JOURNAL OF COMPUTATIONAL PHYSICS 6, 247-267 (1970)

Effects of the Spatial Grid in Simulation Plasmas

A. BRUCE LANGDON

Department of Electrical Engineering and Computer Sciences, Electronics Research Laboratory, University of California, Berkeley, California 94720

Received January 22, 1970; revised April 8, 1970

In earlier studies of simulation plasmas the difference schemes for each step of the calculation have been analyzed, but their over-all performance taken together with plasma behavior has not been treated carefully. We begin with a rigorous treatment of the spatial grid, giving here a formulation which includes most codes now in use. This is done in such a way that the role of each step in the calculation is easily identified in the results, and also the expressions for plasma properties are easily compared with the corresponding "real" plasma properties. Details are given for the electrostatic case. The formulation is applied to the question of energy conservation, and to linear wave dispersion and instability. The effect of the spatial grid is to smooth the interaction force somewhat and to couple plasma perturbations to perturbations at other wavelengths, called aliases. The strength of the coupling depends on the smoothness of the interpolation methods used. Its importance depends roughly on how well the plasma would respond, in the absence of the grid, to wavenumbers $k \sim 2\pi/\Delta x$; e.g., if the Debye length is too small the coupling can destabilize plasma oscillations even in a thermal plasma.

1. INTRODUCTION

A study is under way to understand the physics of plasma simulation models, so that we may better design computer experiments and understand the results, especially where they may differ from real plasma. This work has involved almost no numerical analysis in the usual sense, in which different considerations of accuracy and speed are involved. For instance, the initial-value problem for ordinary differential equations has been extensively studied and a variety of very accurate algorithms are available. Such methods have been used, for example, for single-particle motion in the study of magnetic field configurations in fusion experiment devices. The methods used in many-particle simulation seem comparatively crude and inaccurate. However what is important is not that individual particle orbits be accurate, but that the collective motions of many particles reflect real plasma behavior. When computer time is limited, it has usually been better to use simple and fast difference algorithms rather than having to use fewer particles, say. Further, it is argued elsewhere [1–4] that a modified interaction force can lead to better simulation results than the Coulomb interaction. Even some errors in collective motions, for example oscillation frequencies, may be acceptable if one understands quantitatively their origin and consequences.

On the other hand it is desirable that the codes retain certain physical properties. For instance, while many successful codes are not exactly time reversible, experience has shown often that unacceptable types of errors are avoided when one builds exact reversibility into the difference equations [5]. Similarly, making a smooth interaction force by using finite size particles interacting through the normal electromagnetic fields automatically avoids self-forces and nonphysical instabilities that can arise with other smooth interactions not physically motivated [2].

This paper presents a mathematical framework with which one can apply conventional plasma theory to simulation plasma using a spatial grid on which charge and current densities, and electromagnetic fields, are defined [4, 6, 7]. The use of fields is almost universal even in the electrostatic approximation with simple geometry, rather than summing the Coulomb interaction over all particle pairs (except in the one-dimensional sheet models where the Coulomb force is a simple step function and the particles may be ordered). This paper is directed toward understanding the physical properties of simulation plasma rather than to development of new algorithms for the codes.

Here we treat time as continuous, the rational for this being: it is possible to ignore the space-time grid completely by making it fine enough. This being so, one can study the consequences of finite Δt and finite Δx separately, and should do so initially. In real codes, especially in three dimensions, it is easier to make Δt negligible than Δx; this is similar to the motivation in hydrodynamics for finite-difference schemes of much higher order in x than in t [8]. The condition for treating time as continuous is $\omega_{\max} \Delta t \ll 1$, with $\omega_{\max}$ the largest frequency of concern when $\Delta t \to 0$, assuming the time integration is stable numerically. It is usually true that $\omega_p \Delta t$, $\omega_c \Delta t$, etc., are small, but when $\lambda_D/\Delta x$ is large, $(v_t/\Delta x)\Delta t = (\omega_p \Delta t)(\lambda_D/\Delta x)$ may not be small. However, a plasma does not respond well to frequencies $\gg \omega_p$, ω_c, so that the grid noise may not need to be lower in frequency than Δt^{-1}. The theory to follow will help answer this question of the domain of validity.

The spatial grid is a simple example of a periodic spatial nonuniformity, and we begin with some remarks on the more general case of a plasma with nonuniform interaction. Then each step in the calculation of interactions through a spatial grid is studied (essentially to relate Fourier transforms of densities, forces and fields) with enough generality to include most codes. Next we consider energy conservation. Finally the formalism is applied to linear waves and instabilities.

2. The Effects of a Periodic Spatial Nonuniformity

In this section we will make some general remarks about a plasma system whose interaction force has a spatial nonuniformity which is periodic and time-independent (e.g., a Fermi gas in a crystal, some electron beam devices). Later we will specialize to the grid problem.

Let us consider the interaction force $F(x_1, x_2)$ in one dimension, defined as the force on a particle at x_2 due to a particle at x_1. In a normal physical system, which will be invariant under displacement, F depends only on the separation $x = x_2 - x_1$. However, in computer simulation using a spatial grid, invariance does not exist under all displacements (displacing particles but not the grid). Thus F also depends on $\bar{x} = \frac{1}{2}(x_1 + x_2)$ as well as x. In most simulations a grid with constant spacing Δx is used; in this case $F(\bar{x} - \frac{1}{2}x, \bar{x} + \frac{1}{2}x)$, considered as a function of displacement $\bar{x}$ with separation x constant, is periodic with period Δx.

In order to study the effect of the nonuniformity on a plasma, we need the Fourier transform of $F(x_1, x_2)$. For an infinite system we use a Fourier integral transform in x and a Fourier series in $\bar{x}$.

$$F(\bar{x} - \tfrac{1}{2}x, \bar{x} + \tfrac{1}{2}x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \sum_{p=-\infty}^{\infty} e^{ipk_g\bar{x}} F_p(k) \tag{1}$$

where $k_g = 2\pi/\Delta x$ is the grid wavenumber, and

$$F_p(k) \equiv \int_{-\infty}^{\infty} dx\, F_p(x)\, e^{-ikx}, \tag{2a}$$

$$F_p(x) \equiv \frac{1}{\Delta x} \int_{\Delta x} d\bar{x}\, e^{-ipk_g\bar{x}} F(\bar{x} - \tfrac{1}{2}x, \bar{x} + \tfrac{1}{2}x). \tag{2b}$$

This sign and normalization for the Fourier integral will be followed throughout.

