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EDOT: A CODE TO CALCULATE CHARGED PARTICLE SLOWING DOWN IN A PLASMA

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August 5, 1977

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ABSTRACT

EDOT is a code that calculates the slowing down of a test particle in a Maxwellian plasma utilizing continuous slowing down theory. Both nuclear scattering and reactions are included. The output includes slowing down parameters as well as spectra of knockon ions and in-flight reaction probabilities.

The theory, input, and output for the code are described in this report.

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I. INTRODUCTION

Energetic charged particles, while slowing down in a plasma, give up their energy by scattering to the plasma ions and electrons, as well as to nuclear reactions in which the energetic particle is completely removed. The energy partition to the plasma ions and electrons is further complicated by the fact that ions can be knocked out of the thermal sea, thus creating new sources of energetic particles. It was with the purpose in mind of investigating this phenomenon that the code EDOT was written. This code calculates the slowing down of a test particle in a multi-constituent Maxwellian plasma (different ion and electron temperatures) by continuous slowing down theory. Although for large angle scattering, this approach is not as accurate as other techniques, e.g., multigroup theory or Monte Carlo, it has the advantage of both speed and relatively simple input designation. Both Coulomb and nuclear scattering off of unlike or like particles are considered as well as the energy loss to nuclear reactions. While retaining a degree of simplicity, the resultant equations do take into account important variations such as the energy dependence of all parameters as well as including more than one ion species in the plasma. The complexity this introduces requires numerical rather than an analytic solution to the problem. Output from the code includes the various slowing down parameters (thermalization time, range, energy partitions to electrons, ions, and nuclear reactions). Also on option, the spectra of knockon ions for each constituent in the plasma is given in both energy dependent and multigroup form, the latter furnishing source input to multigroup charged particle transport codes. In-flight reaction probabilities are also calculated for all specified nuclear reactions.

II. THEORY

A. Particle Slowing Down

Consider a test particle of velocity V , mass M , energy $E(= MV^2/2)$, charge number Z , slowing down in a medium composed of electrons (subscript e) and ions (subscript i). The medium will be considered to be a completely stripped nondegenerate Maxwellian plasma under charge neutrality, and electron and ion temperatures which are not necessarily equal. The plasma thermal energy, E_{th} , will be defined as equal to $3kT_i/2$ and the test particle initial energy as E_0 .

The average instantaneous rate of energy loss by the test particle to the plasma is given by (nuclear reactions will be considered later)

$$\left(\frac{\partial E}{\partial t}\right)_{tot} = \left(\frac{\partial E}{\partial t}\right)_e^C + \left(\frac{\partial E}{\partial t}\right)_i^C + \left(\frac{\partial E}{\partial t}\right)_i^N, \quad (1)$$

where the superscripts C and N refer to Coulomb and nuclear scattering, respectively. Note that both ion contributions refer to summations over all ion species, b , in the plasma.

The slowing down time of the test particle to a specific energy E is determined by the relation¹

$$t(E) = \int_{E_0}^E \frac{dE}{\left(\frac{\partial E}{\partial t}\right)_{tot}}, \quad (2)$$

where $0 \leq t(E) \leq t(E_{th})$ and with $t(E_{th})$ being defined as the thermalization

* Throughout this report, kT is to be taken as a single symbol denoting temperature in units of energy.

time. The energy loss by the test particle to the ions by Coulomb scattering is given by (energy loss defined as positive)

$$-\Delta E_i^C(E) = \int_0^{t(E)} \left(\frac{\partial E}{\partial t} \right)_i^C dt, \quad (3)$$

for $0 \leq \Delta E_i^C(E) \leq \Delta E_i^C(E_{th})$, and with a similar expression for the energy loss to the electrons, $\Delta E_e^C(E)$, and additionally for nuclear scattering with the ions, $\Delta E_i^N(E)$. The time, $t(E)$, in Eq. (3) is determined from Eq. (2). However, from this latter expression,

$$dt = \frac{dE}{(\partial E / \partial t)_{tot}}, \quad (4)$$

and Eq. (3) may be written as

$$-\Delta E_i^C(E) = \int_{E_0}^E \frac{\left(\frac{\partial E}{\partial t} \right)_i^C}{(\partial E / \partial t)_{tot}} dE. \quad (5)$$

The ion energy partition function, i.e., the fraction of the test particle's energy going into the ions during the slowing down process is

$$f_i = \frac{\Delta E_i^C(E_{th}) + \Delta E_i^N(E_{th})}{E_0}. \quad (6)$$

The energy loss per unit path length may be written as

$$\left(\frac{\partial E}{\partial s} \right)_{tot} = \left(\frac{\partial E}{\partial t} \right)_{tot} \frac{dt}{ds} = \frac{1}{V} \left(\frac{\partial E}{\partial t} \right)_{tot}, \quad (7)$$

with the range of the test particle then given by

$$R(E) = \int_{E_0}^E \frac{dE}{(\partial E / \partial s)_{\text{tot}}} = \int_{E_0}^E \frac{dE}{\frac{1}{V}(\partial E / \partial t)_{\text{tot}}} \quad (8)$$

