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Charged Particle Mass and Energy Transport in a Thermonuclear Plasma*

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Transport equations for the mass and energy carried by charged particles in a thermonuclear plasma are derived and solved using S_n techniques. Results are in good agreement with an analytic solution to a representative test problem.

I. INTRODUCTION

Growing interest in laser fusion experiments has encouraged the development of computer codes capable of simulating the thermonuclear burn characteristics of the experiments [1]. These computer simulations aid in the design of meaningful experiments and the understanding of their results [2]. Since charged particles borne by thermonuclear reactions within a burning DT sphere carry a significant fraction of the reactions' energy, it is important to accurately simulate how and where the charged particles deposit their energy. Although local deposition has been used in the past [1], recent research has shown this to be an inadequate approximation [3]. In this paper, we show how S_n transport theory can be used to simulate charged particle mass and energy deposition in a thermonuclear plasma.

It is a relatively simple matter to write down the charged particle transport equation and work out a set of difference equations from it; however, it is more difficult to derive a set of difference equations that explicitly conserve mass and energy. In this paper, we illustrate how the conservation requirements can be used to arrive at a set of difference equations that are both mathematically and physically meaningful.

II. DERIVATION OF THE CHARGED PARTICLE TRANSPORT EQUATIONS

To determine the charged particles' mass and energy deposition, it is necessary to solve both the mass and energy transport equations. In this section, we present

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a derivation of those two equations based on conservation arguments analogous to those used in neutron transport theory [4, 5]. Let the charged particle be located at position $\mathbf{r}(t)$ with velocity $\mathbf{v}(t)$ relative to the plasma at time t. The particle experiences an acceleration of the form $\mathbf{a}(\mathbf{r}, \mathbf{v}, t)$ due to its Coulomb interaction with the plasma. Let $N(\mathbf{r}, \mathbf{v}, t)\, d\mathbf{r}\, d\mathbf{v}$ be the number of charged particles with position coordinates between $\mathbf{r}$ and $\mathbf{r} + d\mathbf{r}$, and velocities between $\mathbf{v}$ and $\mathbf{v} + d\mathbf{v}$ at time t. Then the change in the number of charged particles in phase space between times t and $t + \Delta t$ for small Δt is given by

$$N(\mathbf{r} + \Delta\mathbf{r}, \mathbf{v} + \Delta\mathbf{v}, t + \Delta t)\, d\mathbf{r}'\, d\mathbf{v}' - N(\mathbf{r}, \mathbf{v}, t)\, d\mathbf{r}\, d\mathbf{v}, \tag{1}$$

where $d\mathbf{r}'$ and $d\mathbf{v}'$ are volume elements in position and velocity space and are evaluated at $t + \Delta t$. Here,

$$\Delta\mathbf{r} \equiv \mathbf{v}\,\Delta t, \qquad \Delta\mathbf{v} \equiv \mathbf{a}\,\Delta t, \qquad \text{and}$$
$$N(\mathbf{r} + \Delta\mathbf{r}, \mathbf{v} + \Delta\mathbf{v}, t + \Delta t)\, d\mathbf{r}'\, d\mathbf{v}' \equiv N(\mathbf{r}', \mathbf{v}', t + \Delta t)\, d\mathbf{r}'\, d\mathbf{v}'.$$

For small Δt, $d\mathbf{r}'$ and $d\mathbf{v}'$ become

$$d\mathbf{r} = d\mathbf{r}(\partial(\mathbf{r} + \mathbf{v}\, dt)/\partial(\mathbf{r})) \cong d\mathbf{r}(1 + \nabla_r \cdot \mathbf{v}\, dt) = d\mathbf{r}, \tag{2}$$
$$d\mathbf{v}' = d\mathbf{v}(\partial(\mathbf{v} + \mathbf{a}\, dt)/\partial(\mathbf{v})) \cong d\mathbf{v}(1 + \nabla_v \cdot \mathbf{a}\, dt), \tag{3}$$

where

$$\partial(\mathbf{r} + \mathbf{v}\, dt)/\partial(\mathbf{r})$$

represents the Jacobian of the transformation from $\mathbf{r}(t)$ to $\mathbf{r}(t + \Delta t)$. In Eq. (2), $\nabla_r \cdot \mathbf{v} = 0$ because $\mathbf{v}$ and $\mathbf{r}$ are independent variables [5]. Using Eqs. (2) and (3), Eq. (1) becomes

$$\begin{aligned}\{N(\mathbf{r} + \Delta\mathbf{r}, \mathbf{v} + \Delta\mathbf{v}, t + \Delta t)[1 + \nabla_v \cdot \mathbf{a}\, dt] - N(\mathbf{r}, \mathbf{v}, t)\}\, d\mathbf{r}\, d\mathbf{v} \\ = \{\partial N/\partial t + \mathbf{v} \cdot \nabla_r N + \mathbf{a} \cdot \nabla_v N + N\nabla_v \cdot \mathbf{a} + O(dt) + O(dr) + O(dv)\}\, d\mathbf{r}\, d\mathbf{v}\, dt,\end{aligned} \tag{4}$$

where we have used a Taylor expansion of $N(\mathbf{r} + \Delta\mathbf{r}, \mathbf{v} + \Delta\mathbf{v}, t + \Delta t)$ for small Δt. Dropping first-order terms, Eq. (4) becomes

$$\begin{aligned}\{N(\mathbf{r} + \Delta\mathbf{r}, \mathbf{v} + \Delta\mathbf{v}, t + \Delta t)(1 + \nabla_v \cdot \mathbf{a}\, dt) - N(\mathbf{r}, \mathbf{v}, t)\}\, d\mathbf{r}\, d\mathbf{v} \\ = \{(\partial N/\partial t) + \mathbf{v} \cdot \nabla_r N + \mathbf{a} \cdot \nabla_v N + N\nabla_v \cdot \mathbf{a}\}\, d\mathbf{r}\, d\mathbf{v}\, dt.\end{aligned} \tag{5}$$

