v_{\text{th,e}}^{-1}$, where the electric field is calculated, and could therefore be removed without immediately affecting the value of the electric field. As time increases, the solution in velocity space becomes more and more oscillatory, and waves in η space move further away from the origin $\eta = 0\,v_{\text{th,e}}^{-1}$, and in this example they eventually reach the artificial boundary at $\eta = \eta_{\max} = 120\,v_{\text{th,e}}^{-1}$; see Fig. 2.2. The idea, which is explored in the articles [5] and [7], is to solve the Vlasov equation in the Fourier transformed velocity space; wave packets which reach the artificial boundary in η space are allowed to travel over the boundary and to be removed from the solution, while incoming waves are set to zero at the boundary. By choosing a large enough distance from the origin for the artificial η boundary, small enough structures in velocity space are resolved.

The outflow of waves through the η boundary leads to a loss of information in which thermalisation of the Vlasov equation is allowed to occur. The η boundary must be placed at large enough η so that kinetic effects which are important for the physical problem, have the possibility to take place. Effects which explicitly depend on the velocity space filaments are, for example, different cases of recurrence of waves, like the Landau plasma echo effect [16] and the undamped linear waves transverse to a magnetic field [18, 6]. The non-linear Landau damping and the creation of BGK modes, discussed in the present Chapter, and the linear Landau damping [5] are also kinetic effects that could be damped out numerically if a too small domain in η space was used.

In the simulation performed to produce the results in the present section, we used the methods described in [5]. The simulation domain was set to $0 \le x/r_{\text{D}} \le 4\pi$ and $0 \le \eta v_{\text{th,e}} \le 120$ with $N_x = 200$, $N_\eta = 600$, and the time domain was $0 \le \omega_{\text{pe}} t \le 70$ with $N_t = 35000$ and $\Delta t = 0.002\,\omega_{\text{pe}}^{-1}$. The numerical dissipation was set to a small value, $\delta = 0.001\,r_{\text{D}}^{-2}\omega_{\text{pe}}^{-1}$.

2.3.1 The numerical approximation of particle velocities

By inspection of the three panels in Fig. 2.1, one can see that the solution has significantly non-zero values only in the velocity interval $v = -5\,v_{\text{th,e}}$ to $v = 5\,v_{\text{th,e}}$. The initially Maxwellian distribution function has at $t = 70\,\omega_{\text{pe}}^{-1}$ begun to thermalise to a solution which is essentially Maxwellian, except for the two BGK modes. This implies that the Vlasov equation in the Fourier transformed space has a smooth solution. If one assumes that the solution in Fig. 2.1 for all times vanishes as a Maxwellian for large v, with the estimate

$$|f(x,v,t)| < C\exp(-\gamma v^2) \tag{2.14}$$

for some positive constants C and γ, then the η derivatives of the Fourier transformed solution are bounded as

$$\begin{aligned}
&\left|\frac{\partial^n}{\partial\eta^n}\widehat{f}(x,\eta,t)\right| = [\text{Use Eq. (2.10)}] = \left|\frac{1}{2\pi}\int_{-\infty}^{\infty}(\mathrm{i}v)^n e^{\mathrm{i}\eta v} f(x,v,t)\,\mathrm{d}v\right| \\
&< [\text{Use the triangle inequality}] < \frac{1}{2\pi}\int_{-\infty}^{\infty}|(\mathrm{i}v)^n e^{\mathrm{i}\eta v} f(x,v,t)|\,\mathrm{d}v \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty}|v|^n|f(x,v,t)|\,\mathrm{d}v < [\text{By Eq. (2.14)}] \\
&< \frac{1}{2\pi}\int_{-\infty}^{\infty}|v|^n C\exp(-\gamma v^2)\,\mathrm{d}v = \frac{1}{2\pi}\frac{C}{\gamma^{(n+1)/2}}a_n
\end{aligned} \tag{2.15}$$

where the constant

$$a_n = \begin{cases} \sqrt{\pi}\,2^{-n/2}(n-1)!!, & n \text{ even} \\ [(\text{n-1})/2]!, & n \text{ odd} \end{cases} \tag{2.16}$$

