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Energy-Conserving Numerical Approximations for Vlasov Plasmas*

The problem of obtaining useful numerical descriptions of the behavior of high-temperature plasmas is currently of intense interest, especially in the field of controlled thermonuclear fusion research.[1] For sufficiently high temperatures it is appropriate to use the Vlasov approximation, in which the particles can be represented by time-dependent distribution functions, one for each particle species. These distribution functions are functions of position and velocity in a single-particle phase space, and they satisfy collisionless Boltzmann equations in which the electromagnetic field due to the particles is approximated by the so-called *self-consistent* field. A completely equivalent way to represent the particle motion is to specify the trajectories of the points in the single-particle phase space for each species. The trajectories, which are the characteristic curves of the Boltzmann equations, are the solutions of the single-particle equations of motion that are satisfied for each particle when the electromagnetic field due to the particles is replaced by the "self-consistent" field. This latter method of describing the particle motion, that of specifying particle trajectories instead of distribution functions, is being used with increasing favor.

The purpose of this note is to present a unified and general method for deriving numerical approximation schemes within the framework of the trajectory approach. The method is based on the exact Lagrangian that was given independently by Low[2] and Sturrock.[2] A unique system of *ordinary* differential equations is implied by the Lagrangian formulation for any form of approximate representation of the potentials and particle trajectories in terms of time-dependent parameters. A general energy theorem is valid for these systems of ordinary differential equations. For energy-conserving physical situations, situations for which there are no time-dependent external sources, the energy theorem guarantees that classes of energy-conserving approximations can be constructed. This is an important consequence of the Lagrangian formulation. Some simple special cases of the Lagrangian formulation are closely related to other work in this field,

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[1] For a recent survey of activity in this area, see Los Alamos Scientific Laboratory Report LA-3990: "Proceedings of the APS Topical Conference on Numerical Simulation of Plasma, September 18–20, 1968."

[2] F. E. Low, *Proc. Roy. Soc. (London)* **A248**, 282 (1958); P. A. Sturrock, *Ann. Phys. (New York)* **4**, 306 (1958).

for example, to numerical simulation of Vlasov plasmas by a finite number of particles with the particle-in-cell (PIC) method or the cloud-in-cell (CIC) method. The burden of this paper is to explain how Hamilton's variational principle can be used to replace the integro-partial differential equations that describe Vlasov plasmas by an approximating system of ordinary differential equations in time. We do not propose difference schemes for solving these ordinary differential equations numerically.

We begin by describing the physical problem and outlining the application of Hamilton's principle to the derivation of approximation schemes.[3] Then the energy theorem is discussed. Finally, an example appropriate to numerical simulation by a finite number of particles is presented.

We consider a plasma consisting of N species of particles and denote the mass and charge of particles of species i by M_i and Q_i, respectively. The initial distribution function for particles of species i in the phase space of position $\mathbf{r}$ and velocity $\mathbf{v}$ is denoted by $f_i(\mathbf{r}, \mathbf{v}, 0)$. The particles move in the "self-consistent" electromagnetic field and, possibly, in generalized nonelectromagnetic potentials that we denote by $U_i(\mathbf{r}, \mathbf{v}, t)$ for species i. We also allow the possibility of external (prescribed) charge and current densities $\rho_0(\mathbf{r}, t)$ and $\mathbf{j}_0(\mathbf{r}, t)$. The Lagrangian for this system[2,3] is expressed in terms of the electromagnetic scalar and vector potentials $\phi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$, and in terms of functions $\mathbf{R}_i(\mathbf{r}', \mathbf{v}', t)$ that describe the particle trajectories as functions of time and the initial conditions. The vectors $\mathbf{r} = \mathbf{R}_i(\mathbf{r}', \mathbf{v}', t)$ and $\mathbf{v} = \dot{\mathbf{R}}_i(\mathbf{r}', \mathbf{v}', t)$, where the dot denotes differentiation with respect to t, are the position and velocity vectors, respectively, of that particle of species i whose initial position and velocity vectors were $\mathbf{r}'$ and $\mathbf{v}'$. For simplicity of notation, the arguments of $\mathbf{R}_i(\mathbf{r}', \mathbf{v}', t)$ will be omitted in the following formulas. The Lagrangian is[4]