The properties of the plasma which are little affected by the lack of displacement invariance are expected to be similar to those of a plasma with two-particle force equal to the averaged force $F_0(x)$ [1, 2]. We can analyze those properties by the gridless theory [2]. The difference $\delta F = F - F_0$ is an unphysical grid force. In some respects it is like a "noise" force; however it is coherent with the plasma perturbation. More will be said about this later.

For a particle density $n(x)$ (time dependence is ignored for now), the force $F(x)$ on a particle at x is

$$F(x) = \int dx'\, F(x', x)\, n(x').$$

When transformed this becomes, using Eq. (1),

$$F(k) = \sum_{p=-\infty}^{\infty} F_p(k - \tfrac{1}{2}pk_g)\, n(k_p), \tag{3}$$

where $k_p \equiv k - pk_g$. We see that the effect of δF (corresponding to the $p \neq 0$ terms) is to *couple density perturbations and forces at wavenumbers which differ by integral multiples of the grid wavenumber k_g*. Such wavenumbers are said to be *aliases* of one another [9].

As an illustration we will derive a dispersion relation for small amplitude plasma oscillations. Linearizing the Vlasov equation and adding time dependence $\exp(-i\omega t)$ to n and F, we find the density response $n(k, \omega)$, of an unmagnetized uniform plasma, to the force field $F(k, \omega)$ to be, in the usual notation

$$n(k, \omega) = F(k, \omega)\, \psi(k, \omega)$$

where

$$\psi(k, \omega) = \frac{n_0}{im} \int dv \frac{f_0'}{\omega + i0 - kv}, \qquad \mathrm{Im}\,\omega \geqslant 0. \tag{4}$$

For $\mathrm{Im}\,\omega < 0$ this must be analytically continued from the upper half ω plane. Equations (3) and (4) may be combined to yield

$$n(k, \omega) = \psi(k, \omega) \sum_p F_p(k - \tfrac{1}{2}pk_g)\, n(k_p, \omega)$$

or, alternatively,

$$F(k, \omega) = \sum_p F_p(k - \tfrac{1}{2}pk_g)\, F(k_p, \omega)\, \psi(k_p, \omega).$$

If one replaces k by $k_q \equiv k - qk_g$ and p by $p - q$ ($q = 0, \pm 1, \pm 2, \ldots$), each set of equations may be written in infinite matrix form

$$\begin{aligned} 0 &= \sum_p \{\delta_{q,p} - F_{p-q}(\tfrac{1}{2}[k_p + k_q])\, \psi(k_q, \omega)\}\, n(k_p, \omega), \\ 0 &= \sum_p \{\delta_{q,p} - F_{p-q}(\tfrac{1}{2}[k_p + k_q])\, \psi(k_p, \omega)\}\, F(k_p, \omega). \end{aligned} \tag{5}$$

We can now see several important features.

The possible free oscillations of the plasma are given by the zeros of the determinant of either matrix. The presence of off-diagonal terms, due to the coupling together of many wavelengths, shows that the normal coordinates (in the terminology of the small-oscillation problem in classical mechanics) for n and F are not the exponentials $\exp(ik_p x - i\omega t)$, but are some (as yet unknown) linear combinations of such exponentials, so that n or F varies as $\exp(ikx - i\omega t)$ times a periodic function of x with period Δx (Bloch function). Thus we have brought our problem into the classical form [10].

If $|k| \ll |k_g|$, one may expect the $p = q = 0$ element to be much the largest in the matrix. Also, if $k_g v_t \gg \omega_p$, i.e., Debye length $\lambda_D = v_t/\omega_p \gg \Delta x$, we expect $n(k_p, \omega)$ to be largest when $p = 0$. Therefore we have an approximate dispersion relation $\epsilon_0 = 0$, where $\epsilon_0 \equiv 1 - F_0(k)\,\psi(k, \omega)$. This is exactly the same as we would get for a uniform system whose interaction force is F_0. The validity of this approximation will become clearer in Section 5.

At this point it is best to make use of the simplification which results when the particle forces are found from a function defined on a discrete grid. Therefore we now analyze each step of the interaction calculation to interrelate the Fourier transforms of the several quantities.

3. Interactions Through a Spatial Grid

A. *The Grid Electric Field and Particle Force Field*

We define an electric field $\{E_j\}$ on a discrete spatial grid whose j'th grid point is located at $x_j = j\,\Delta x$ (for simplicity we develop the principal results in an infinite one-dimensional system and generalize later). We can see easily the significance for the field of the aliases k_p of k: for any p, $\exp(ik_p x_j) = \exp(ikx_j)$. Thus the aliases are different wavenumbers which produce identical variations of grid quantities [9–11]. We will find that this equivalence simplifies the results of the last section. The appropriate Fourier transform is,[1] again temporarily suppressing time dependence,

$$E(k) = \Delta x \sum_{j=-\infty}^{\infty} E_j e^{-ikx_j}. \tag{6}$$

Note that $E(k)$ is periodic, $E(k_p) = E(k)$. In the inverse transform we integrate over one period

$$E_j = \int_g \frac{dk}{2\pi} E(k)\, e^{ikx_j}. \tag{7}$$

[1] Some expressions should be interpreted as generalized functions [12]. All results are well behaved for finite systems; see Appendix I.

If necessary, we might choose this period to be

$$\int_g dk = \int_{-\frac{1}{2}k_g}^{\frac{1}{2}k_g} dk,$$

which Brillouin calls the first zone [10].

We derive the particle force field from the grid field by interpolation.

$$F(x) = q \sum_j E_j w_j(x). \tag{8}$$

The weights w_j are usually zero if $| x - x_j |$ is larger than $2\,\Delta x$ or so. If all the grid points are treated equivalently, the weights are shifted copies of each other and so may all be expressed in terms of the $j = 0$ weight

$$w_j(x) = w_0(x - x_j). \tag{9}$$

The transform of Eq. (8) is

$$\begin{aligned} F(k) &= \int dx\, e^{-ikx} q \sum w_j(x) \int_g \frac{dk'}{2\pi} E(k')\, e^{ik'x_j} \\ &= qE(k) \frac{w_0(k)}{\Delta x} \\ &= qE(k)\, I(-k), \end{aligned} \tag{10}$$

where $I(k) \equiv w_0(-k)/\Delta x$ is an interpolation function, and we have used Eqs. (7)–(9), the periodicity of $E(k')$, and the Poisson summation formula [12].