and where symbols ! for the factorial and !! for the semi-factorial have their usual meaning. Thus, by the assumption (2.14) for $f(x,v,t)$ it follows that $\widehat{f}(x,\eta,t)$ is infinitely differentiable with respect to η with the estimate (2.15) for the derivatives. It is now possible to make an error estimate of the truncation error of a difference scheme used to approximate the η derivative in Eq. (2.11). The compact Padé scheme [11], which in the present thesis is used to perform numerical approximations of the first derivatives in $\boldsymbol{\eta}$ space (see [5] and [7]) has a truncation error of size

$$|\varepsilon| \leq \frac{1}{120}\Delta\eta^4 \max\left|\frac{\partial^5\widehat{f}}{\partial\eta^5}\right| \tag{2.17}$$

where the fifth derivative gives $n = 5$ in formula (2.15). This gives the estimate

$$|\varepsilon| < \frac{1}{2\pi}\frac{\Delta\eta^4}{60}\frac{C}{\gamma^3} \tag{2.18}$$

for the truncation error. It is thus possible to make an error estimate for the numerical differentiation in the Fourier transformed velocity η space in Eq. (2.11), which is not possible for a numerical differentiation in the original velocity v space in Eq. (2.1).

The next question is how well a numerical scheme resolves the particle velocities in the Vlasov equation. The advection of particles in x space is performed by the second term in the Vlasov equation (2.1). Particles are transported in x space with velocity v, according to Eq. (2.3).

The product by the velocity v in the Vlasov equation (2.1), is transformed into a differentiation with respect to η in the Fourier transformed Vlasov equation (2.11),

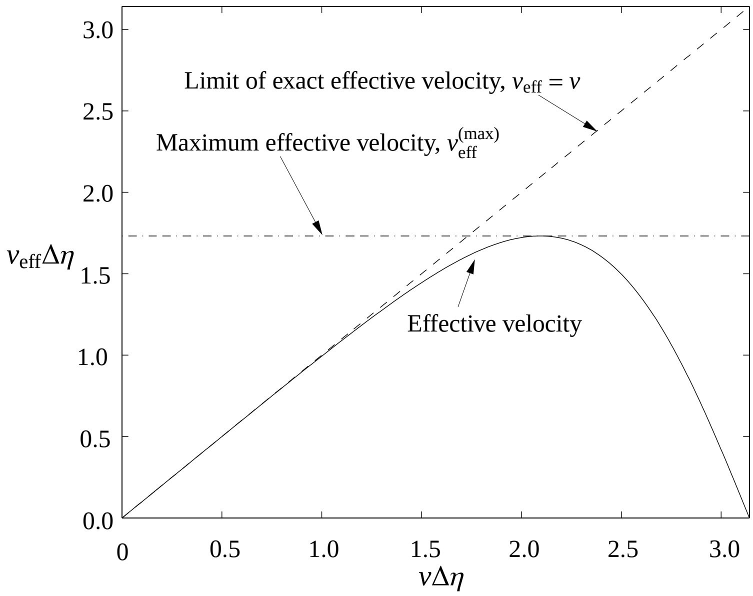

Figure 2.4: The effective particle velocities produced by the Padé difference scheme.

and in the numerical solution of the equation, the η derivative is approximated by a difference scheme. In order to investigate the impact of the difference scheme on effective particle velocities, we study an approximation of the Fourier transformed Vlasov equation, in which the x and t derivatives are performed exactly, while the η derivative is approximated by a difference scheme D_η, giving rise to the difference-differential equation

$$\frac{\partial \widehat{f}}{\partial t} - \mathrm{i}\frac{\partial}{\partial x}(D_\eta \widehat{f}) + \mathrm{i}\frac{eE}{m}\eta \widehat{f} = 0 \tag{2.19}$$

In order to study the effect of the difference approximation D_η on the solution in v space, the definition (2.10) is inserted into Eq. (2.19), giving

