FLOW COMPUTATIONS WITH ACCURATE SPACE DERIVATIVE METHODS

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Abstract

This paper is concerned with the numerical solution of partial differential equations describing fluid flow problems in real space and in phase space. One important goal is to show conclusively that the Accurate Space Derivative methods can be used with success for solving such problems numerically. We describe a method for the numerical solution of the Korteweg-de Vries-Burgers equation. We show numerically that the solution of this equation evolves asymptotically into a steady shock wave with monotonic and oscillatory profile. We present numerical solutions of the Vlasov-Poisson system of equations which describes the motion of an ideal incompressible fluid in phase space. These problems are related to longitudinal oscillations in two- and three-dimensional phase space.

I. INTRODUCTION

Partial differential equations describing fluid flow problems have been solved successfully by: (1) transform methods, in which the variables are expressed in terms of orthogonal polynomials; and (2) finite difference methods. The former approach proved to be very accurate in Fluid Mechanics [23] and in Plasma Physics [1] for problems with simple boundaries. Although finite difference methods are well suited to solving realistic problems with complex boundaries, [5, 10, 26] they seldom achieve more than a rather modest accuracy in practice [26, p. 24]. The significantly larger error terms in finite difference methods are due to the approximation of the space derivatives by some finite difference expressions. Space differencing errors can be reduced substantially by the accurate computation of the space derivative terms. A numerical method based on this principle can be expected to possess similar accuracy as the corresponding transform method if similar time differencing methods are employed. Indeed, it was found by Orszag[25] that the pseudospectral (collocation) approximation[24] and the spectral (Galerkin) approximation[23] give similar errors. In the pseudospectral approximation the space derivatives are computed by Fourier methods[24] and "leapfrog" (or midpoint rule) time differencing is used to march forward in time.

Recently the author reported on higher order (in time) numerical schemes[12,13] based on the Accurate Space Derivative (ASD) method. In this approach to time differencing we start from a Taylor series in t, following in principle Lax and Wendroff [26, p. 302]. The time derivatives are then substituted by expressions containing only space derivative terms. The numerical evaluation of the space derivative terms is based on the use of finite Fourier series. In this respect our method is similar to the pseudospectral approximation.[24,25]

The role of the finite Fourier transform techniques in the ASD methods is limited to the efficient computation of the space derivative terms. In the case of nonrectangular coordinate systems other types of orthogonal polynomials may prove to be more convenient than finite Fourier series. Nevertheless, the application of the ASD methods over such a computational grid appears to be entirely feasible, so long as the space derivatives are evaluated at the grid points by making use of all the information that can be supported by the computational grid. It is, therefore, incorrect to regard the ASD method as a spectral method. The fast Fourier transform algorithm is merely a tool, i.e., a "black box," for the procedure of differentiation.

The ASD methods have been applied successfully to one-dimensional problems.[12-15] In this paper we study numerical solutions to nonlinear differential equations with one, two, and three space variables. In Section II we discuss a numerical method for the Korteweg-de Vries-Burgers (KdVB)[18] equation. This type of equation occurs in some classes of nonlinear dispersive systems with dissipation. We show numerically that the solution of the KdVB equation evolves asymptotically into a steady shock wave with monotonic or oscillatory profile. Sections III and IV are devoted to the numerical simulation of the Vlasov-Poisson system of equations, which describes the behavior of collisionless fully ionized plasmas. The electron velocity distribution function is commonly referred to as "phase space" fluid, since the Vlasov equation describes the flow of an ideal incompressible fluid in phase space.[3,22] In Section III, we present results on linear and nonlinear Landau damping of electrostatic oscillations in unmagnetized plasma. In Section IV we consider electrostatic waves in a magneto-plasma. These simulations require one space variable, x, and two velocity variables v_x and v_y. Here we show results related to perpendicularly propagating cyclotron harmonic waves.