$$L = \sum_{k=1}^{N} \int d^3\mathbf{r}'\, d^3\mathbf{v}' f_k(\mathbf{r}', \mathbf{v}', 0) \left\{ \frac{1}{2} M_k \dot{\mathbf{R}}_k^2 - U_k(\mathbf{R}_k, \dot{\mathbf{R}}_k, t) - Q_k \phi(\mathbf{R}_k, t) + \frac{1}{c} Q_k \dot{\mathbf{R}}_k \cdot \mathbf{A}(\mathbf{R}_k, t) \right\} + \int_V d^3\mathbf{r} \left\{ \frac{1}{8\pi} [\mathbf{E}^2(\mathbf{r}, t) - \mathbf{B}^2(\mathbf{r}, t)] - \rho_0(\mathbf{r}, t)\, \phi(\mathbf{r}, t) + \frac{1}{c} \mathbf{j}_0(\mathbf{r}, t) \cdot \mathbf{A}(\mathbf{r}, t) \right\}, \tag{1}$$

[3] Details will appear in a chapter of a forthcoming book: B. Alder, S. Fernbach, and M. Rotenberg, eds., "Methods in Computational Physics," Academic Press, New York, Vol. 9. Some details can be found in H. Ralph Lewis, Los Alamos Scientific Laboratory Report LA-3803 (1967).

[4] The Lagrangian formulation for the electromagnetic field can be extended to include any of a certain class of material media that exhibit nonlinear polarizability and magnetizability. (See Footnote 3.) This extension is not included here, although there may be useful applications to the numerical study of nonlinear optical phenomena.

where **E** and **B** are to be expressed in terms of ϕ and **A** by

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\dot{\mathbf{A}} \qquad \text{and} \qquad \mathbf{B} = \nabla \times \mathbf{A}, \tag{2}$$

and where appropriate boundary conditions have been specified on the boundary of the volume V. The equations of motion for the particles and the Maxwell equations for the fields can be obtained with this Lagrangian via Hamilton's variational principle in which the functions to be varied independently are ϕ, **A**, and the $\mathbf{R}_k$:

$$\delta \int_{t_2}^{t_2} L\, dt = 0. \tag{3}$$

The initial and boundary conditions on the variations are discussed in the reference given in Footnote 3.

The first step in using the variational principle to obtain a system of ordinary differential equations whose solutions will provide approximations to ϕ, **A**, and the $\mathbf{R}_k$ is to choose a specific type of approximation of those functions in terms of time-dependent parameters whose time dependence is to be found. That is, we choose functions Φ, $\mathcal{A}$, and $\mathcal{R}_k$ whose dependence on their arguments is specified, and demand that ϕ, **A**, and $\mathbf{R}_k$ be approximated as

$$\phi(\mathbf{r}, t) \cong \Phi[\mathbf{r}, t, \{\alpha_n(t)\}], \qquad \mathbf{A}(\mathbf{r}, t) \cong \mathcal{A}[\mathbf{r}, t, \{\beta_m(t)\}],$$

and

$$\mathbf{R}_k(\mathbf{r}', \mathbf{v}', t) \cong \mathcal{R}_k[\mathbf{r}', \mathbf{v}', t, \{\gamma_{kl}(t)\}], \tag{4}$$

where the sets of functions $\alpha_n(t)$, $\beta_m(t)$, and $\gamma_{kl}(t)$ are to be determined. Equations for these functions shall be obtained through use of the variational principle. The functions Φ, $\mathcal{A}$ and $\mathcal{R}_k$, and the initial conditions on the $\alpha_n(t)$, $\beta_m(t)$, and $\gamma_{kl}(t)$, must be chosen to satisfy the boundary and initial conditions on the potentials and trajectories. The simplest *example* is to choose Φ, $\mathcal{A}$, and the $\mathcal{R}_k$ without explicit time dependence as linear combinations of a finite number of linearly independent basis functions with time-dependent coefficients:

$$\Phi[\mathbf{r}, t, \{\alpha_n(t)\}] = \sum_{n=1}^{N_1} \alpha_n(t)\, \Phi_n(\mathbf{r}), \qquad \mathcal{A}[\mathbf{r}, t, \{\beta_m(t)\}] = \sum_{m=1}^{N_2} \beta_m(t) \mathcal{A}_m(\mathbf{r}),$$

$$\mathcal{R}_k[\mathbf{r}', \mathbf{v}', t, \{\gamma_{kl}(t)\}] = \sum_{l=1}^{N_3} \gamma_{kl}(t)\, \mathcal{R}_{kl}(\mathbf{r}', \mathbf{v}'). \tag{5}$$

If the basis functions Φ_n , $\mathcal{A}_m$, and $\mathcal{R}_{kl}$ were infinite in number and formed complete sets of functions, then no approximation would be involved. The approximation enters by not choosing complete sets of functions.