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\frac{\partial f}{\partial t}e^{\mathrm{i}\eta v} - \mathrm{i}\frac{\partial f}{\partial x}D_\eta(e^{\mathrm{i}\eta v}) + \frac{eE}{m}\mathrm{i}\eta f e^{\mathrm{i}\eta v}\right]\mathrm{d}v = 0 \tag{2.20}$$

where the difference operator gives $D_\eta(e^{\mathrm{i}\eta v}) = \mathrm{i}v_{\text{eff}}(v)e^{\mathrm{i}\eta v}$ with the eigenvalue $\mathrm{i}v_{\text{eff}}(v)$, and the term $\mathrm{i}\eta f e^{\mathrm{i}\eta v}$ gives $-e^{\mathrm{i}\eta v}\partial f/\partial v$ by an integration by parts, yielding

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\frac{\partial f}{\partial t} + v_{\text{eff}}(v)\frac{\partial f}{\partial x} - \frac{eE}{m_{\text{e}}}\frac{\partial f}{\partial v}\right]e^{\mathrm{i}\eta v}\,\mathrm{d}v = 0 \tag{2.21}$$

The requirement that Eq. (2.21) should be valid for all η gives that the integrand must be zero. The resulting equation is

$$\frac{\partial f}{\partial t} + v_{\text{eff}}(v)\frac{\partial f}{\partial x} - \frac{eE}{m_{\text{e}}}\frac{\partial f}{\partial v} = 0 \tag{2.22}$$

which is an approximation of the Vlasov equation (2.1), with the *effective velocity* $v_{\text{eff}}(v)$ produced by the numerical differentiation in η space. For the Padé scheme used [5, 7], one can show that

$$v_{\text{eff}}(v) = \frac{3}{\Delta\eta}\frac{\sin(v\Delta\eta)}{[2+\cos(v\Delta\eta)]} \tag{2.23}$$

where $\Delta\eta$ is the grid size in η space. In the limit $v\Delta\eta \to 0$, then $v_{\text{eff}} \to v$; see Fig. 2.4 where $v_{\text{eff}}\Delta\eta$ has been plotted as a function of $v\Delta\eta$. The equations for the characteristic curves in (x, v) space, produced by Eq. (2.22), are

$$\dot{x}(t) = v_{\text{eff}}(v(t)) = \frac{3}{\Delta\eta}\frac{\sin(v(t)\Delta\eta)}{[2+\cos(v(t)\Delta\eta)]} \tag{2.24}$$

$$\dot{v}(t) = -\frac{e}{m_{\text{e}}}E(x(t), t) \tag{2.25}$$

Thus the particles are transported in x space with the effective velocity v_{eff}, which is periodic with respect to v. One can note that the velocity field produced by the numerical approximation is still incompressible, i.e., the phase space divergence for the velocity field (2.24–2.25) vanishes in a similar manner as in Eq. (2.6); thus, the approximation of the η derivative does not contribute directly to the increasing or decreasing of phase volumes. If the product $v\Delta\eta$ is too large, then the approximation $v_{\text{eff}} \approx v$ breaks down; see Fig. 2.4. A maximum effective velocity, $v_{\text{eff}}^{(\text{max})}\Delta\eta = \sqrt{3} \approx 1.73$, can be found for $v\Delta\eta = 2\pi/3 \approx 2.09$. It means that even though the largest *represented* velocity is given by the Nyqvist limit $v_{\text{max}} = \pi/\Delta\eta \approx 3.14/\Delta\eta$, the highest effective velocity for transport of particles in x space is $v_{\text{eff}}^{(\text{max})} = \sqrt{3}/\Delta\eta$. In numerical experiments, one has to choose a small enough $\Delta\eta$, so that important phenomena in velocity space, for example beams of particles, are well resolved, i.e., the velocities of these particles must fulfil $v < v_{\text{eff}}^{(\text{max})}$ with some margin.