A statement of mass conservation is that the change in the number of charged particles (Eq. (1)) in an element of phase space ($d\mathbf{r}\, d\mathbf{v}\, dt$) is equal to the sum of any sources of particles into that element minus the losses due to scattering. Thus, we may write the conservation statement as

$$N(\mathbf{r} + \Delta\mathbf{r}, \mathbf{v} + \Delta\mathbf{v}, t + \Delta t)\, d\mathbf{r}'\, d\mathbf{v}' - N(\mathbf{r}, \mathbf{v}, t)\, d\mathbf{r}\, d\mathbf{v} = S_M\, d\mathbf{r}\, d\mathbf{v}\, \Delta t - v\sigma N\, d\mathbf{r}\, d\mathbf{v}\, \Delta t, \tag{6}$$

where $S_M\, d\mathbf{r}\, d\mathbf{v}\, \Delta t$ represents the total source introduced into the element of phase space, $v = |\mathbf{v}|$, and σ is the scattering cross section. Using Eq. (5) in (6), dividing both sides by $d\mathbf{r}\, d\mathbf{v}\, \Delta t$, and taking the limit $\Delta t \to 0$, we have

$$(\partial N/\partial t) + \mathbf{v} \cdot \nabla_r N + \mathbf{a} \cdot \nabla_v N = S_M - v\sigma N - N\nabla_v \cdot \mathbf{a}, \tag{7}$$

which is the transport equation for charged particles subjected to an acceleration $\mathbf{a}(\mathbf{r}, \mathbf{v}, t)$ in a stationary plasma. Equation (7) may be written in the conservative form as

$$(\partial N/\partial t) + \nabla_r \cdot (\mathbf{v}N) + \nabla_v \cdot (\mathbf{a}N) = S_M - v\sigma N, \tag{8}$$

since $\nabla_r \cdot \mathbf{v} = 0$. The term $\mathbf{a} \cdot \nabla_v N$ in Eq. (7) corresponds to "streaming" of particles in velocity space, playing the same role as the $\mathbf{v} \cdot \nabla_r N$ term in position space. The term $N\nabla_v \cdot \mathbf{a}$ represents a sink in the element of phase space due to the deceleration force acting on the charged particles. For the limiting case $\mathbf{a} \to 0$, Eqs. (7) and (8) reduce to the familiar form of the neutron transport equation.

The transport equation for the energy carried by charged particles is derived through an application of the first law of thermodynamics. Let $\psi(\mathbf{r}, \mathbf{v}, t)\, d\mathbf{r}\, d\mathbf{v}$ represent the kinetic energy carried by charged particles with position coordinates between $\mathbf{r}$ and $\mathbf{r} + d\mathbf{r}$, and velocities between $\mathbf{v}$ and $\mathbf{v} + d\mathbf{v}$ at time t. The energy deposited by the field of charged particles to the plasma as heat due to the coulomb drag is given by

$$2\mathbf{v} \cdot \mathbf{a}\, \Delta t\, \psi/v^2.$$

The statement of energy conservation is written

$$\begin{aligned} &\psi(\mathbf{r} + \Delta\mathbf{r}, \mathbf{v} + \Delta\mathbf{v}, t + \Delta t)\, d\mathbf{r}'\, d\mathbf{v}' - \psi(\mathbf{r}, \mathbf{v}, t)\, d\mathbf{r}\, d\mathbf{v} \\ &\qquad - (2\mathbf{v} \cdot \mathbf{a}\psi/v^2)\, d\mathbf{r}\, d\mathbf{v}\, \Delta t = (S_E - v\sigma\psi)\, d\mathbf{r}\, d\mathbf{v}\, \Delta t, \end{aligned} \tag{9}$$

where the energy source S_E is given by $S_E \equiv \frac{1}{2}Mv^2 S_M$. Equation (9) simply states that the increase in kinetic energy carried by the field of charged particles plus the heat energy deposited to the plasma (note that $\mathbf{v} \cdot \mathbf{a} < 0$) equals the source of energy minus scattering losses. The derivation of the transport equation proceeds as before, resulting in the expression

$$(\partial\psi/\partial t) + \mathbf{v} \cdot \nabla_r \psi + \mathbf{a} \cdot \nabla_v \psi = S_E - v\sigma\psi - \psi\nabla_v \cdot \mathbf{a} + (2/v^2)\, \mathbf{v} \cdot \mathbf{a}\psi. \tag{10}$$

Equation (10) may be written in the conservative form

$$(\partial\psi/\partial t) + \nabla_r \cdot (\mathbf{v}\psi) + \nabla_v \cdot (\mathbf{a}\psi) = S_E - v\sigma\psi + (2/v^2)\, \mathbf{v} \cdot \mathbf{a}\psi. \tag{11}$$

The term $(2/v^2)\, \mathbf{v} \cdot \mathbf{a}\psi$ acts as a "sink" in the transport equation and explicitly accounts for the energy lost by the field of charged particles due to the coulomb drag. The fact that this term does not occur in Eq. (8) is indicative of the fact that mass is conserved in this problem, whereas kinetic energy is not conserved.