II. NUMERICAL SOLUTION OF THE KORTEWEG-DE VRIES-BURGERS EQUATION

In this section we consider the Korteweg-de Vries-Burgers equation[18]

$$\frac{\partial u}{\partial t} + 2u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} + \mu\frac{\partial^3 u}{\partial x^3} = 0, \tag{1}$$

where ν is the coefficient of diffusivity and μ is the dispersive parameter. This type of equation occurs in some classes of nonlinear dispersive systems with dissipation. The steady state version of Eq. (1) has been used by Grad and Hu[17] to describe a weak shock profile in plasmas. Propagation of waves on an elastic tube filled with viscous fluid is also described by the KdVB equation in a particular limit.[18] In more recent studies[19] it has been found that the surface profile above a fully developed Poiseuille channel flow is also described approximately by the KdVB equation.

Our problem is defined by fixing the upstream and downstream boundary conditions that must be satisfied by Eq. (1) at all time, $t \geqq 0$. These are

$$\lim_{x\to-\infty} u(x,t) = u_\infty^-, \quad \lim_{x\to+\infty} u(x,t) = u_\infty^+, \quad u_\infty^- > u_\infty^+. \tag{2}$$

For simplicity, we choose $u_\infty^- = 1$, and $u_\infty^+ = 0$.

The steady-state solutions of the KdVB equation have been studied in some detail by Johnson.[19,20] For nonzero dissipation, $\nu \neq 0$, the steady-state solution is of the following two types: (a) a monotonic shock wave if $\nu^2 \geqq 4\mu$; or (b) a shock wave oscillatory upstream and monotonic downstream when $\nu^2 < 4\mu$. One of the goals of this study is to show numerically that for any initial data satisfying (2), e.g.,

$$u(x,0) = \begin{cases} 1, & x < x_0 \\ 0, & x > x_0 \end{cases} \tag{3}$$

the solution of Eq. (1) evolves asymptotically into the steady shock wave with the predicted monotonic or oscillatory profile.

The initial value problem stated in Eqs. (1) and (3) is solved by the Accurate Space Derivative (ASD) method[12] of order three. By this method, $u(x,t+\Delta t)$ is computed from $u(x,t)$ by means of the following expression

$$u(t+\Delta t) = u(t) + \frac{\partial u(t)}{\partial t}\Delta t + \frac{\partial^2 u(t)}{\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^3 u(t)}{\partial t^3}\frac{\Delta t^3}{3!} \tag{4}$$

The time derivatives in Eq. (4) are computed from Eq. (1) by successive differentiation as follows;

$$\frac{\partial u}{\partial t} = -2u\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2} - \mu\frac{\partial^3 u}{\partial x^3} \tag{5}$$

$$\frac{\partial^2 u}{\partial t^2} = -2\frac{\partial u}{\partial t}\frac{\partial u}{\partial x} - 2u\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial t}\right) + \nu\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial t}\right) - \mu\frac{\partial^3}{\partial x^3}\left(\frac{\partial u}{\partial t}\right) \tag{6}$$

$$\frac{\partial^3 u}{\partial t^3} = -2\frac{\partial^2 u}{\partial t^2}\frac{\partial u}{\partial x} - 4\frac{\partial u}{\partial t}\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial t}\right) - 2u\frac{\partial}{\partial x}\left(\frac{\partial^2 u}{\partial t^2}\right) + \nu\frac{\partial^2}{\partial x^2}\left(\frac{\partial^2 u}{\partial t^2}\right) - \mu\frac{\partial^3}{\partial x^3}\left(\frac{\partial^2 u}{\partial t^2}\right) \tag{7}$$

The x derivative terms in Eqs. (5-7) are computed by Fourier methods. Let U(k,t) be the finite Fourier transform of u(x,t) defined over the computational domain D. The ℓ^{th} order derivative of u(x,t) is given by

$$\frac{\partial^\ell u}{\partial x^\ell} = \sum_k (ik)^\ell \, U(k,t) \, \exp(ikx) \tag{8}$$

where $i = (-1)^{1/2}$ and the summation in (8) is carried out for all wave numbers k which can be represented over the computational mesh without ambiguity. This method of computing the space derivatives gives results which are substantially more accurate than those obtained from finite difference expressions.