Now let the particles be finite size rigid "clouds" which pass freely through each other [6].[2] Their charge density is spread out; $qS(x)$ is the charge density of a cloud with total charge q whose "center" is at the origin [1, 2]. If we use the interpolation of Eq. (8) to find the force on each element $S(x' - x)\,dx'$ of a cloud whose center is at x, the total *cloud* force is

$$F(x) = \int dx'\, S(x' - x) q \sum_j E_j w_j(x'),$$

and the transform $F(k)$ is Eq. (10) with the additional factor $S(-k)$. It is convenient to introduce[3]

$$S_e(k) = I(k)\, S(k) \tag{11}$$

[2] Historically there has been a tendency to separate the interpolation and particle size considerations. In [7] the particles are not considered finite in size and the whole matter is considered one of interpolation. In [6] the particles are considered to be square clouds and nearest-grid-point (NGP) interpolation is used for each elemental area of a cloud. Our discussion will at first include both viewpoints, and later combine the two aspects.

[3] The functions $w_0(x)$, $S(x)$ and therefore also $S_e(x)$, are usually even, so that their transforms are real and even, but this is not assumed here.

the effective cloud shape in the grid-particle calculation, so that

$$F(k) = qS_e(-k)\,E(k). \tag{12}$$

This form is like that of a gridless cloud plasma [2], and emphasizes the similar roles played by smoothing thought of as interpolation [7], and smoothing introduced by smearing out the particle [6]. In choosing the cloud viewpoint we keep in mind that the weights, and therefore S_e, should satisfy certain conditions not required of S_e in a gridless system, such as the normalization

$$\sum_j w_j(x) = 1 \qquad \text{for all } x. \tag{13}$$

Our discussion does not depend on this condition, but without it the force is not constant in space for a particle in a uniform field.

It is interesting to examine this condition in transform space. Using the Poisson summation formula one can show that Eq. (13) implies conditions on $I(k)$ which are satisfied also by $S_e(k)$, since $S(k = 0) = 1$, namely:

$$\begin{aligned} S_e(k) &= 1 \qquad \text{for} \quad k = 0, \\ &= 0 \qquad \text{for} \quad k = pk_g\,, \qquad p \neq 0. \end{aligned} \tag{14}$$

Since $E(k)$ is periodic, F will normally contain many wavelengths. This is just another way of saying $F(x)$ is never sinusoidal. For a constant field $E_j = E$, we have $E(k) = 2\pi E \sum \delta(k_p)$, and thus $F(k) = 2\pi qE \sum S_e(-pk_g)\,\delta(k_p)$. Because of Eq. (14) only one term survives, and $F(k) = 2\pi qE\,\delta(k)$ as it should.

For linear interpolation [6, 7] one has $\sum x_j w_j(x) = x$, which means $S_e'(pk_g) = 0$, i.e., the zeros of $S_e(k)$ at $k = pk_g$ are of order two. Then, for small k, $S_e(k_p)$, $p \neq 0$, is smaller, and therefore $F(x)$ smoother, as expected, than when the interpolation is not at least linearly exact.

In gridless models the zeros of $S(k)$ for square clouds may make them seem unattractive [2]; we see here that in a gridded model these zeros of $S_e(k)$ are beneficial.

B. *The Grid Charge Density and Particle Density*

The grid charge density for a zero-size particle at x is

$$\rho_j = \frac{q}{\Delta x}\, w_j(x). \tag{15}$$

Although using the same weight function as for the force is not a necessary feature of this discussion, there are good reasons for doing so. Using a different weight function corresponds to using a different cloud shape, which can lead to a gravitation-like instability [2]. Also, if the difference equations relating ρ_j to E_j are symmetric in space, use of the same weight function eliminates self-forces and ensures conservation of momentum.

The normalization condition Eq. (13) makes the total charge on the grid, $\Delta x \sum \rho_j$, equal to the particle charge q.

The transformed charge density for clouds is

$$\rho(k) = q \sum_{p=-\infty}^{\infty} S_e(k_p)\, n(k_p) \tag{16}$$

where n is the density of cloud centers. It is here that the aliases become coupled through the grid. One can think of the infinite sum in this way: We are taking information defined on a continuum and trying to squeeze it onto a discrete grid. The difficulty shows itself here in that different particle wavelengths (aliases) appear the same at the grid points.

The same phenomenon is familiar in the analysis of sampled time series [9]. If one does not sample often enough, differing frequencies become indistinguishable. This can be improved by low-pass filtering the signal before sampling, and that is what one is doing here with a smooth S_e.

In simulation models the sampling effects are fed back into the system. A sinusoidal density perturbation produces forces with many wavelengths, which cause density perturbations at the new wavelengths, and all these perturbations act back on the original perturbations.

Let us consider some common cases. The simplest interpolation satisfying Eq. (13) is nearest-grid-point (NGP), Fig. 1. When NGP is used with no further smoothing the effective cloud is as shown in Fig. 2 [4] and $S_e(k) = \mathrm{dif}(\frac{1}{2}k\,\Delta x)$,

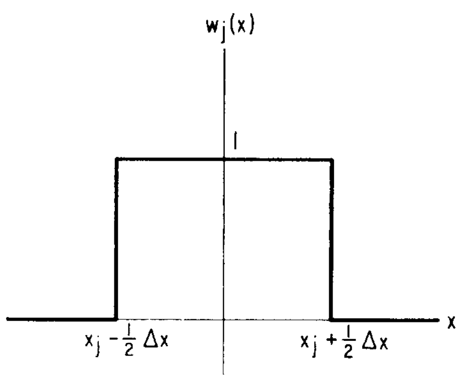

FIG. 1. Nearest-grid-point interpolation weight function.