III. Reduction to a Spherically Symmetric, One-Dimensional Coordinate System

Let the charged particle's location $\mathbf{r}$ be expressed in terms of the coordinates (r, μ), where $\mu = \mathbf{r} \cdot \mathbf{v}/rv$. Assuming spherical symmetry we have

$$\mathbf{a} = a(\mathbf{v}/v). \tag{12}$$

The number density of charged particles $N(\mathbf{r}, \mathbf{v}, t)$ may be written $N(r, v, \mu, t)$, and the velocity $\mathbf{v}$ may be expressed in terms of the $\mathbf{r}$ and $\boldsymbol{\theta}$ directions by using the relations $v_r = v \cos\theta$, and $v_\theta = v \sin\theta$, where $\mu = \cos\theta$.

With these definitions, the directional derivative $\mathbf{v} \cdot \nabla_r$ becomes

$$\mathbf{v} \cdot \nabla_r = \left(v_r \frac{\partial}{\partial r} + \frac{v_\theta}{r} \frac{\partial}{\partial \theta}\right) = \frac{v\mu}{r^2} \frac{\partial}{\partial r} r^2 + \frac{v}{r} \frac{\partial}{\partial \mu} (1 - \mu^2). \tag{13}$$

The term $\mathbf{a} \cdot \nabla_v$ is given by

$$\mathbf{a} \cdot \nabla_v = a \left(\frac{\partial}{\partial v} + \frac{\mu}{v} \frac{\partial}{\partial \mu}\right) - a \frac{\mu}{v} \frac{\partial}{\partial \mu} = \frac{a}{v^2} \frac{\partial}{\partial v} v^2 - 2 \frac{a}{v} = 0. \tag{14}$$

Finally, the term $\nabla_v \cdot \mathbf{a}$ is easily seen to be

$$\nabla_v \cdot \mathbf{a} = (1/v^2)(\partial/\partial v)\, v^2 a. \tag{15}$$

Using these results, the mass transport equation (7) can be written in spherical coordinates as

$$\frac{\partial N}{\partial t} + \frac{\mu v}{r^2} \frac{\partial}{\partial r} (r^2 N) + \frac{v}{r} \frac{\partial}{\partial \mu} [(1 - \mu^2)\, N] + \frac{1}{v^2} \frac{\partial}{\partial v} (a v^2 N) = S_M - v\sigma N. \tag{16}$$

Similarly, the energy transport equation (10) becomes

$$\frac{\partial \psi}{\partial t} + \frac{\mu v}{r^2} \frac{\partial}{\partial r} (r^2 \psi) + \frac{v}{r} \frac{\partial}{\partial \mu} [(1 - \mu^2)\, \psi] + \frac{1}{v^2} \frac{\partial}{\partial v} (a v^2 \psi) = S_E - v\sigma\psi + \frac{2}{v} a\psi. \tag{17}$$

It is customary [4, 5] to express the neutron transport equation in terms of the flux ϕ of neutrons, where $\phi = vN$. Using this relation, the charged particle transport equation (16) becomes

$$\frac{1}{v}\frac{\partial\phi}{\partial t} - \frac{a}{v^2}\phi + \frac{\mu}{r^2}\frac{\partial}{\partial r}(r^2\phi) + \frac{1}{r}\frac{\partial}{\partial\mu}[(1-\mu^2)\phi] + \frac{1}{v^2}\frac{\partial}{\partial v}av\phi = S_M - \sigma\phi. \quad (18)$$

This equation is stated only to illustrate the use of the conservation requirement in a later section. The numerical solution of Eq. (18) for charged particle transport leads to erroneous results, as will be demonstrated later (e.g., Eq. (53)).

IV. Functional Form of the Coulomb Drag

The Coulomb drag term **a** is given by

$$\mathbf{a} = \frac{d\mathbf{v}}{dt} = \frac{1}{M}\frac{dE}{dr}\frac{\mathbf{v}}{v} \quad (19)$$

and $dE/dr < 0$. In a recent paper, Evans [3] summarized the derivation of the functional form of dE/dr and discussed its effect on the energy deposition of a charged particle in a fully ionized plasma. In the following paragraphs, we summarize his results in a form suited to our needs.