Having decided on some specific functions Φ, $\mathcal{A}$, and $\mathcal{R}_k$, we substitute Eqs. (4) into Eq. (1) to obtain a new Lagrangian which we also denote by L. The new Lagrangian is a function of generalized coordinates α_n, β_m, and γ_{kl}, and generalized velocities $\dot{\beta}_m$ and $\dot{\gamma}_{kl}$. We demand exact satisfaction of Hamilton's principle, Eq. (3), for arbitrary variations of the α_n, β_m, and γ_{kl}. This is the same as demanding exact satisfaction for arbitrary variations of ϕ, $\mathbf{A}$, and the $\mathbf{R}_k$ within the *restricted* class of functions defined by Eqs. (4). The system of ordinary differential equations for the time-dependent parameters are the Euler-Lagrange equations associated with the new Lagrangian:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\gamma}_{kl}} - \frac{\partial L}{\partial \gamma_{kl}} = 0, \qquad \frac{d}{dt}\frac{\partial L}{\partial \dot{\beta}_m} - \frac{\partial L}{\partial \beta_m} = 0, \qquad \frac{\partial L}{\partial \alpha_n} = 0. \tag{6}$$

The energy theorem can be demonstrated by going to a Hamiltonian formulation. We define generalized momenta σ_m and τ_{kl} by

$$\sigma_m = \frac{\partial L}{\partial \dot{\beta}_m} \qquad \text{and} \qquad \tau_k = \frac{\partial L}{\partial \dot{\gamma}_{kl}}. \tag{7}$$

In terms of them we define a Hamiltonian function H by

$$H = \sum_m \dot{\beta}_m \sigma_m + \sum_{k,l} \dot{\gamma}_{kl} \tau_{kl} - L, \tag{8}$$

where H is to be considered a function of the α_n, β_m, γ_{kl}, σ_m, τ_{kl}, and, possibly, t. By using Eqs. (6), (7), and (8), it is easy to verify the following equations:

$$\dot{\gamma}_{kl} = \frac{\partial H}{\partial \tau_{kl}}, \qquad \dot{\tau}_{kl} = -\frac{\partial H}{\partial \gamma_{kl}}, \qquad \dot{\beta}_m = \frac{\partial H}{\partial \sigma_m}, \qquad \dot{\sigma}_m = -\frac{\partial H}{\partial \beta_m}, \qquad \frac{\partial H}{\partial \alpha_n} = 0. \tag{9}$$

These equations imply

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}. \tag{10}$$

Equation (10) is a statement of the energy theorem. It applies for *arbitrary* choice of the functions Φ, $\mathcal{A}$, and $\mathcal{R}_k$ in Eqs. (4). An important special case is that in which none of the functions Φ, $\mathcal{A}$, and $\mathcal{R}_k$ have explicit time dependence. If, in addition, ρ_0, $\mathbf{j}_0$, and U_k are not explicitly time-dependent, so that the physical system is energy-conserving, then Eq. (10) reduces to

$$\frac{dH}{dt} = 0, \tag{11}$$

which shows that the approximation scheme, like the physical system, is energy-conserving.

This formalism is being applied to a numerical investigation of the cold two-

stream instability with a continuum of particles,[5] and there are many other possible applications. As an illustration, we consider here the numerical simulation of plasmas by a finite number of particles. In that case, Eqs. (6) or (9) yield the equations of motion for each particle and a definite approximation scheme for the electromagnetic potentials. To be specific, we specialize to the simple case of one spatial dimension, x, with periodic boundary conditions at $x = 0$ and $x = \lambda$, and we consider a single species of particles in the presence of a fixed, uniform background charge density ρ_0. Because there is only one dimension, we can set the vector potential identically equal to zero. The initial distribution function is a sum of δ-functions,

$$f(x, v, 0) = \sum_i \delta(x - x_i)\, \delta(v - v_i), \tag{12}$$

where x_i and v_i are the initial position and velocity of the i-th particle, respectively. There is only one function $\mathbf{R}_k$. We denote its x component by $\chi(x', v', t)$, and choose representations of χ and ϕ in the form of Eqs. (5):

$$\phi(x, t) = \sum_{n=1}^{N_1} \alpha_n(t)\, \Phi_n(x), \qquad \chi(x', v', t) = \sum_{l=1}^{N_3} \gamma_l(t)\, X_l(x', v'). \tag{13}$$