In the simulation performed to produce the results in the present section, particles were accelerated to velocities somewhat less than $v = 5v_{\text{th,e}}$; see the left-hand panel of Fig. 2.3. The grid size was $\Delta\eta = (120/600)v_{\text{th,e}}^{-1} = 0.2v_{\text{th,e}}^{-1}$, which gives that $v\Delta\eta \approx 1.0$ for these particles. According to the diagram in Fig. 2.4, the effective velocity is close to the limit of exact velocity for the value $v\Delta\eta = 1.0$, and thus the particle velocities for the fastest particles are well resolved. The maximum effective velocity produced in the simulation was $v_{\text{eff}}^{(\text{max})} = \sqrt{3}/\Delta\eta \approx 8.6v_{\text{th,e}}$.

The dispersive properties of the Padé scheme and many other high-order schemes have been analysed by Lele [11], who has produced diagrams similar to Fig. 2.4 for these schemes. If these schemes are to be used for the solution of the present problem, the effective velocities of particles produced by the schemes can be read off in these diagrams. The nice dispersive properties of these schemes make them interesting for the solution of the present problem, since the dispersions of the schemes have their direct interpretations in the approximations of particle velocities, similarly as in Eq. (2.24) for the Padé scheme.

2.4 The outflow boundary condition and its relation to the Hilbert transform

The outflow boundary condition [5, 7] at the artificial boundary $\eta = \eta_{\text{max}}$ can be formulated with the help of projection operators in the form

$$\widehat{f} = \mathrm{F}^{-1} H(k_x) \mathrm{F} \widehat{f}, \qquad \eta = \eta_{\text{max}} \tag{2.26}$$

where the spatial Fourier transform and inverse spatial Fourier transform is defined as

$$\mathrm{F}\phi = \int_{-\infty}^{\infty} \phi(x) e^{-\mathrm{i}k_x x} \mathrm{d}x \tag{2.27}$$

and

$$\mathrm{F}^{-1}\widetilde{\phi} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \widetilde{\phi}(k_x) e^{\mathrm{i}k_x x} \mathrm{d}k_x \tag{2.28}$$

respectively, and where the Heaviside function is defined as

$$H(k_x) = \begin{cases} 1, & k_x > 0 \\ 0, & k_x \leq 0 \end{cases} \tag{2.29}$$

In [7] the boundary condition is instead formulated in terms of Fourier series/integral pairs, with the same result, and the argument of H contains an extra term, which does not change the discussion here. The projection operator $\mathcal{G} \equiv \mathrm{F}^{-1} H(k_x) \mathrm{F}$, acting on $\widehat{f}$ as

$$\mathcal{G}[f](x) = \mathrm{F}^{-1} H(k_x) \mathrm{F} f \tag{2.30}$$

projects the function $\widehat{f}$ onto the space of functions with only positive Fourier components in x space. In other words, the projection removes components with negative wave vectors at the boundary and leaves components with positive wave vectors unchanged. The analysis in [5] and [7] shows that the flow of data at the boundary is separated in exactly this way; wave packets having positive wave vectors in x space will travel in the direction of higher η and should be allowed to travel over the boundary at $\eta = \eta_{\max}$, and waves with negative wave vectors in x space will travel into the domain and should therefore be set to zero at the boundary.

The *Hilbert transform*

$$\mathcal{H}[f](x) = \frac{1}{\pi}\mathsf{p}\int_{-\infty}^{\infty} \frac{f(y)}{x-y}\mathrm{d}y \tag{2.31}$$

where p denotes the *Cauchy principal value*, has the property that

$$\mathcal{H}[e^{ikx}](x) = \mathrm{sign}(k)\mathrm{i}e^{ikx} \tag{2.32}$$

and it follows that the boundary operator $\mathcal{G}$ can be expressed in terms of the Hilbert transform as

$$\mathcal{G}[f](x) = \frac{1}{2}\left[f(x) - \mathrm{i}\mathcal{H}[f](x)\right] = \frac{1}{2}\left[f(x) - \mathrm{i}\frac{1}{\pi}\mathsf{p}\int_{-\infty}^{\infty}\frac{f(y)}{x-y}\mathrm{d}y\right] \tag{2.33}$$

i.e., as an operator in real x space. In the Fourier transform formulation of the boundary operator $\mathcal{G}$, the domain in x is assumed to be infinite or periodic, which is problematic if the domain in the physical problem is bounded and non-periodic. The integral formulation (2.33) of the boundary operator may open up the possibility to construct well-posed boundary conditions also for non-periodic problems, if the integral in the Hilbert transform is restricted to bounded limits; this idea needs more research though, and is not explored further here.