In order to satisfy the conditions expressed in Eq. (2), the principle domain

$$D = \{x; \quad 0 \leq x \leq L\} \tag{9}$$

is partitioned into two subdomains

$$D = D_0 + D_1$$

as shown in Figure 1. Here D_1 is the true computational domain over which new u values are computed. The values of u over D_0 are fixed and are being kept constant throughout the entire computation. The unique purpose of D_0 is to provide a smooth transition between the two end points of D_1 and to assure periodicity over D. This configuration permits the computation of the space derivatives of u by the Fourier method outlined above.

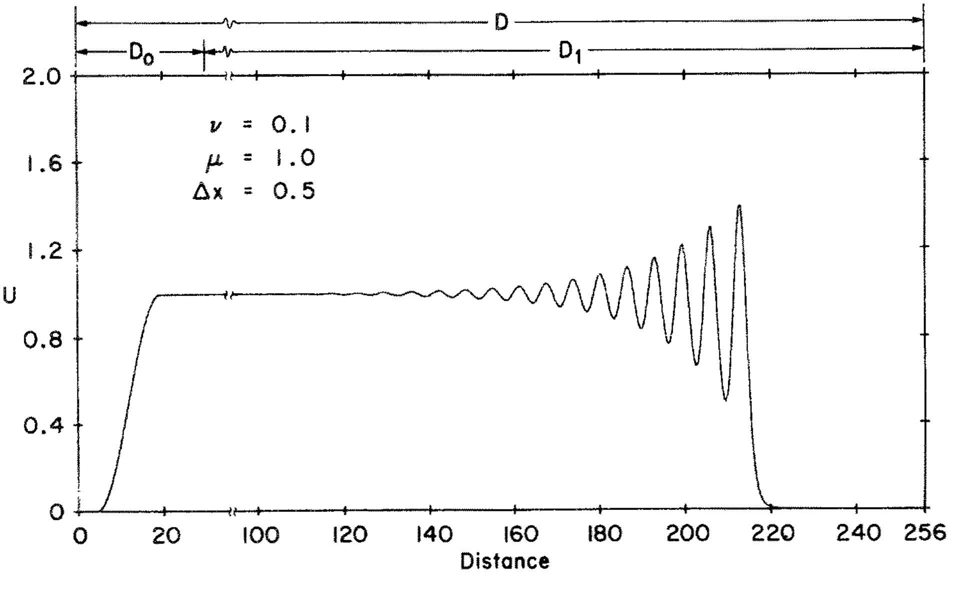

Figure 1. An oscillatory wave solution of the Korteweg-de Vries-Burgers equation at t = 65.

Our numerical results confirm that for any initial condition satisfying Eq. (2) the solution of Eq. (1) evolves asymptotically into a steady state shock wave with the predicted monotonic or oscillatory profile.[18] The dispersion parameter was set $\mu = 1$ in all cases with $u_{\infty}^{-} = 1$ and $u_{\infty}^{+} = 0$. Under these conditions the theoretical speed of propagation is unity, i.e., $c = 1$. Figure 1 shows an oscillatory profile, $\nu = 0.1$, as it evolved from a step function, Eq. (3), after 65 time units. The computations were done with time step $\Delta t = 0.005$. The speed of propagation of this wave at this point is $c = 0.994$. In Figure 2 we show the profiles of a mildly oscillatory case, $\nu = 0.5$, at different times. The speed of propagation of this wave at $t = 50$ is $c = 0.997$. The evolution of a monotonic shock wave is shown in Figure 3. Note that the initial conditions are somewhat different from a step function in that $u(x,0) = 1.2$ for $160 \leq x < 200$. The speed of wave propagation in this case (ν=6) was $c = 0.998$. The space and time increments were $\Delta x = 2$ and $\Delta t = 0.02$.

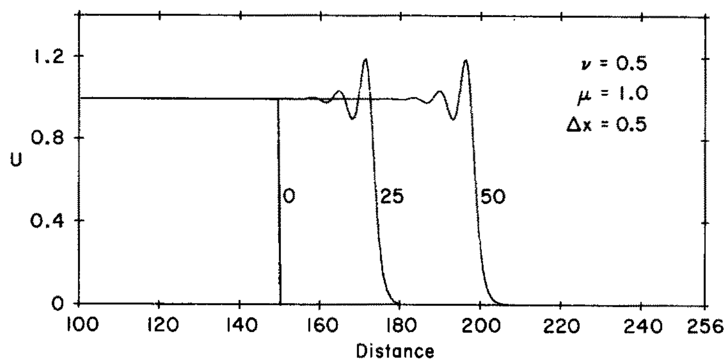

Figure 2. Evolution of a mildly oscillatory wave solution of the KdVB equation. The time separation between plots is 25 time units; the numbers on the curves are values of time.