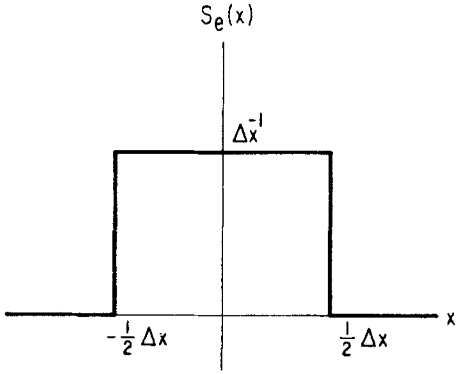

FIG. 2. The effective cloud for straightforward NGP [5]. This is also the square cloud S of [6].

where we have introduced the diffraction function

$$\operatorname{dif}\theta \equiv \frac{\sin\theta}{\theta}$$

which will arise frequently.

When NGP interpolation is used for each element of a square cloud of width Δx (S like S_e of Fig. 2; the usual CIC or "charge-sharing" case [6]) one has $S = I$ and $S_e = \operatorname{dif}^2(\frac{1}{2}k\,\Delta x)$, shown in Fig. 3.

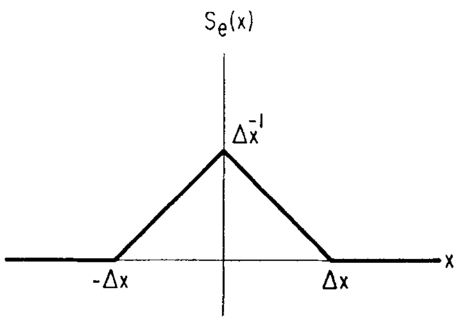

FIG. 3. The effective cloud for CIC of [6] and PIC [7].

In one dimension the area-weighting of PIC [7] is just linear interpolation (Fig. 4) and S_e is the same as for the CIC case above. Thus PIC and this example of CIC are computationally identical, although there are important differences in viewpoint.

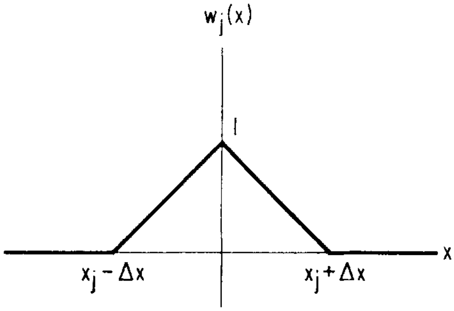

FIG. 4. The weight function for one-dimensional PIC (linear interpolation).

C. *The Field Equations*

The relations between grid quantities may be written in a form that looks like the gridless case

$$4\pi\rho(k) = K^2(k)\,\phi(k), \tag{17}$$

$$E(k) = -i\kappa(k)\,\phi(k). \tag{18}$$

These relations then define K and κ, which are therefore periodic. In a normal code at long wavelengths $K \approx \kappa \approx k$ (but see, e.g., [13]).

When the grid quantities are related by finite-difference formulas one can find the functions K and κ simply by assuming the grid quantities vary as $\exp(ikx_j)$ (like finding transfer functions in [11]). For example, substituting $\phi_j = \phi \exp(ikx_j)$ and $\rho_j = \rho \exp(ikx_j)$ into the common Poisson difference equation

$$-4\pi\rho_j\,\Delta x^2 = \phi_{j+1} - 2\phi_j + \phi_{j-1}$$

yields $K = k \operatorname{dif}(\frac{1}{2}k\,\Delta x)$. Similarly, $E_j = -(\phi_{j+1} - \phi_{j-1})/(2\,\Delta x)$ yields $\kappa = k \operatorname{dif} k\,\Delta x$.

If, on the other hand, we use the fast Fourier transform [14][4] to solve for the field, we can choose K and κ freely (over one period in k space) to best achieve the desired physics, even though there may not be any reasonable corresponding finite-difference relation involving a small number of grid points. For instance, one can get more interaction smoothing, corresponding to widening the cloud, by truncating the k space here in some smooth manner. This is computationally cheaper than using a complicated grid-particle interpolation involving many grid points. At least in one dimension, the most economical way to get a smooth interaction without grid effects may be to use a fine mesh, NGP interpolation, and do the smoothing in k space as just described. Note that then E in the model corresponds more closely to F rather than E in the gridless cloud system.

[4] This review paper is very readable as well as containing information unavailable elsewhere.

We now have a complete formulation of interactions in most one-dimensional models. The generalization to 2 or 3 dimensions is given next.

D. *Generalization to More Dimensions*

The grid label j becomes a vector $\mathbf{j} = (j_x, j_y, j_z)$ with integer components. The coordinate of grid point $\mathbf{j}$ is, in a three dimensional oblique[5] grid,

$$\mathbf{x}_\mathbf{j} = \mathbf{j} \cdot \mathbf{\Delta x} \tag{19}$$

where the rows of the tensor $\mathbf{\Delta x}$ are the basis vectors for the grid [15], defining the edges of a grid cell whose volume is

$$V_c = \det \mathbf{\Delta x}.$$

In the usual rectangular grid we have

$$\mathbf{\Delta x} = \begin{pmatrix} \Delta x & 0 & 0 \\ 0 & \Delta y & 0 \\ 0 & 0 & \Delta z \end{pmatrix}. \tag{20}$$

The transform becomes, for example,

$$\mathbf{E}(\mathbf{k}) = V_c \sum_\mathbf{j} \mathbf{E}_\mathbf{j} e^{-i\mathbf{k}\cdot\mathbf{x}_\mathbf{j}}. \tag{6'}$$

For a point particle at $\mathbf{x}$,

$$\mathbf{F}(\mathbf{x}) = q \sum_\mathbf{j} w_\mathbf{j}(\mathbf{x})\, \mathbf{E}_\mathbf{j} \tag{8'}$$

$$\rho_\mathbf{j} = \frac{q}{V_c} w_\mathbf{j}(\mathbf{x}) \tag{15'}$$

where

$$w_\mathbf{j}(\mathbf{x}) = w_0(\mathbf{x} - \mathbf{x}_\mathbf{j}). \tag{9'}$$

For clouds the transforms are

$$\mathbf{F}(\mathbf{k}) = qS_e(-\mathbf{k})\, \mathbf{E}(\mathbf{k}) \tag{12'}$$

$$\rho(\mathbf{k}) = q \sum_p S_e(\mathbf{k}_p)\, n(\mathbf{k}_p) \tag{16'}$$

[5] For instance, triangular meshes have also been used.