2.5 The reduction of dimensions

In the present section, we discuss shortly the possibilities to simplify the Vlasov equation by the reduction of the number of velocity dimensions for different cases. Most of this is well-known theory [8], and is repeated here only for clarity.

In the study of problems with certain symmetries, it is sometimes possible to make a choice of the coordinate system so that the the problem can be analysed in a smaller number of dimensions. Numerically (and analytically), this is very convenient because unnecessary information is removed from the problem and a smaller number of sampling points is needed to represent the solution on a numerical grid.

One such assumption is that the problem is *homogeneous* in one or more dimensions, in which derivatives in these dimensions vanish. In the study of plane waves in plasma, the number of dimensions in $\mathbf{x} = (x_1, x_2, x_3)$ space can be reduced to one dimension, $\mathbf{x} = (x_1, 0, 0)$, so that only derivatives with respect to x_1 (and not x_2 and x_3) remain. In this manner, the Vlasov equation can be reduced from three spatial and velocity dimensions, to one spatial and three velocity dimensions, plus time.

For the non-relativistic Vlasov equation, studied numerically in the present thesis, it turns out that it is also possible to reduce the number of velocity dimensions, but in a different manner than for the spatial dimensions. For electrostatic electron waves in an unmagnetised plasma, the reduction to one spatial dimension x_1 also leads to that terms containing factors of v_2 and v_3, and derivatives with respect to v_2 and v_3, also vanish, giving rise to the system

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} - \frac{eE_1}{m_e} \frac{\partial f}{\partial v_1} = 0 \tag{2.34}$$

$$\frac{\partial E_1}{\partial x_1} = \frac{e}{\varepsilon_0} \left[n_0 - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x_1, v_1, v_2, v_3, t)\, \mathrm{d}v_1\, \mathrm{d}v_2\, \mathrm{d}v_3 \right] \tag{2.35}$$

The dependence on (v_2, v_3) only appears in the integral over all velocity space for calculating the electric field E_1. Similarly, for waves in a magnetised plasma, propagating in the (x_1, x_2) plane perpendicular to the magnetic field directed in the x_3 direction and with the electric field directed in the (x_1, x_2) plane perpendicular to the magnetic field, any dependences on the distribution in v_3 vanish in the Vlasov equation, and one has one Vlasov equation in (x_1, x_2, v_1, v_2, t) space for each value on v_3. In these cases, it is possible (and convenient) to reduce the number of dimensions also in $\mathbf{v}$ space.

In the study of collective phenomena in plasma, the electromagnetic fields do not depend explicitly on the exact velocity distribution of particles but on the charge and velocity densities in $\mathbf{x}$ space, calculated as integrals (moments) of the distribution function. This makes it possible to reduce the number of velocity dimensions in the Vlasov equation. For the case of electrostatic waves in an unmagnetised plasma discussed above, it is simple to show that linear combinations of distribution functions with different (v_2, v_3) are solutions to the one-dimensional Vlasov equation (2.34), because these distribution functions separately are solutions to the same Vlasov equation. In particular, taking the limit of a continuous "linear combination," the one-dimensional distribution function

$$f^{1\mathrm{D}}(x_1, v_1, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x_1, v_1, v_2, v_3, t)\, \mathrm{d}v_2\, \mathrm{d}v_3 \tag{2.36}$$

is a solution to the one-dimensional Vlasov equation (2.34) because the function $f(x_1, v_1, v_2, v_3, t)$ is a solution to the the Vlasov equation (2.34) for each value on (v_2, v_3). The electric field is calculated from Eq. (2.35) where, by Eq (2.36),