These numerical results demonstrate the feasibility of the ASD method for the numerical solution of nonlinear partial differential equations with other than periodic boundary conditions. It should be noted that the coefficients μ and ν need not be constants. The numerical method outlined above can be applied to problems whose coefficients are functions of x, i.e., $\mu = \mu(x)$ and $\nu = \nu(x)$. We found considerably better agreement between exact and computed speeds of the wave propagation for the Burgers equation[12] than for the KdVB equation. The most probable cause for this is the presence of the third derivative term whose computation may result in more round-off errors.

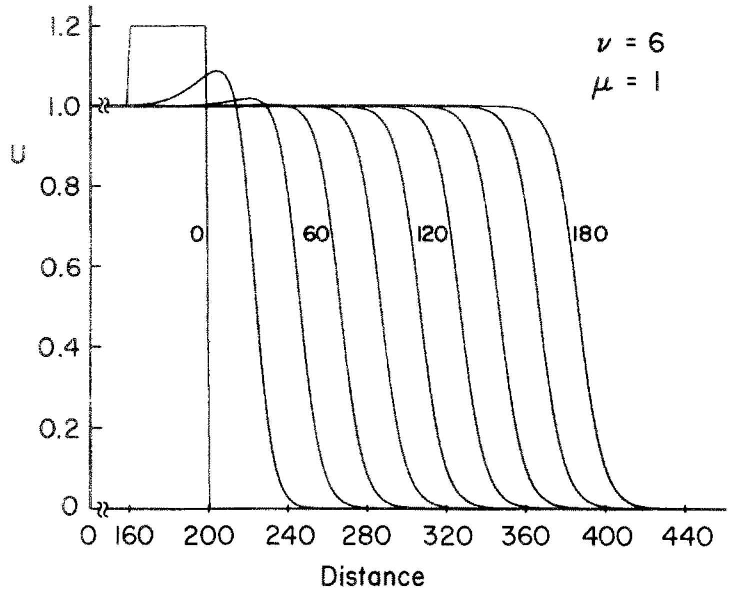

Figure 3. Evolution of a monotonic wave solution of the KdVB equation. Time separation between plots is 20 time units; the numbers on the curves are values of time.

III. ELECTROSTATIC OSCILLATIONS IN UNMAGNETIZED PLASMAS

The system of equations under consideration consists of the Vlasov equation for the electron distribution $f(x,v,t)$,

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - E \frac{\partial f}{\partial v} = 0 \tag{10}$$

and the Poisson equation for the electric field $E(x,t)$

$$\frac{\partial E}{\partial x} = 1 - \int f \, dv \tag{11}$$

These equations are written in dimensionless units.[1] The basic unit of time t and velocity v are the reciprocal of the plasma frequency $(\omega_p)^{-1}$ and the mean thermal velocity v_t. Length x is measured in units of the Debye length. The equilibrium electron distribution in all our computations is Maxwellian, i.e.,

$$f_0(v) = (2\pi)^{-\frac{1}{2}} \exp(- \tfrac{1}{2} v^2) \tag{12}$$

and the initial condition for the electron distribution is

$$f(x,v,o) = f_0(v) \; (1 + \alpha \cos k x) \tag{13}$$

where k is the wavenumber and α is the initial perturbation amplitude. The initial electric field amplitude is