The drag experienced by a charged particle moving through a plasma is due to its interaction with both electrons and ions in the plasma. Let Ze and A be the charge and the atomic weight of the particle, let Z_je, A_j, and N_j be the charge, atomic weight, and number density of the jth ionic constituent of the plasma. The drag experienced by the charged particle due to the ionic constituents of the plasma is given by

$$-\langle dE/dr\rangle_i = B_i/E \qquad (\text{MeV/cm}), \quad (20)$$

where

$$B_i = 0.130284AZ^2 \sum_j (Z_j^2/A_j)\, N_jF_j(y_j)\,\Lambda_j\,, \quad (21)$$

with

$$y_j^2 = (A_j/A)(E/kT_i), \quad (22)$$

$$F_j(y_j) = \Phi(y_j) - [1 + (A_j/A)]\, y_j\Phi'(y_j), \quad (23)$$

and Φ is the error function, Φ' its derivative, kT_i the ion temperature (in MeV), and N_j is expressed in units of 10^{24} cm^{-3}. The ion term Λ_j is

$$\begin{aligned} \Lambda_j = \Lambda_{qj} &= \kappa_j{}^I + \tfrac{1}{2}\ln(EkT_e/N_e), \qquad E/E^* > 1 \\ \kappa_j{}^I &= 14.9984 + \ln(A^{1/2}A_j/(A + A_j)) \\ = \Lambda_{cj} &= \Lambda_{qj} + \tfrac{1}{2}\ln(E/E^*), \qquad E/E^* < 1, \end{aligned} \quad (24)$$

where kT_e is the electron temperature in MeV, N_e is the number density of electrons (in 10^{24} cm^{-3}) and $E/E^* = (\lambda\!\!\!^{-}/2L)^2$, where

$$\lambda\!\!\!^{-}/2L = (137/2)\, ZZ_j(C/v) \tag{25}$$

and C is the speed of light.

The drag due to electrons in the plasma is given by

$$-\langle dE/dr\rangle_e = B_e/E, \qquad \text{(MeV/cm)}, \tag{26}$$

where

$$B_e = 239.216 AZ^2 N_e F_e(y_e)\, \Lambda_e \tag{27}$$

with

$$y_e{}^2 = (M_e/M_p)(E/kT_e), \tag{28}$$

$$F_e(y_e) = \Phi(y_e) - [1 + (M_e/AM_p)]\, y_e \Phi'(y_e), \tag{29}$$

where M_p is the mass of a proton and M_e is the mass of an electron. The electron term Λ_e is given by

$$\begin{aligned} \Lambda_e &= \Lambda_{qe} = K^{\Pi} + \ln(kT_e/(N_e)^{1/2}), \qquad kT_e > kT_e{}^*, \qquad K^{\Pi} = 11.4434, \\ &= \Lambda_{ce} = \Lambda_{qe} + \tfrac{1}{2}\ln(kT_e/kT_e{}^*), \qquad kT_e < kT_e{}^*, \end{aligned} \tag{30}$$

where $kT_e{}^* = 3.62822 \times 10^{-5} Z^2$ (MeV).

With the functional form of **a** defined by Eqs. (19)–(30), we now proceed to derive the difference equations from the charged particle transport equations.

V. Derivation of the Difference Equations

Following the standard method [4] for differencing the transport equation, phase space is partitioned by the discrete ordinates $\{r_i\}_{i=1}^{I}$, $\{\mu_m\}_{m=1}^{M}$, $\{t_s\}_{s=1}^{S}$, and $\{v_g\}_{g=1}^{G}$, where $r_i < r_{i+1}$, $\mu_m < \mu_{m+1}$, $t_s < t_{s+1}$, and $v_g > v_{g+1}$. The quantities $t_{s+1/2}$, $r_{i+1/2}$, $\mu_{m+1/2}$, and $v_{g+1/2}$ are defined by

$$\begin{aligned} t_{s+1/2} &= \tfrac{1}{2}(t_s + t_{s+1}), \qquad & r_{i+1/2} &= \tfrac{1}{2}(r_i + r_{i+1}), \\ \mu_{m+1/2} &= \tfrac{1}{2}(\mu_m + \mu_{m+1}), \qquad & v_{g+1/2} &= \tfrac{1}{2}(v_g + v_{g+1}). \end{aligned} \tag{31}$$

Half-integral subscripts correspond to cell boundaries, integral subscripts correspond to cell centered quantities. The conservative difference form of the transport equations are now derived using the discrete ordinate method as in neutron transport theory [4, 5].

The conservative differencing operator K is defined by

$$K = (1/\beta) \int_{t_{s-1/2}}^{t_{s+1/2}} dt \int_{r_{i-1/2}}^{r_{i+1/2}} r^2\, dr \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} d\mu \int_{v_{g+1/2}}^{v_{g-1/2}} v^2\, dv, \tag{32}$$

where

$$\beta = \Delta t_s\, \Delta r_i^3/3\, \Delta\mu_m\, \Delta v_g^3/3.$$

The quantities Δt_s, Δr_i^3, $\Delta\mu_m$, and Δv_g^3 are given by

$$\begin{aligned} \Delta t_s &= t_{s+1/2} - t_{s-1/2}, \qquad & \Delta r_i^3 &= r_{i+1/2}^3 - r_{i-1/2}^3, \\ \Delta\mu_m &= \mu_{m+1/2} - \mu_{m-1/2}, \qquad & \Delta v_g^3 &= v_{g-1/2}^3 - v_{g+1/2}^3. \end{aligned} \tag{33}$$

The operator K is used to difference both the mass transport equation (16) and the energy transport equation (17). This operator averages the expression it is applied to over the phase space cell $\Delta t_s\, \Delta r_i^3\, \Delta\mu_m\, \Delta v_g^3$. The fact that K is conservative will be proved in the following section.