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f\, \mathrm{d}v_1\, \mathrm{d}v_2\, \mathrm{d}v_3 = \int_{-\infty}^{\infty} f^{1\mathrm{D}}\, \mathrm{d}v_1 \tag{2.37}$$

and the resulting one-dimensional Vlasov-Poisson system is

$$\frac{\partial f^{1D}}{\partial t} + v_1 \frac{\partial f^{1D}}{\partial x_1} - \frac{eE_1}{m_e} \frac{\partial f^{1D}}{\partial v_1} = 0 \tag{2.38}$$

$$\frac{\partial E_1}{\partial x_1} = \frac{e}{\varepsilon_0} \left[n_0 - \int_{-\infty}^{\infty} f^{1D}(x_1, v_1, t)\, \mathrm{d}v_1 \right] \tag{2.39}$$

for the unknown function f^{1D}.

For waves propagating perpendicularly to a magnetic field, mentioned above, it is possible to derive the two-dimensional Vlasov-Maxwell system, which depends on the distribution functions in the form

$$f^{2D}(x_1, x_2, v_1, v_2, t) = \int_{-\infty}^{\infty} f(x_1, x_2, v_1, v_2, v_3, t)\, \mathrm{d}v_3 \tag{2.40}$$

For waves propagating with some angle to the magnetic field, it is not possible (or much harder) to reduce the number of velocity dimensions in the manner described above, since all three velocity components will appear explicitly in the resulting Vlasov equation, making the superposition technique impossible.

The one- and two-dimensional Vlasov equation is studied numerically in the present thesis [5, 7].

2.5.1 Relativistic effects

For physical situations with high velocity beams of particles or with hot plasma, and very near cyclotron harmonic frequencies [17], it may be necessary to take relativistic effects into account. This increases the difficulties, since the reduction of velocity dimensions cannot be performed as easily as for the non-relativistic case above. This is due to the fact that particles with high velocities appear to be "heavier" and therefore the velocity dimensions couple to each other.

The distribution function for electrons, $\widehat{f}_e(\mathbf{x}, \mathbf{p}, t)$, moving with inertia

$$\mathbf{p} = \gamma m_e \mathbf{v} \tag{2.41}$$

with rest mass m_e and the relativistic γ factor

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}} = \sqrt{1 + p^2/(m_e^2 c^2)} \tag{2.42}$$

is governed by the relativistic Vlasov equation

$$\frac{\partial \widehat{f}_e}{\partial t} + \left(\frac{\mathbf{p}}{\gamma m_e} \cdot \nabla \right) \widehat{f}_e - e \left(\mathbf{E} + \frac{\mathbf{p}}{\gamma m_e} \times \mathbf{B} \right) \cdot \boldsymbol{\nabla}_{\mathbf{p}} \widehat{f}_e = 0 \tag{2.43}$$

where $\nabla_{\mathbf{p}}$ denotes the gradient with respect to **p**. (It is more common, and convenient, to use the independent variable **p** than **v** in the relativistic Vlasov equation.)

The γ factor contains all three components of **p** (or **v**) which means that the relativistic equation will contain expressions of all components of the known variable **p**, even in the case of electrostatic waves in an unmagnetised plasma, which was discussed for the non-relativistic case above. Therefore solutions with different values on (p_2, p_3), giving rise to different values on γ, will obey *different* one-dimensional Vlasov equations, and the superposition technique which worked for the non-relativistic Vlasov equation above, will not work in the relativistic case. The reduction of the number of velocity dimensions is therefore more difficult in the relativistic case than in the non-relativistic case.

The dispersive properties of linear waves in an un-magnetised, relativistic plasma was studied by Bergman and Eliasson [2]; it illustrates the increase of difficulties in the relativistic case, due to the coupling of velocity dimensions via the γ factor.

In the Fourier transform technique in velocity space, studied in the present thesis, the γ factor will give rise to a convolution by a function, which is a problem to be solved if the Fourier transform technique is to be generalised to relativistic cases.