$$E_0 = \frac{\alpha}{k} \; . \tag{14}$$

One can linearize Eq. (10) by holding $\frac{\partial f}{\partial v}$ constant $\left(\text{i.e., replacing } \frac{\partial f}{\partial v} \text{ by } \frac{\partial f_0}{\partial v}\right)$.[1,27] This procedure gives the well known result that the amplitude of the wave damps as $\exp(\gamma t)$ where the Landau damping coefficient is determined by the wavenumber k.[9] On the other hand, if we linearize Eq. (10) by holding the amplitude of the wave constant (i.e., replacing $E(t) \cos(kx - \omega t)$ by $E_0 \cos(kx - \omega t)$), we find that the distribution function is strongly modified in the resonant region. The time scale for this modification is the oscillation period for the resonant electron in a trough of the wave

$$\tau = \omega_B^{-1} = \alpha^{-\frac{1}{2}} \tag{15}$$

where ω_B is the bounce frequency.[7,9,27] According to this analysis, which is valid when $|\gamma\tau| << 1$ and also when $E_0 << 1$, the electric field damps according to the linear Landau theory for times less than τ. For times greater than the bounce time τ there is an oscillatory modulation of $E(t)$ with period of the order of τ.

According to a recent numerical study[7] using the Fourier-Hermite method[1] the critical value $\gamma\tau \approx 0.5$ separates the oscillatory ($\gamma\tau < 0.5$) from the monotonically damped behavior ($\gamma\tau > 0.5$) of the electric field. However, the numerical simulation of the oscillatory behavior for one complete cycle (or longer) of the modulating frequency proved to be computationally unfeasible with the Fourier-Hermite method. We shall present in this paper results obtained by the ASD method in which the above described oscillatory behavior is clearly observable.

The numerical method used for the solution of the Vlasov-Poisson system of equations is a third order ASD method, which is similar to the one described for the KdVB equation. The electron distribution function is advanced by approximating $f(x,v,t+\Delta t)$ from $f(x,v,t)$ by means of the expression

$$f(x,v,t+\Delta t) = \sum_{\ell=0}^{3} \frac{\partial^\ell f(x,v,t)}{\partial t^\ell} \frac{(\Delta t)^\ell}{\ell!} \tag{16}$$

The time derivatives in Eq. (16) are obtained from Eq. (10) by means of successive differentiation, i.e.,

$$\frac{\partial f}{\partial t} = - v \frac{\partial f}{\partial x} + E \frac{\partial f}{\partial v} \tag{17}$$

$$\frac{\partial^2 f}{\partial t^2} = - v \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial t}\right) + E \frac{\partial}{\partial v}\left(\frac{\partial f}{\partial t}\right) + \frac{\partial E}{\partial t}\left(\frac{\partial f}{\partial v}\right) \tag{18}$$

$$\frac{\partial^3 f}{\partial t^3} = - v \frac{\partial}{\partial x}\left(\frac{\partial^2 f}{\partial t^2}\right) + E \frac{\partial}{\partial v}\left(\frac{\partial^2 f}{\partial t^2}\right) + 2 \frac{\partial E}{\partial t}\frac{\partial}{\partial v}\left(\frac{\partial f}{\partial t}\right) + \frac{\partial^2 E}{\partial t^2}\frac{\partial f}{\partial v} \tag{19}$$

The derivatives with respect to x and v are computed by using finite Fourier transform methods.[12] The electric field $E(x,t)$ and its derivatives with respect to t are obtained from $f(x,v,t)$ and its time derivatives, Eqs. (17) and (18). This we do by using standard Poisson solver techniques.[1,5,22]

In the first example considered here the amplitude of the perturbation is very small, $\alpha = 0.001$. In this case $\gamma\tau = 4.85$ and the electric field undergoes exponential damping until $t \cong 55$ as shown in Figure 4. After a short transition region an approximate recurrence of the initial state can be observed at $t \cong 75$. This apparent explosive growth of the electric field was sometimes mistaken for beaming instability, a physical phenomenon.[21] It was shown recently that the reason behind this phenomenon is entirely numerical, which is related to the velocity resolution of the numerical procedure.[8] The above computation was performed by using an 8×64 grid to represent the (x,v) phase plane with time step $\Delta t = 0.05$. When the same computer experiment was repeated over an 8×256 grid, oscillation frequency and damping rate obtained from the numerical output averaged over the peaks from $t = 4.7$ to $t = 26.9$ were $\omega = 1.417$ and $-\gamma = 0.1537$, respectively. The exact values obtained from Landau's dispersion equation are $\omega = 1.416$ and $-\gamma = 0.1534$.