The $\Phi_n(x)$ must satisfy the boundary conditions at $x = 0$ and $x = \lambda$. Because of the singular initial distribution function, a convenient set of X_l are

$$X_l(x', v') = \begin{cases} 1, & \text{if } x' = x_l\,,\ v' = v_l \\ 0, & \text{otherwise,} \end{cases} \tag{14}$$

in which case the initial conditions on the $\gamma_l(t)$ are

$$\gamma_l(0) = x_l\,, \qquad \dot{\gamma}_l(0) = v_l\,. \tag{15}$$

Clearly, $\gamma_l(t)$ is the position of the l-th particle at time t.

The Euler–Lagrange equations for γ_l and α_n are

$$M\ddot{\gamma}_l = -Q \sum_i \alpha_i(t)\, \Phi_i'[\gamma_l(t)], \tag{16a}$$

and

$$\frac{1}{4\pi} \sum_{i=1}^{N_1} \alpha_i(t) \int_0^\lambda dx\, \Phi_i'(x)\, \Phi_n'(x) = \rho_0 \int_0^\lambda dx\, \Phi_n(x) + Q \sum_{l=1}^{N_3} \Phi_n[\gamma_l(t)], \tag{16b}$$

where $\Phi_i'(x) \equiv (d/dx)\, \Phi_i(x)$. Equation (16a) is the equation of motion for the l-th particle, and Eq. (16b) is a definite approximation scheme for solving Poisson's equation. The equations are energy-conserving.

[5] H. Ralph Lewis and K. J. Melendez, paper B1 of the reference in Footnote 1.

Simple special cases of Eqs. (16), and of their analogues in two and three dimensions, are related to procedures that have been used in numerical simulation work.[6] Our Lagrangian approach provides energy-conserving versions of those procedures, as well as a wide variety of energy-conserving generalizations. As an example that provides an energy-conserving version of the one-dimensional particle-in-cell (PIC) method, let us take a piecewise linear approximation for the scalar potential. It is then convenient to choose the $\Phi_n(x)$ to be the following local basis for periodic, piecewise-linear functions:

$$\Phi_n(x) = \begin{cases} \dfrac{1}{\Delta}[x - (n-1)\Delta], & \text{if } (n-1)\Delta \leqslant x \leqslant n\Delta \\ \dfrac{1}{\Delta}[(n+1)\Delta - x], & \text{if } n\Delta \leqslant x \leqslant (n+1)\Delta \\ 0, & \text{otherwise} \end{cases} \tag{17}$$

where $\Delta = \lambda/(N_1 + 1)$. With this set of basis functions, $\alpha_n(t)$ is the value of the potential at $x = n\Delta$. The integrals occurring in Eq. (16b) are:

$$\int_0^\lambda dx\, \Phi_n(x) = \Delta, \tag{18a}$$

$$\int_0^\lambda dx\, \Phi_i'(x)\, \Phi_n'(x) = \begin{cases} \dfrac{2}{\Delta}, & \text{if } i = n \\ -\dfrac{1}{\Delta}, & \text{if } |i - n| = 1 \\ 0, & \text{otherwise} \end{cases} \tag{18b}$$

The matrix defined by Eq. (18b) represents the usual central difference approximation for the second derivative. As a consequence of these formulas, Eq. (16b) is identical to the "area-weighting" approximation for Poisson's equation.[6,7]

Further examples will be presented in a later publication.[3]

In conclusion, we express the expectation that the Lagrangian approach to deriving numerical approximation schemes for Vlasov plasmas will be of practical advantage in solving complicated problems.

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[6] See, for example, the reference in Footnote 1. In particular, paper A4 by R. L. Morse and C. W. Nielson, and paper D1 by C. K. Birdsall and D. Fuss.

[7] We acknowledge helpful discussions with C. W. Nielson on this point.