CHAPTER 3

Summaries of the Papers

Paper I

Outflow Boundary Conditions for the Fourier Transformed One-Dimensional Vlasov-Poisson system

B. Eliasson. *J. Sci. Comput.*, 16(1):1–28, 2001.

This paper is devoted to well-posed outflow boundary conditions in the Fourier transformed velocity space, for the one-dimensional Vlasov equation. Numerical simulations are performed to assess stability of the numerical scheme, that the code produces known linear and non-linear results, and that the numerical recurrence phenomenon is reduced.

Paper II

Outflow Boundary Conditions for the Fourier Transformed Two-Dimensional Vlasov Equation

B. Eliasson. *J. Comput. Phys.*, 181:98–125, 2002.

The Fourier transform technique in velocity space is generalised to the two-dimensional Vlasov equation. The Vlasov equation is rewritten in a form so that well-posed boundary conditions, similar to those for the one-dimensional Vlasov equation, can be derived. Numerical simulations are performed to assess stability, and that the numerical recurrence phenomenon is reduced. Linear dispersion laws for magnetised and unmagnetised plasma are compared with the numerical results.

Paper III

Linear wave dispersion laws in unmagnetized relativistic plasma: Analytical and numerical results

J. Bergman and B. Eliasson. *Phys. Plasmas*, 8(5):1482–1492, 2001.

This article is devoted to the linear dispersion laws for relativistic plasma. The treatment is more complicated than in the non-relativistic case, since the velocity dimensions cannot be separated. Simple approximative dispersion laws are derived for electrostatic and electromagnetic waves, and these laws are compared with numerical evaluations of the full dispersion laws.

Paper IV

Numerical Modelling of the Two-Dimensional Vlasov-Maxwell System

B. Eliasson. *IT Scientific Report 2002-028*, ISSN 1404-3203, Department of Information Technology, Uppsala University, November 2002. Downloadable from Web site http://www.it.uu.se/research/reports/

The two-dimensional Vlasov equations for electrons and ions are solved together with the fully electromagnetic Maxwell equations. Special attention is devoted to the divergence problem of the Maxwell equations. The Maxwell equations are rewritten by means of the Lorentz potentials in a form which conserves the divergences of the electric and magnetic fields up to the local truncation error of the scheme, regardless of the numerical scheme used.

Paper V

Domain Decomposition of the Padé Scheme and Pseudo-Spectral Method, Used in Vlasov Simulations

B. Eliasson. *IT Scientific Report 2002-029*, ISSN 1404-3203, Department of Information Technology, Uppsala University, November 2002. Downloadable from Web site http://www.it.uu.se/research/reports/

This report contains an analysis of the parallel algorithms used to integrate the one-dimensional Vlasov equation in time. The parallel algorithm is based on domain decomposition of the two-dimensional problem, where derivatives in one dimension are performed by pseudo-spectral methods and in the other dimension by the compact Padé scheme which gives rise to linear tri-diagonal equation systems. In the parallelisation of the pseudo-spectral method, it is not possible to avoid a large amount of communication due to the FFTs used, and therefore this method gives speedup only on the shared memory machines tested, and not on clusters of computers. The parallelisation of the Padé scheme can be performed efficiently by the solution of the tri-diagonal linear systems of equations by the method of domain decomposition; the resulting Schur complement systems are symmetric, tri-diagonal and strongly diagonally dominant and can therefore be solved by a few Jacobi iterations. This method gave a large (often super-linear) speedup on both shared memory computers and clusters of computers. A students project using the Globus Toolkit for parallelisation over the Internet is also discussed.

CHAPTER 4

Conclusions and future perspectives

The subject of the present thesis has been to investigate methods to efficiently solve the Vlasov-Maxwell system numerically, and to study linear and nonlinear physical problems with the code with the main objective to interpret ionospheric interaction experiments. The method has been, firstly to rewrite the equations in a form suitable for numerical integration:

- The Vlasov equation is Fourier transformed in velocity $\mathbf{v}$ space, giving a new equation with smoother solutions in the Fourier transformed velocity $\boldsymbol{\eta}$ space. The Fourier transform technique is an old technique, but previous algorithms have run into problems because of reflectrions of "waves" against the artificial boundary at the highest component of the Fourier transformed velocity domain. This problem is here solved by the introduction of absorbing outflow boundaries. These allow outgoing waves to propagate over the boundary and to be removed from the calculation, while incoming waves are set to zero. In physical terms, the Vlasov equation is allowed to partially thermalise, because the information about the highest frequency components in velocity space is lost.