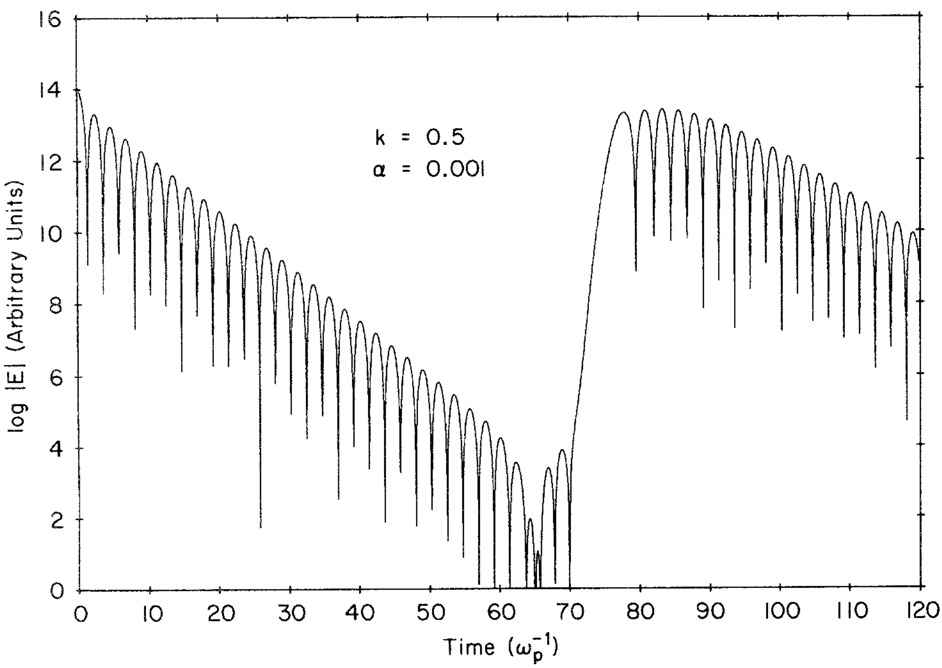

Figure 4. The numerical solution of the Vlasov equation for Maxwellian distribution shows the classical linear Landau damping. The explosive growth at $t = 70$ is the recurrence of the initial state due to aliasing effects in velocity space.

In Figure 5 we show the results of a nonlinear problem characterized by the parameter values $k = 0.5$, $\alpha = 0.1$. For this case $\gamma\tau = 0.485$. We compared these results with those obtained from the Fourier-Hermite method. We found a three significant figure agreement in the peak values of the electric field obtained from these two methods up to t = 35. There is a minimum value of the wave amplitude at t ≈ 56 after which a slight growth can be observed, indicating that the value $\gamma\tau = 0.485$ is close to the critical value. In the Fourier-Hermite code we used 1200 Hermite terms and three Fourier terms. In the ASD method we used a 16 × 128 grid which assures about twice the resolution in both x as well as in v. The third order ASD method was found 2.35 times faster. Thus for comparable space and velocity resolution in this range the third order ASD method appears to be an order of magnitude faster than the Fourier-Hermite method.