Applying K to both sides of Eq. (16), the mass transport equation becomes

$$\begin{aligned} &\frac{1}{\Delta t_s}(N_{s+1/2} - N_{s-1/2}) + \frac{\mu_m}{V_i}\left(\frac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)(A_{i+1/2}N_{i+1/2} - A_{i-1/2}N_{i-1/2}) \\ &+ \frac{(A_{i+1/2} - A_{i-1/2})}{V_i}\left(\frac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\left(\frac{\alpha_{m+1/2}N_{m+1/2} - \alpha_{m-1/2}N_{m-1/2}}{W_m}\right) \\ &+ \frac{3}{\Delta v_g^3}(a_{g-1/2}v_{g-1/2}^2 N_{g-1/2} - a_{g+1/2}v_{g+1/2}^2 N_{g+1/2}) = S_M - \frac{\Delta v_g^4/4}{\Delta v_g^3/3}\,\sigma N, \end{aligned} \tag{34}$$

where $V_i = \Delta r_i^3/3$

$$\begin{aligned} A_{i+1/2} &= r_{i+1/2}^2, \\ N &= N(t_s, r_i, \mu_m, v_g), \\ N_{s+1/2} &= N(t_{s+1/2}, r_i, \mu_m, v_g), \\ N_{i+1/2} &= N(t_s, r_{i+1/2}, \mu_m, v_g), \\ N_{m+1/2} &= N(t_s, r_i, \mu_{m+1/2}, v_g), \\ N_{g+1/2} &= N(t_s, r_i, \mu_m, v_{g+1/2}), \qquad \text{etc.} \end{aligned} \tag{35}$$

and the values of W_m and $\alpha_{m\pm1/2}$ are defined in the standard way [4, 5] so as to assure rotation–reflection invariance. In a similar manner, the differenced form of the energy transport equation is obtained by applying K to both sides of Eq. (17). The result is

$$\frac{1}{\Delta t_s}(\psi_{s+1/2} - \psi_{s-1/2}) + \frac{\mu_m}{V_i}\left(\frac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)(A_{i+1/2}\psi_{i+1/2} - A_{i-1/2}\psi_{i-1/2})$$
$$+ \frac{(A_{i+1/2} - A_{i-1/2})}{V_i}\left(\frac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\left(\frac{\alpha_{m+1/2}\psi_{m+1/2} - \alpha_{m-1/2}\psi_{m-1/2}}{W_m}\right) + \left(\frac{3}{\Delta v_g^3}\right)$$
$$\times (a_{g-1/2}v_{g-1/2}^2\psi_{g-1/2} - a_{g+1/2}v_{g+1/2}^2\psi_{g+1/2}) = \frac{M}{2}\frac{(\Delta v_g^5/5)}{(\Delta v_g^3/3)} S_M - \left(\frac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\sigma\psi$$
$$+ 2\left(\frac{3}{\Delta v_g^3}\right)\left(\frac{\Delta v_g^2}{2}\right) a_g\psi, \tag{36}$$

where $a_g = a(v_g)$. The term $2(3/\Delta v_g^3)(\Delta v_g^2/2)\, a_g\psi$ acts as an absorption in the difference equation and accounts for the energy lost to the coulomb drag.

VI. Conservation Requirements

To demonstrate that Eqs. (34) and (36) satisfy the conservation requirements, we analyze an idealized "thought problem." Consider a burning DT sphere enclosed by a sphere of lead in an otherwise empty region of space (see Fig. 1).

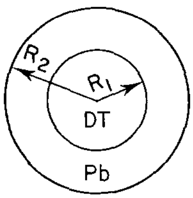

FIG. 1. Burning DT sphere with radius R_1 enclosed by a sphere of lead with radius R_2.

Both the mass and the energy of the charged particles born by thermonuclear reactions within the DT sphere remain within the gas–lead system. Suppose that the charged particles are born with velocity V and are degraded in energy by the coulomb drag force until they reach velocity V_T, which is their thermal velocity. Consider the operator

$$L = \int_{T_0}^{T} dt \int d^3r \int d^3v, \tag{37}$$

where the integration limits of r extend from the center of the spheres to the surface S_r at R_2, and the integration limits of v extend from $V_{G+1/2}$ to $v_{1/2}$, where

$v_{G+1/2} < V_T$ and $v_{1/2} > V$. Applying L to Eq. (8), the conservation statement becomes

$$\mathscr{N}_T - \mathscr{N}_{T_0} = \mathscr{S}_M \tag{38}$$

since

$$\begin{aligned} L(\nabla_r \cdot \mathbf{v}N) &= \int_{S_r} N\mathbf{v} \cdot d\hat{S}_r = 0, \\ L(\nabla_v \cdot \mathbf{a}N) &= \int_{S_v} N\mathbf{a} \cdot d\hat{S}_v = 0, \end{aligned} \tag{39}$$

where $d\hat{S}_r$ and $d\hat{S}_v$ are outward directed elements of surface area in position and velocity space with unit normal directions, $\sigma = 0$, and S_v is the surface in velocity space defined by $|\mathbf{v}| = v_{1/2}$. The quantities $\mathscr{N}_T$ and $\mathscr{S}_M$ are defined by

$$\begin{aligned} \mathscr{N}_T &= \int d^3r \int d^3v\, N(r, v, T), \\ \mathscr{S}_M &= \int_{T_0}^{T} dt \int d^3r \int d^3v\, S_M(r, v, t). \end{aligned} \tag{40}$$

Equations (39) state that no charged particles flow into or out of the surface at R_2, nor is there a source of charged particles with velocity $v > v_{1/2}$. Equation (38) states that the increase in charged particles within the gas–lead system during the time interval $(T - T_0)$ equals the integrated source of charged particles during that time.