where

$$S_e(\mathbf{k}) = I(\mathbf{k})\, S(\mathbf{k}) \tag{11'}$$

$$I(\mathbf{k}) = \frac{1}{V_c}\, w_0(-\mathbf{k})$$

$$\mathbf{k_p} = \mathbf{k} - \mathbf{p} \cdot \mathbf{k}_g \tag{21}$$

$$\mathbf{k}_g = 2\pi(\mathbf{\Delta x}^{-1})^T \tag{22}$$

and $\mathbf{p}$ is a vector with integer components. The rows of tensor $\mathbf{k}_g$ are basis vectors, reciprocal [15] to those given by $\mathbf{\Delta x}$, times 2π. They define the periodicity of transforms of grid quantities, since

$$\exp(i\mathbf{k_p} \cdot \mathbf{x_j}) = \exp(i\mathbf{k} \cdot \mathbf{x_j} - 2\pi i \mathbf{p} \cdot \mathbf{j}) = \exp(i\mathbf{k} \cdot \mathbf{x_j}).$$

For a rectangular grid

$$\mathbf{k}_g = 2\pi \begin{pmatrix} \Delta x^{-1} & 0 & 0 \\ 0 & \Delta y^{-1} & 0 \\ 0 & 0 & \Delta z^{-1} \end{pmatrix}.$$

The integral in the inverse transform is taken over one period in $\mathbf{k}$ space.

$$\mathbf{E_j} = \int_g \frac{d\mathbf{k}}{(2\pi)^3}\, \mathbf{E}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x_j}} \tag{7'}$$

The forms taken in one, two, or three dimensions are simply seen if one remembers that $d\mathbf{k}/(2\pi)^3 \to d\mathbf{k}/(2\pi)^d$, where d is the dimensionality.

The relations between transformed grid quantities are

$$4\pi\rho(\mathbf{k}) = K^2(\mathbf{k})\, \phi(\mathbf{k}), \tag{17'}$$

$$\mathbf{E}(\mathbf{k}) = -i\boldsymbol{\kappa}(\mathbf{k})\, \phi(\mathbf{k}). \tag{18'}$$

Quantities $\phi_\mathbf{j}$, $\mathbf{E_j}$, and $\boldsymbol{\rho}_\mathbf{j}$ are defined only on the grid, while $n(\mathbf{x})$ and $\mathbf{F}(\mathbf{x})$ are defined on a continuum of particle positions.

In our simplest example, the effective cloud for NGP becomes, in a three-dimensional rectangular grid,

$$S_e(\mathbf{k}) = \operatorname{dif}(\tfrac{1}{2}k_x\, \Delta x)\, \operatorname{dif}(\tfrac{1}{2}k_y\, \Delta y)\, \operatorname{dif}(\tfrac{1}{2}k_z\, \Delta z).$$

The field finite-difference equations, in their simplest generalization, yield

$$K^2 = k_x^2 \operatorname{dif}^2 \tfrac{1}{2}k_x\, \Delta x + k_y^2 \operatorname{dif}^2 \tfrac{1}{2}k_y\, \Delta y + k_z^2 \operatorname{dif}^2 \tfrac{1}{2}k_z\, \Delta z$$

and $\kappa_x = k_x \operatorname{dif} k_x\, \Delta x$, etc.

E. *An Alternative Viewpoint*

Having seen how the product $S_e = IS$ arises naturally in both force and charge interpolation, we will not be surprised if it is simpler to deal with the grid-particle problem in terms of S_e from the outset. The transforms of Eqs. (12′) and (16′) are

$$\mathbf{F}(\mathbf{x}) = qV_c \sum_j \mathbf{E}_j S_e(\mathbf{x}_j - \mathbf{x}) \tag{23}$$

$$\rho_j = qS_e(\mathbf{x}_j - \mathbf{x}) \tag{24}$$

for a cloud with center at $\mathbf{x}$. The first expression may be regarded as the simplest discrete analogue to the continuum result $qS_e(-\mathbf{x}) * \mathbf{E}(\mathbf{x})$ (where * denotes convolution) for a cloud with shape factor $S_e(\mathbf{x})$ [2]. The second expression is the continuum charge density for the cloud, sampled at the grid point, and is the same as $\rho_j(x)$ in [6].

In this viewpoint Hockney's particles are squares with size equal to one grid cell (as he has already argued [4]), and the particles in CIC as normally used [6] and in PIC [7] are the convolution of two such squares (see [6, Fig. 6]).

Having drawn the gridded and gridless models as close together as possible, we recall however that the grid imposes on S_e conditions such as Eq. (13), which is equivalent to

$$V_c \sum_j S_e(\mathbf{x}_j - \mathbf{x}) = 1. \tag{13′}$$

This is automatically satisfied when S_e is the convolution of several cloud S functions, at least one of which satisfies such a condition.

4. Energy Conservation

We desire some combination of grid quantities which will function as a field energy. Two commonly used candidates are

$$\frac{\Delta x}{8\pi} \sum E_j^2 \quad \text{and} \quad \frac{\Delta x}{2} \sum \rho_j \phi_j .$$

We quickly discover that either of these (they are normally unequal) when added to the kinetic energy does not give a constant, no matter how accurate the time integration may be. To see why the sum is not exactly constant, but is often very nearly so, we express the rates of change in terms of the particle current density J and particle force F, again in one dimension:

$$\frac{d}{dt}\frac{\Delta x}{8\pi}\sum_j E_j^2 = \frac{d}{dt}\int_g \frac{dk}{2\pi}\frac{|E(k)|^2}{8\pi} = -\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{F(-k)}{q}J(k)\frac{k\kappa}{K^2}, \tag{25}$$

$$\frac{d}{dt}\frac{\Delta x}{2}\sum_j \rho_j\phi_j = \frac{d}{dt}\int_g \frac{dk}{2\pi}\frac{1}{2}\rho(k)\,\phi^*(k) = -\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{F(-k)}{q}J(k)\frac{k}{\kappa}, \tag{26}$$

whereas

$$\frac{d}{dt}\,\mathrm{K.E.} = \int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{F(-k)}{q}J(k) \tag{27}$$

which is $\int dx\,\mathbf{E}\cdot\mathbf{J}$ for a real plasma. The integrands are equal only for $k = 0$. This cannot be corrected by redefining κ and K because they must be periodic; e.g., we can define $\kappa = K = k$ only in the first zone, while the integrals are over all k.