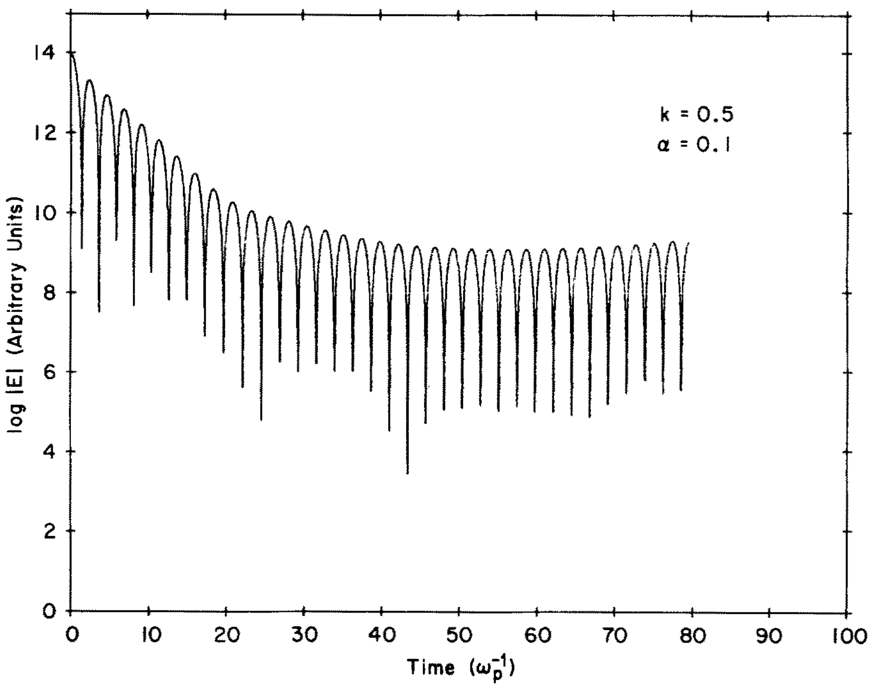

Figure 5. Electric field versus time for a nonlinear wave.

In Figure 6 we show the results of a strongly nonlinear problem. The parameter values are $k = 0.5$, $\alpha = 0.3$, and $\gamma\tau \approx 0.343$. The oscillatory behavior of the modulating envelope over these oscillations is observable showing a good qualitative agreement with theoretical predictions.

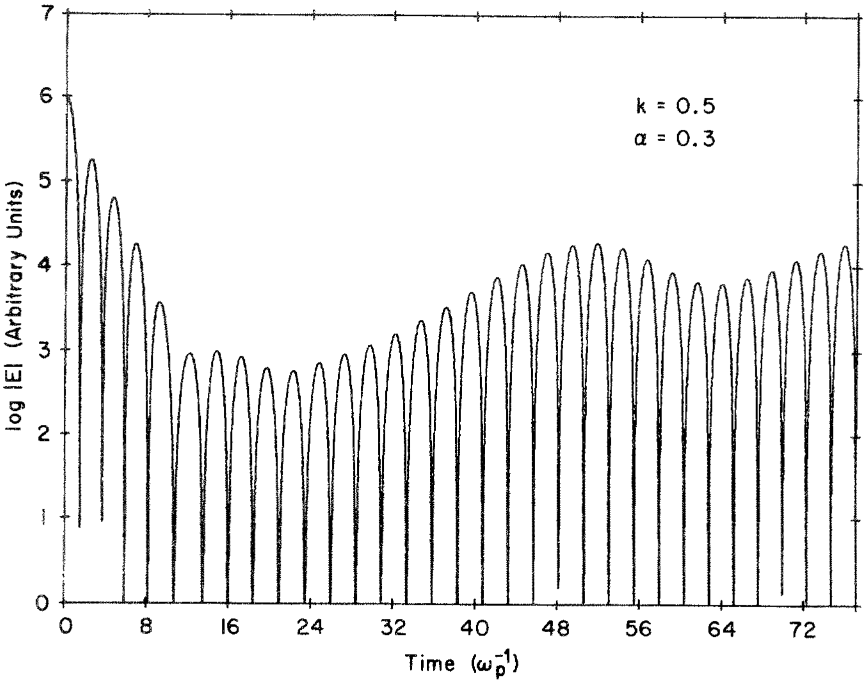

Figure 6. Electric field for a strongly nonlinear wave.

IV. ELECTROSTATIC OSCILLATIONS IN A MAXWELLIAN MAGNETO-PLASMA

In this section, we shall consider longitudinal electrostatic waves in a warm magneto-plasma. We assume an infinite collisionless Maxwellian plasma with an externally applied uniform magnetic field B. There is no damping for waves propagating at right angles to the magnetic field. These waves, first predicted by Bernstein,[4] are restricted to passbands associated with the harmonics of the electron cyclotron frequency ω_c.[2] For this reason they have been referred to as Cyclotron Harmonic Waves (CHW). Computer simulations of these waves were carried out by using particle methods.[11,16] Particle simulation models are subject to fluctuations which interfere with externally excited small amplitude perturbations. For this reason the particle models permitted only the observation of the undriven Bernstein modes obtained from the fluctuations of the computer plasma.[11,16] Here we shall consider electrostatic oscillations excited by means of small amplitude perturbations similar to those in the previous section.