In a similar manner, L may be applied to Eq. (11) with the result

$$\Psi_T - \Psi_{T_0} + \mathscr{H} = \mathscr{S}_E, \tag{41}$$

$$\begin{aligned} \Psi_T &= \int d^3r \int d^3v\, \psi(r, v, T), \\ \mathscr{H} &= -\int_{T_0}^{T} dt \int d^3r \int d^3v (2/v)\, a\psi, \\ \mathscr{S}_E &= \int_{T_0}^{T} dt \int d^3r \int d^3v\, S_E. \end{aligned} \tag{42}$$

Equation (41) states that the increase in kinetic energy by the field of charged particles plus the energy deposited to the gas–lead system as heat due to the coulomb drag equals the total integrated source of energy. It is crucial that any difference equations derived from Eqs. (8) and (11) explicitly retain these conservation properties. Otherwise, the solution will be erroneous.

The operator L is also given by

$$L = \sum_s \sum_i \sum_m \sum_g \beta K, \tag{43}$$

where $t_{1/2} = T_0$, $t_{S+1/2} = T$, $r_{1/2} = 0$, and $r_{I+1/2} = R_2$. Thus, the application of L to Eqs. (8) and (11) corresponds to the application of operator L' to Eqs. (34) and (36), where

$$L' = \sum_s \sum_i \sum_m \sum_g \beta. \tag{44}$$

Applying L' to Eq. (34) results in the expression

$$\sum_{img} (\Delta r_i^3/3)\, \Delta\mu_m (\Delta v_g^3/3)\{N_{S+1/2} - N_{1/2}\} = \sum_{simg} \beta S_M, \tag{45}$$

since the other terms telescope and the boundary conditions are specified to be

$$\begin{aligned} &N(t, r, \mu, v_{1/2}) = 0, \qquad N(t, R_2, \mu, v) = 0, \\ &\psi(t, r, \mu, v_{1/2}) = 0, \qquad \psi(t, R_2, \mu, v) = 0, \qquad \text{etc.} \end{aligned} \tag{46}$$

Similarly, applying L' to Eq. (36) results in the expression

$$\begin{aligned} &\sum_{img} (\Delta r_i^3/3)\, \Delta\mu_m (\Delta v_g^3/3)\{\psi_{S+1/2} - \psi_{1/2}\} - \sum_{simg} 2\, \Delta t (\Delta r_i^3/3)\, \Delta\mu_m (\Delta v_g^2/2)\, a_g \psi \\ &\quad = \sum_{simg} \beta \frac{M}{2} \frac{(\Delta v_g^5/5)}{(\Delta v_g^3/3)} S_M. \end{aligned} \tag{47}$$

Equations (45) and (47) correspond to Eqs. (38) and (41), respectively. This correspondence reveals that Eqs. (34) and (36) explicity conserve the mass and energy of the charged particles.

The energy deposited as heat to a particular zone of the gas–lead system is given by

$$-\sum_{smg} 2\, \Delta t (\Delta r_i^3/3)\, \Delta\mu_m (\Delta v_g^2/2)\, a_g \psi. \tag{48}$$

To obtain the amount of mass deposited by the field of charged particles to a particular zone of the system, we chose $v_G > V_T$. This choice ensures that $a_{g\pm 1/2} < 0$ for all groups g. The mass deposited to a particular zone is then given by

$$\sum_{sm} M\, \Delta t_s (\Delta r_i^3/3)\, \Delta\mu_m\, v_{G+1/2}^2 a_{G+1/2} N_{G+1/2}. \tag{49}$$

The effective source of energy in Eq. (41)

$$\sum_{simg} \beta \frac{M}{2} \frac{\Delta v_1^5/5}{\Delta v_1^3/3} S_M , \tag{50}$$

does not equal the exact energy source

$$\sum_{simg} \beta \frac{M}{2} V^2 S_M , \tag{51}$$

due to discretization error. This error is remedied by replacing the source term S_M in Eq. (50) by the fictitious source S_M', where

$$S_M' = V^2((\Delta v_1^3/3)/(\Delta v_1^5/5))\, S_M . \tag{52}$$

Returning now to Eq. (18), the alternate form of the mass transport Eq. (16), we readily find that the application of L to Eq. (18) results in the expression

$$\sum_{img} (\Delta r_i^3/3)\, \Delta\mu_m (\Delta v_g^2/2)\{\phi_{S+1/2} - \phi_{1/2}\} + \sum_{simg} \Delta t(\Delta r_i^3/3)\, \Delta\mu_m\, \Delta v\, a_g \phi = \sum_{simg} \beta\, S_M . \tag{53}$$

Due to the presence of the absorption

$$\sum_{simg} \Delta t(\Delta r_i^3/3)\, \Delta\mu_m\, \Delta v\, a_g \phi,$$

Eq. (52) does not correspond to the conservation statement given by Eq. (38). From this, it is clear that Eq. (18), though apparently mathematically equivalent to Eq. (16), does not lead to a conservative difference equation and cannot be used to obtain a numerical solution of the transport equation (8). Thus, the conservation requirements place a powerful restriction on the form of the difference equations representing the transport equations (8) and (11).