Although we see that energy is not conserved microscopically, in many simulations the observed macroscopic "total energy" changes by amounts small compared to other energies of importance. When this is so, our results suggest that most of the exchange of energy between fields and particles has taken place at long wavelengths. Since this is where the model most accurately simulates the plasma, a good energy check gives credibility to the simulation.

Through a Lagrangian formulation, Lewis [16] has shown how to change the model so that there will be an exact energy constant (for exact time integration, $\Delta t \to 0$).[6] We can find the modification by examining Eq. (26); if the transformed force is $\mathbf{F} = -i\mathbf{k}S_e(-\mathbf{k})\,\phi(\mathbf{k})$ instead of Eq. (12′) then the integrand is identical to that of Eq. (27). This means that the force is derivable from the potential[7] V

$$\mathbf{F} = -\frac{\partial V}{\partial \mathbf{x}}, \tag{28}$$

$$V = qV_c\sum_{\mathbf{j}} S_e(\mathbf{x_j} - \mathbf{x})\,\phi_{\mathbf{j}}. \tag{29}$$

[6] Note that energy conservation does not imply numerical stability in plasma models.

[7] Note that deriving the force from a potential is not quite sufficient to ensure energy conservation in artificial systems. The potential field depends on the particle positions $\{x_i\}$, i.e., $V = V(x; \{x_i\})$. The system conserves energy, and the energy is

$$\sum\left[\tfrac{1}{2}mv_i^2 + \tfrac{1}{2}V(x = x_i, \{x_{i'}\})\right], \text{ if } (\partial V/\partial x)_{x=x_i} = \sum_{i'}(\partial V/\partial x_i)_{x=x_{i'}}$$

This is true in normal physical situations where, for instance, V is a sum of two-particle interaction potentials which are even functions.

The grid electric field is not used. Lewis's Lagrangian treatment prescribes the form of Poisson's equation also, but we require only that Poisson's equation be symmetric in space in deriving Eqs. (25) and (26).

With this single modification the model is also Hamiltonian. As a result the theoretical description is simpler and formally closer to that of gridless plasmas [2].

However these codes do not conserve momentum, whereas the usual codes do. Furthermore, momentum is still conserved in some numerical methods of integrating the equations of motion, whereas in Lewis's case it may be that energy conservation is less than in the usual models due to the effect of the less smooth forces on the accuracy of the time integration.

The lack of momentum conservation becomes less important for large $N_D \equiv n\lambda_D$, the number of particles per Debye length. For instance the self force gives a slight jiggle in velocity $\Delta v \ll v$ for a thermal particle if $(n\lambda_D)(\lambda_D/\Delta x) \gg 1$. However this condition may be required in all methods in order that fluctuations due to δF have small enough amplitudes to be described by linear theory.

Further study should be made of Lewis's codes.

5. Linear Wave Dispersion and Instabilities

If we use Eq. (12) in Eq. (5) we find for each row the same result

$$\epsilon(k, \omega)\, qS_e(-k)\, E(k) = 0,$$

so that $\epsilon = 0$ is the dispersion relation, where

$$\epsilon(k, \omega) = 1 - S_e^{-1}(-k) \sum_p F_p(k - \tfrac{1}{2}pk_g)\, S_e(-k_p)\, \psi(k_p, \omega).$$

The solutions $\omega(k)$ are (multivalued) periodic functions of k.

The same result may be obtained more directly by eliminating n, F, ρ, and ϕ from Eqs. (4), (12), and (16)–(18) yielding the more useful expression

$$\epsilon(\mathbf{k}, \omega) = 1 + \frac{4\pi i q^2}{K^2} \boldsymbol{\varkappa} \cdot \sum_{\mathbf{p}} | S_e(\mathbf{k}_p)|^2\, \boldsymbol{\psi}(\mathbf{k}_p, \omega),$$

where $n(\mathbf{k}, \omega) = \boldsymbol{\psi}(\mathbf{k}, \omega) \cdot \mathbf{F}(\mathbf{k}, \omega)$. The linear density response function ψ may be found from the relation $\boldsymbol{\psi} = \mathbf{k} \cdot \boldsymbol{\sigma}/\omega q^2$, where $\boldsymbol{\sigma}$ is the gridless real plasma conductivity tensor defined by $\mathbf{J}(\mathbf{k}, \omega) = \boldsymbol{\sigma}(\mathbf{k}, \omega) \cdot \mathbf{E}(\mathbf{k}, \omega)$.

The normal modes are given by a simple equation $\epsilon = 0$ rather than an infinite determinant because the aliases are equivalent for grid quantities. The normal modes are sinusoidal in space for grid quantities, though not for particle quantities due to the alias coupling. In this respect the situation is like that for the vibrations of the atoms in a crystal rather than for wave propagation in a continuum having a periodic nonuniformity [10].

We emphasize that the only approximation is that the linearized plasma response is used; no approximation is made about the smallness of the grid effects.

The function $\epsilon(\mathbf{k}, \omega)$, for grid quantities, plays the usual role of dielectric function in kinetic theory results on fluctuations etc., to be reported in a later paper.

For an unmagnetized electrostatic Vlasov plasma we have

$$\epsilon(\mathbf{k}, \omega) = 1 + \frac{\omega_p^2}{K^2(\mathbf{k})} \sum_{\mathbf{p}}^{n} | S_e(\mathbf{k}_p)|^2 \int \frac{d\mathbf{v}}{\omega + i0 - \mathbf{k}_p \cdot \mathbf{v}} \boldsymbol{\varkappa} \cdot \frac{\partial f_0}{\partial \mathbf{v}}, \qquad \operatorname{Im} \omega \geqslant 0$$

which we will study in some detail for a Maxwellian velocity distribution with no drift. Then

$$\epsilon(\mathbf{k}, \omega) = 1 - \frac{\omega_p^2}{2K^2 v_t^2} \sum_{\mathbf{p}} | S_e |^2 \frac{\boldsymbol{\varkappa} \cdot \mathbf{k}_p}{k_p^2} Z' \left(\frac{\omega}{\sqrt{2}\, | \mathbf{k}_p | \, v_t} \right)$$

where Z is the plasma dispersion function [17].