- The Maxwell equation is rewritten in a form which conserves the divergences of the electric and magnetic fields, with the help of the Lorentz potentials. This form makes it possible to use any consistent and stable numerical scheme to integrate the equations.

Secondly, because the Fourier transformed Vlasov equation has a smoother solution in the Fourier transformed velocity $\boldsymbol{\eta}$ space, a high-order standard method (the Padé scheme) can be employed to perform approximations of derivatives in $\boldsymbol{\eta}$ space. The Padé scheme has nice dispersive properties and is therefore comparable with spectral methods. This is important because the dispersion of the Padé scheme has a direct physical interpretation in the approximation of velocities of particles in the present problem. The numerical methods used are:

- Derivatives in the Fourier transformed velocity space $\boldsymbol{\eta}$ are calculated with the fourth order compact Padé difference scheme.

- Derivatives and other operators in $\mathbf{x}$ space are calculated with pseudo-spectral methods.

- The time integration is performed with the fourth order Runge-Kutta method.

Lastly, the algorithm for solving the one-dimensional Vlasov equation is parallelised in order to test performance with different methods of parallelisation. Derivatives in the Fourier transformed velocity space are approximated by the compact Padé scheme, giving rise to tri-diagonal equation systems, and derivatives in x space are approximated by a pseudo-spectral mathod by the use of FFTs. The parallel algorithm for the compact Padé scheme was compared with the parallel algorithm for the pseudo-spectral method:

- The parallelisation in the Fourier transformed velocity η space could be made efficiently, with good speedup on both shared memory machines and clusters of computers. In η space, derivatives are calcuated by the compact Padé scheme, which gives rise to a large number of tri-diagonal linear equation systems. These tri-diagonal systems are parallelised by the method of domain decomposition, giving rise to tri-diagonal and strongly diagonally dominant Schur complement systems which can be solved efficiently in parallel by a few Jacobi iterations. The only communication needed is a few vectors communicated between the nearest neighbours of processors. Therefore the efficiency of the parallel algorithm for the semi-implicit Padé scheme is comparable to the efficiencies of parallel algorithms for explicit difference schemes.

- The parallelisation in x space gives speedup on some shared memory computers but not on clusters of computers. The problem is that FFTs are performed in the pseudo-spectral method used. The FFTs are global operators which act on the whole domain in x space, leading to a heavy load on the communication where all processors in the x direction have to communicate a large amount of data to all other processors in its processor row. On the other hand, tests where the pseudo-spectral method is replaced with a high-order difference scheme show excellent speedup on all types of computer systems tested. The difference scheme is bounded in x space, and therefore the processors only have to communicate a few vectors to its neighbouring processors, making the parallelisation efficient. However, more research is needed to generalise this idea to higher dimensions.

The conclusion is that parallelisation in higher dimensions should be performed in the Fourier transformed velocity space, because the compact Padé scheme can be parallelised very efficiently, compared to the efficiency of parallelising the pseudo-spectral method in x space.

In order to assess that the numerical code produces known results, numerical benchmarks have been performed on linear and non-linear physical problems, and the results have been compared with theory and with previously published results by other authors. The computer code has been generalised to simulate a two-dimensional Vlasov plasma with mobile electrons and ions, and with a fully electromagnetic treatment of the fields. The code can therefore be used to simulate realistic linear and nonlinear problems in two dimensions.

For the future, the generalisation of the Vlasov-Maxwell simulations to the full three velocity and spatial dimensions is a natural extension. With today's computers, it is possible to solve only small "model" problems in the full dimensions. However, the rate of development of faster computers does not show any sign of decreasing, so it is not a waste of time to develop the numerical tools for the future generations of computers. The development of the Internet with high bandwidth communication opens up for the sharing of computing resources over the Internet, with the possibility to run problems on a mixture of cheaper clusters of computers and faster parallel computers.

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