The conservation requirements also demand the solution of both Eqs. (34) and (36) in order to determine the charged particle mass and energy deposition in the plasma. Although numerous formulae may be written that express the energy deposition in terms of the values of $N(t, r, \mu, v)$ and $a(r, v, t)$, these formulas cannot be proved to conserve energy (as done in this section) and do not conserve energy when used in a code. Such formulas can be normalized by the prior knowledge of $\mathscr{S}_E$ and forced to conserve energy; however, the results do not enjoy excellent agreement with the results of Cooper and Evans [7]. Results using the solution of Eq. (36) do enjoy such agreement and are presented in Section VIII.

VII. Step Function Solution of the Difference Equations

For the sake of illustration, Eqs. (34) and (36) will be solved using step function extrapolation. More sophisticated methods of solution including the LS_n [6] method will be described in future publications. In Eq. (34), let $N_{s+1/2} = N_{i+1/2} = N_{g+1/2} = N$ for $\mu_m > 0$. Similarly, in Eq. (36), let $\psi_{s+1/2} = \psi_{i+1/2} = \psi_{g+1/2} = \psi$. Then, Eqs. (34) and (36) may be solved for N and ψ, resulting in the expressions

$$N = \frac{\left[\begin{array}{l} S_M + \dfrac{1}{\Delta t_s} N_{s-1/2} + \dfrac{\mu_m}{V_i}\left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right) A_{i-1/2} N_{i-1/2} + \dfrac{(A_{i+1/2} - A_{i-1/2})}{V_i} \\ \qquad \times \left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right) \dfrac{\alpha_{m-1/2}}{W_m} N_{m-1/2} + \left(\dfrac{3}{\Delta v_g^3}\right) a_{g-1/2} v_{g-1/2}^2 N_{g-1/2} \end{array}\right]}{\left[\begin{array}{l} \dfrac{1}{\Delta t_s} + \dfrac{\mu_m}{V_i}\left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right) A_{i+1/2} + \dfrac{(A_{i+1/2} - A_{i-1/2})}{V_i}\left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\dfrac{\alpha_{m+1/2}}{W_m} \\ \qquad + \left(\dfrac{3}{\Delta v_g^3}\right) a_{g+1/2} v_{g+1/2}^2 + \left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\sigma \end{array}\right]}, \tag{54}$$

$$\psi = \frac{\left[\begin{array}{l} \dfrac{M}{2}\dfrac{(\Delta v_g^5/5)}{(\Delta v_g^3/3)} S_M + \dfrac{1}{\Delta t_s}\psi_{s-1/2} + \dfrac{\mu_m}{V_i}\left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right) A_{i-1/2}\psi_{i-1/2} \\ \qquad + \dfrac{(A_{i+1/2} - A_{i-1/2})}{V_i}\left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\dfrac{\alpha_{m-1/2}}{W_m}\psi_{m-1/2} \\ \qquad + \left(\dfrac{3}{\Delta v_g^3}\right) a_{g-1/2} v_{g-1/2}^2 \psi_{g-1/2} \end{array}\right]}{\left[\begin{array}{l} \dfrac{1}{\Delta t_s} + \dfrac{\mu_m}{V_i}\left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3)}\right) A_{i+1/2} + \dfrac{(A_{i+1/2} - A_{i-1/2})}{V_i}\left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\dfrac{\alpha_{m+1/2}}{W_m} \\ \qquad + \left(\dfrac{3}{\Delta v_g^3}\right) a_{g+1/2} v_{g+1/2}^2 + \left(\dfrac{\Delta v_g^4/4}{\Delta v_g^3/3}\right)\sigma - 2\left(\dfrac{3}{\Delta v_g^3}\right)\left(\dfrac{\Delta v_g^2}{2}\right) a_g \end{array}\right]}. \tag{55}$$

For $\mu_m < 0$, the relations $N_{i-1/2} = N$ and $\psi_{i-1/2} = \psi$ are used to determine the values of N and ψ. Using Eqs. (54) and (55) to obtain the values of $N_{s+1/2}, \ldots, N_{g+1/2}$, $\psi_{s+1/2}, \ldots, \psi_{g+1/2}$, the transport equations (34) and (36) may be solved throughout the regions of interest.

During an actual calculation, values of S_m are supplied to the subroutine performing charged particle transport from a driver program using calculated values of the zonal thermonuclear burn rates. Methods for calculating these rates are given in [1]. Since we have assumed the charged particles interact with the plasma only by small angle scattering (resulting in the coulomb drag term **a**), the value of σ used in our calculations is $\sigma \equiv 0$. We have investigated the numerical simulation of large angle scattering of charged particles, but due to storage limitations, these effects are not presently included in our computer program.