When $\lambda_D \gtrsim \Delta x$ the principal term is the one whose $\mathbf{k}_p$ is nearest $\mathbf{k}$. The modes are heavily damped when $\mathbf{k}$ differs much from this $\mathbf{k}_p$. In this case we expect no important interaction among the different aliases. In the first zone we would take only the $\mathbf{p} = \mathbf{0}$ term, obtaining the average force $\mathbf{F}_0$ dielectric function ϵ_0 discussed earlier. One could then view the model as approximately a gridless cloud plasma with Coulomb interaction; e.g., for the Maxwellian

$$\epsilon_0 = 1 - \frac{\omega_p^2}{2k^2 v_t^2} | S_0 |^2 Z' \left(\frac{\omega}{\sqrt{2}\, k v_t} \right),$$

with

$$| S_0 |^2 = | S_e |^2 \frac{\mathbf{k} \cdot \boldsymbol{\varkappa}}{K^2}$$

where S_d is the cloud shape to be used in the dispersion relation (called S_e in [1]).

In Fig. 5 are shown solutions of these two dispersion relations for the Maxwellian in one dimension with $S_e = \operatorname{dif}(\frac{1}{2}k\, \Delta x)$ [4]. The difference between $\operatorname{Im} \omega$ in the two cases is too small to be shown on the graph, and $\operatorname{Re} \omega$ differs significantly only where the wave is heavily damped. Thus alias coupling is not very important here, and the averaged force works very well. This conclusion is stronger for CIC–PIC.[8]

[8] Some of these remarks may need qualification before application to models in which Landau damping and phase mixing of short wavelengths are inhibited, e.g., when all spatial variation is perpendicular to a strong steady magnetic field.

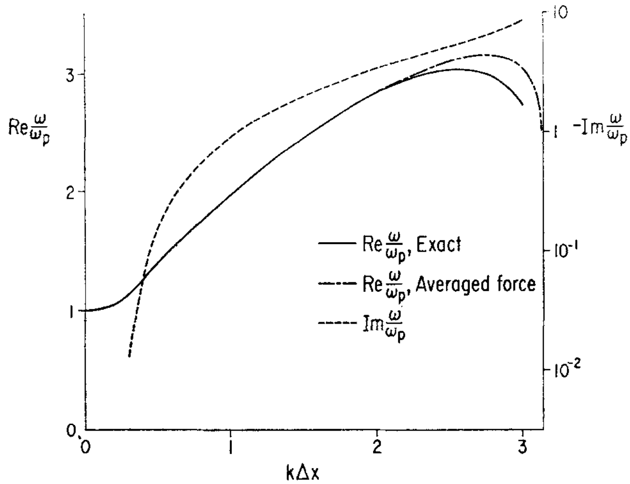

FIG. 5. Solutions of the exact and average-force dispersion relations for a Maxwellian velocity distribution with $\lambda_D = \Delta x$ and NGP interpolation [5].

An interesting qualitative difference introduced by the alias coupling is that for half the aliases $\mathbf{k}_p$ has the opposite direction to $\boldsymbol{\varkappa}$ so that the factor $\boldsymbol{\varkappa} \cdot \mathbf{k}_p/k_p^2$ has the wrong sign. For small $k\Delta x$ this can make $\omega \operatorname{Im} \epsilon$ negative, while $\omega\partial \operatorname{Re} \epsilon/\partial\omega$ remains positive, leading to an instability. In the jargon of real plasmas, the wave has positive energy and experiences negative absorption. The growth rate was negligible in Fig. 5 but becomes significant when $\lambda_D/\Delta x$ is decreased, as we see in Fig. 6 for $\lambda_D = 0.1\, \Delta x\, (2\pi v_t/\Delta x \sim \omega_p)$. The averaged force description

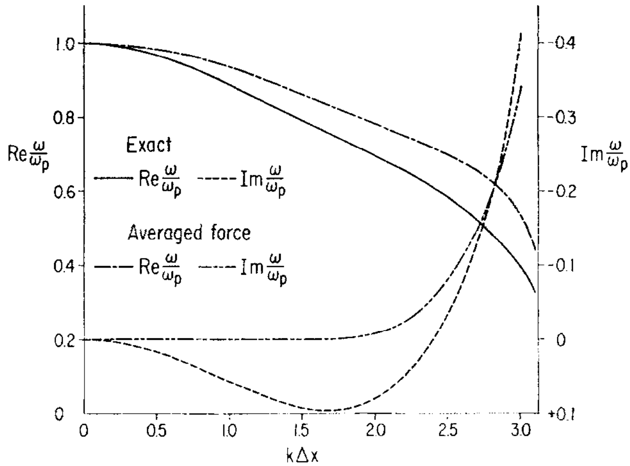

FIG. 6. Solutions of the exact and average-force dispersion relations with $\lambda_D = 0.1\, \Delta x$.

is not very good now. The maximum growth rate is about $0.1\omega_p$. If we go to CIC–PIC the alias coupling is weaker and the maximum growth rate is about $0.014\omega_p$.

We have not yet studied this instability experimentally. There would probably be some difficulty in doing so without a very large number of particles to ensure that the linear approximation is not violated by too-large fluctuations and grid noise forces or that the instability is not damped by collisions. One wonders what an instability looks like in a plasma which is already Maxwellian. Perhaps it just gives enhanced fluctuations. These might cause a gradual heating of the plasma. This is not forbidden since the codes are not energy conserving. In the energy conserving codes the destabilizing factor $\kappa \cdot \mathbf{k}_p/\mathbf{k}_p^2$ is absent, so that there is no grid-induced instability unless the plasma is drifting through the grid.

6. Conclusions

We have begun a mathematical description of many-particle simulation codes to supplement the present heuristic and pragmatic experimental criteria on which algorithm design has been based. This paper deals primarily with the spatial grid and its influence on plasma behavior. Applications are made to the question of energy conservation and to linear plasma oscillations. Here one sees how and when plasma properties, especially the lack of response to short-wavelength or high-frequency forces, help overcome the apparent inaccuracies of the algorithms to give model behavior which is at least qualitatively like that of real plasma. Our approach is applicable to other gridded models, e.g., in which E is defined on a separate interlaced grid whose points are at the centers of the cells of the grid for ρ and ϕ, or in which the fields are magnetic or electromagnetic. Qualitative features brought out in the general discussion of Section 2 may be expected to persist. While we can now obtain good understanding of the quantitative differences in short-term small amplitude plasma properties due to the simulation model, we cannot at present make much claim to even a good qualitative understanding of the modification of long-time or highly-nonlinear plasma evolution. However, where appropriate theory is available for real plasma, our formalism could be used to apply the theory to the model. Further study of the grid effects will be desirable as more ambitious simulations (e.g., three-dimensional models) force us to use very coarse grids.