If we assume that B is directed along the z axis and all quantities to be functions only of the spatial dimension x, and the velocity dimensions v_x, v_y, the Vlasov-Poisson system can be written in dimensionless variables as

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} - E \frac{\partial f}{\partial v_x} + \omega_c \left(v_y \frac{f}{\partial v_x} - v_x \frac{\partial f}{\partial v_y} \right) \tag{20}$$

$$\frac{\partial E}{\partial x} = 1 - \int f \, dv_x \, dv_y \tag{21}$$

where ω_c is the cyclotron frequency.

The numerical method followed here is the same (3rd order ASD) as in the previous section generalized to include three phase space variables. The equilibrium distribution function used is

$$f_0(v_x,v_y) = (2\pi)^{-1} \exp\left(-\frac{1}{2}(v_x^2 + v_y^2)\right) \tag{22}$$

and the initial condition for the electron distribution is

$$f(x,v_x,v_y,0) = f_0(v_x,v_y)\ (1 + \alpha \cos k\, x) \tag{23}$$

where k is the wavenumber of the longest wave and the perturbation amplitude was set $\alpha = 0.001$.

The time behavior of the electric field amplitude is characterized by steady, undamped oscillations. These oscillations are not monochromatic, and therefore, the E vs. time plots are not very informative. After accumulating the E values (i.e., its first spatial Fourier coefficient) over 4096 time steps, the Fourier transform of the time sequence was found and the spectrum was computed. The spectrum of a representative spatial mode is shown in Figure 7. The position of peaks indicates frequencies at which cyclotron harmonic waves can propagate. We compared these values with those predicted by small amplitude perturbation theory,[2,11] and found that they agreed within 1% expressed in units of ω_c.

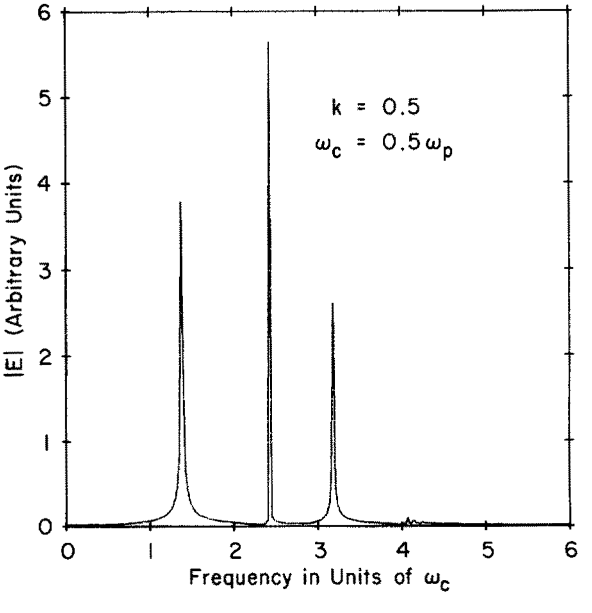

Figure 7. Spectrum of longitudinal oscillations in a magneto-plasma.

V. CONCLUSIONS

In this paper we demonstrated that ASD methods can be applied with success to fluid flow type problems, i.e., problems in which the convective term plays a dominant role. Our results from the numerical study of the KdVB equation suggest that the method is well suited to nonlinear partial differential equations with shock-like solutions. From these results it is also clear that periodic boundary conditions are not prerequisites for these methods. The only purpose of the finite Fourier transform algorithm is to compute the space derivatives efficiently. It is quite conceivable to think of situations in which other (than Fourier) techniques are preferable.

According to our experience, the ASD method in plasma computations proved to be superior to the Fourier-Hermite method[1] or to finite difference methods.[5] The computation of strongly nonlinear problems (e.g., the one shown in Figure 6)* with the third order ASD method requires about one tenth of the CPU time required by the other numerical methods in order to attain similar overall accuracy.

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