Values of Δr_i and M required to achieve acceptable accuracy are problem dependent; however, some insight can be gained from the values used in calculations described in the following sections. Values of Δt_s are customarily chosen dynamically by methods described in [1].

VIII. Results

A computer program designed to transport charged particles based on the mathematical results of the previous sections has been written and is in use at our laboratory. We have used this code to calculate alpha particle energy deposition in a reacting DT sphere. The sphere contains equal numbers of deuterium and tritium atoms and is assumed to be fully ionized at a uniform temperature and density. The alpha particles are created uniformly in the sphere with an initial energy of 3.51 MeV and an isotropic angular distribution. Fig. 2 is a graph of the

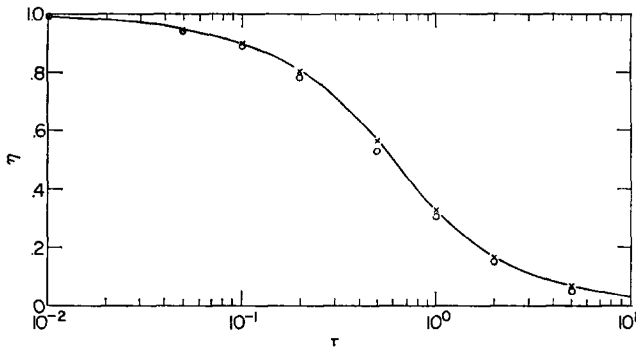

Fig. 2. Fraction of energy η escaping a burning DT sphere at a temperature of 5 keV and a density of 0.2125 g/cm^3 with radius τ in mean free paths. ———, analytic result; ○, step function solution; ×, LSN solution.

fraction of energy η escaping the sphere as a function of the sphere's radius τ in mean free paths. The results of LS_n charged particle transport are in excellent agreement with the analytic results of Cooper and Evans [7], while the use of the step function solution of the transport equation results in moderately good agreement with the analytic solution.

Figure 3 is a graph of the fraction of energy deposited within a subsphere of the burning DT sphere with radius $\tau = 2$. Again, the results of LS_n charged particle transport are in excellent agreement with analytic results. The step function solution enjoys surprisingly good agreement with the results of Cooper and Evans

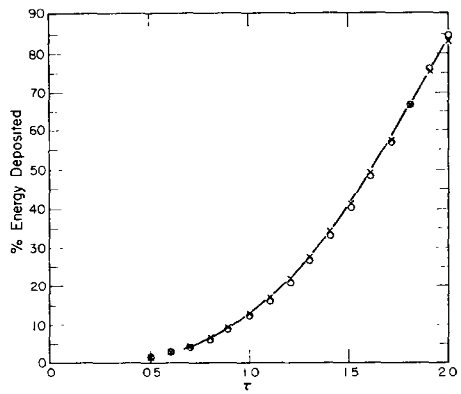

FIG. 3. Percentage of the total energy born within a burning DT sphere with radius $\tau = 2.0$ deposited within a subsphere with radius τ. The sphere has a density of 0.2125 g/cm^3 and a temperature of 5 KeV. ———, analytic result; ○, step function solution; ×, LSN solution.

for this particular problem. These example calculations show that S_n techniques are able to model correctly both the global and local energy deposition of charged particles in a burning DT plasma.

Both of the calculations described above were performed using an S_4 approximation ($M = 5$) with 20 zones ($I = 21$) in the burning DT sphere and 18 groups ($G = 19$). Time steps on the order of $\Delta t = 10^{-10}$ seconds were used; however, larger values result in little change. Increasing the values of I or M result in no visible change on the graphs, so that convergence appears to have been obtained for these problems. We have not made a detailed study of the dependence of the convergence of the calculation on values of I, M, G, and Δt; the modest values mentioned here have been adequate for all the calculations we have made to date. The calculation of Fig. 3 required 16 sec of CPU time on a CDC 7600 machine. Inclusion of the charged particle transport package described in this paper to a one-dimensional laser fusion code (such as described in [1]) typically doubles the running time for representative problems.

IX. CONCLUSIONS

The charged particle mass and energy transport equations have been derived and differenced in a conservative manner. Future papers will present results using these equations to obtain the mass and energy deposition for a number of physically interesting problems. Charged particle momentum transport and deposition will also be discussed.

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References

1. J. P. Christiansen, D. E. T. F. Ashby, and K. U. Roberts, *Comp. Phys. Com.* **7** (1974), 271.
2. G. S. Fraley, E. J. Linnebur, R. J. Mason, and R. L. Morse, *Phys. Fluids* **17** (1974), 474.
3. F. Evans, *Phys. Fluids* **16** (1973), 1011.
4. C. E. Lee, "The Discrete S_n Approximation to Transport Theory," Los Alamos Scientific Laboratory Report LA-2595, unpublished, 1962.
5. G. I. Bell and S. Glasstone, "Nuclear Reactor Theory," Van Nostrand Reinhold, New York, 1970.
6. C. E. Lee, *Amer. Nucl. Soc. Trans.* **18** (1974), 149.
7. R. Cooper and F. Evans, *Phys. Fluids* **18** (1975), 332.