APPENDIX. Finite Periodic Systems

Let us see how to adapt the results of this paper to finite periodic systems. In one dimension, for simplicity, let all quantities have period $L = N\Delta x$; i.e., a particle function satisfies $P(x + L) = P(x)$ and a grid function satisfies $G_{j+N} = G_j$. The transforms $P(k)$ and $G(k)$ become sums of δ functions and the inverse transforms are therefore sums also. The coefficients of the δ functions are $2\pi/L$ times what one obtains by integrating or summing the transforms over only one period:

$$P(k) = \int_0^L dx\, P(x)\, e^{-ikx},$$
$$G(k) = \Delta x \sum_{j=0}^{N-1} G_j e^{-ikx_j}, \tag{A.1}$$

with $k = 2\pi n/L$, $n = 0, \pm 1, \pm 2,\ldots$. In terms of the above new $P(k)$ and $G(k)$, the inverse transforms are

$$P(x) = \frac{1}{L} \sum_{n=-\infty}^{\infty} P(k)\, e^{ikx},$$
$$G_j = \frac{1}{L} \sum_{n=0}^{N-1} G(k)\, e^{ikx_j}. \tag{A.2}$$

The first is of course the conventional Fourier series and the second is the finite discrete Fourier transform which is performed by the so-called fast Fourier transform algorithm [14].

In summary the expressions for $P(k)$ and $G(k)$ differ from the infinite case only in the limits and in that they are evaluated only for $k = 2\pi n/L$. The k integrals become sums according to the rule

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \rightarrow \frac{1}{L} \sum_{n=-\infty}^{\infty}, \tag{A.3a}$$

$$\int_g \frac{dk}{2\pi} \rightarrow \frac{1}{L} \sum_{n=0}^{N-1}. \tag{A.3b}$$

The periodicity in k of $G(k)$ becomes a periodicity in n of length N.

As an example, let us look at field energy fluctuations in an energy-conserving code. It can be shown that the energy density spatial fluctuation spectrum, for a Maxwellian velocity distribution not drifting through the grid, is formally identical to the gridless result

$$\left(\frac{1}{2}\rho\phi\right)_k = \frac{\theta}{2}\left(1 - \frac{1}{\epsilon(k, 0)}\right). \tag{A.4}$$

This is normalized so that the average energy density is

$$\left\langle \frac{1}{2} \rho_j \phi_j \right\rangle = \int_g \frac{dk}{2\pi} \left(\frac{1}{2} \rho \phi \right)_k .$$

The average total field energy in the system is then

$$\Delta x \sum_N \langle \tfrac{1}{2} \rho_j \phi_j \rangle = \sum_{n=0}^{N-1} (\tfrac{1}{2} \rho \phi)_k$$

according to our rule (A.3b). Thus (A.4) gives the average field energy per mode. (If the length of the system is doubled, the number of modes is also doubled, so that the average total field energy is doubled, as it should be.)

Acknowledgments

This work was supported in part by the United States Atomic Energy Commission, Contract AT-(04-3)-34 (Proj. 128). It arose out of an earlier collaboration with C. K. Birdsall and has benefitted greatly from his interest since. A few of the ideas presented here evolved elsewhere independently, or in conversations with the author, over several years; while it is difficult to assign individual credit, the author would like to acknowledge helpful conversations with J. P. Boris, J. M. Dawson, C. F. McKee, and H. Okuda.

References

1. C. K. Birdsall *et al.*, *Proc. Amer. Phys. Soc. Topical Conf. Numerical Simulation of Plasma*, paper D2, Los Alamos Rep. LA-3990, Sept. 1968; J. M. Dawson *et al.*, *ibid.*, paper A1 (abstracts in *Bull. Amer. Phys. Soc.* **13** (1968), 1744, 1747).
2. A. B. Langdon and C. K. Birdsall, *Phys. Fluids* **13**, 2115 (1970).
3. H. Okuda and C. K. Birdsall, *Phys. Fluids* **13**, 2123 (1970).
4. R. W. Hockney, *Phys. Fluids* **9** (1966), 1826.
5. O. Buneman, *J. Comput. Phys.* **1** (1967), 517.
6. C. K. Birdsall and D. Fuss, *Proc. Amer. Phys. Soc. Topical Conf. Numerical Simulation of Plasma*, paper D1 Los Alamos Rep. LA-3990, Sept. 1968; *J. Comput. Phys.* **3**, 494 (1969).
7. R. L. Morse and C. W. Nielson, *Proc. Amer. Phys. Soc. Topical Conf. Numerical Simulation of Plasma*, paper A4 Los Alamos Rep. LA-3990, Sept. 1968.
8. K. V. Roberts and N. O. Weiss, *Math. Comput.* **20** (1966), 272.
9. R. B. Blackman and J. W. Tukey, "The Measurement of Power Spectra." Dover, New York, 1958.
10. L. Brillouin, "Wave Propagation in Periodic Structures." Dover, New York, 1953.
11. R. W. Hamming, "Numerical Methods for Scientists and Engineers," part III. McGraw-Hill, New York, 1962.
12. M. J. Lighthill, "Fourier Analysis and Generalized Functions." Cambridge Univ. Press, London, 1962.
13. R. C. Harding and H. L. Berk, *Bull. Amer. Phys. Soc.* **14** (1969), 1024.

14. W. M. Gentleman and G. Sande, in American Federation of Information Processing Societies, *1966 Fall Joint Computer Conference*, Vol. 29, p. 563. Spartan Books, New York, 1966.
15. L. Brand, "Vector Analysis." Wiley, New York, 1957.
16. H. R. Lewis, *J. Comp. Phys.* **6** (1970), 136–141.
17. B. D. Fried and S. D. Conte, "The Plasma Dispersion Function." Academic, New York, 1961.