B. Coulomb Energy Loss

The average instantaneous rate of energy loss by the test particle to the plasma electrons is given by (see Section 7-11 of Ref. 2)

$$-\left(\frac{\partial E}{\partial t}\right)_e^C = \left[\frac{4\pi e^4 Z^2}{V} \right] \frac{G(x_e)}{m_e} L_e \sum_b n_{e_b} \quad (9)$$

and to the plasma ions,

$$-\left(\frac{\partial E}{\partial t}\right)_i^C = \left[\frac{4\pi e^4 Z^2}{V} \right] \sum_b \frac{z_b^2 n_{i_b} L_{i_b} G(x_{i_b})}{m_{i_b}} \quad (10)$$

The summations are over all ion species, b . In these two equations (j refers to either e or i_b),

$$G(x_j) = \phi(x_j) - \left(1 - \frac{m_j}{M}\right) x_j \phi'(x_j) \quad (11)$$

$$\phi(x_j) = \text{erf}(x_j) \quad (12)$$

$$x_j = v \left(\frac{m_j}{2kT_j} \right)^{1/2} \quad (13)$$

and L is the Coulomb logarithmic term,³ i.e.,

$$L_j = \ln \left(1 + \Lambda_j^2 \right)^{1/2} \quad (14)$$

The argument of the log is given by the ratio (Sections 7-3 and 7-11 of Ref. 2)

$$\Lambda_j = \frac{\ell_D}{b_{oj}} , \quad (15)$$

where ℓ_D is the Debye shielding length which is

$$\ell_D = \ell_{De} \gamma_c \quad (16)$$

with

$$\ell_{De} = \left(\frac{kT_e}{4\pi n_e e^2} \right)^{1/2} , \quad (17)$$

$$\gamma_c = \left[\frac{1}{1 + \frac{kT_e}{kT_i} \frac{\bar{Z}^2}{\bar{Z}}} \right]^{1/2} , \quad (18)$$

the latter term yielding the screening action of the ions. Furthermore,

$$\bar{Z}^2 = \sum_b N_{fb} Z_b^2 , \quad (19)$$

and

$$\bar{Z} = \sum_b N_{fb} Z_b , \quad (20)$$

$N_{fb} \left(\equiv n_{ib} / n_i \right)$ being the atom fraction of particles b in the plasma. The classical value for b_o , the distance of closest approach, is the minimum impact parameter, given by

$$b_{oj} = \frac{ZZ_j e^2}{2E_{rj}} \equiv b_{oj} \text{ (classical)} , \quad (21)$$

with E_{rj} being the relative energy between the test particle and the particle of species j . We have

$$E_{rj} = \frac{1}{2} \mu_j v_{rj}^2 , \quad (22)$$

with the reduced mass

$$\mu_j = \frac{M m_j}{M + m_j} , \quad (23)$$

and the relative velocity

$$\vec{v}_{rj} = \vec{v}_j - \vec{V} . \quad (24)$$

Correctly averaging over the relative velocity is a complicated procedure, e.g., Doppler broadening of neutron cross sections. However, a first order approximation may be made by angle averaging Eq. (24) to yield^{1,11}

$$\langle v_{rj}^2 \rangle = v_j^2 + V^2 , \quad (25)$$

and substituting this result into Eq. (22), along with Eq. (23) and noting that $E_j = \frac{3}{2} kT_j$, we obtain

$$E_{rj} = \frac{m_j}{m_j + M} E - \frac{M}{m_j + M} \frac{3}{2} kT_j . \quad (26)$$

There is a quantum mechanical diffractive correction that applies only to electrons for our range of temperature interest (Section 7-3 of Ref. 2 and Section 5.2 of Ref. 5). If $\lambda_j (\equiv \hbar/\mu_j v_{rj}) > 2b_{oj}$ (classical); or equivalently, if $E_{rj} > 2Z^2 Z_j^2 (\mu_j c^2) \alpha^2$ where α is the fine structure constant and E_{rj} and $\mu_j c^2$ are in the same units; then $2b_{oj} = \lambda_j$.

The electron density is, using Eq. (20),

$$n_e = \sum_b n_{e_b} = \sum_b Z_b n_{i_b} = n_i \sum_b Z_b N_{F_b} = n_i \bar{Z} \quad , \quad (27)$$

and for the ion density,

$$n_i = \sum_i n_{i_b} = \rho \frac{N_a}{A} \quad , \quad (28)$$

where

$$\bar{A} = \sum_b N_{f_b} A_b \quad , \quad (29)$$

and A is the atomic weight, ρ is the material density, and N_a is Avogadro's number.

Our basic equations, Eq. (9) and (10), may now be written as⁶

$$-\left(\frac{\partial E}{\partial t}\right)_e^C = \left(\frac{4\pi e^4}{m_e}\right) \frac{Z^2}{V} n_i L_e G(x_e) \bar{Z} \quad , \quad (30)$$

and

$$-\left(\frac{\partial E}{\partial t}\right)_i^C = \left(\frac{4\pi e^4}{m_e}\right) A_e \frac{Z^2}{V} n_i \sum_b \frac{Z_b^2 N_{f_b} L_{i_b} G(x_{i_b})}{A_b} \quad , \quad (31)$$

where

$$x_e = \left(\frac{A_e}{A} \frac{E}{kT_e} \right)^{1/2}, \quad (32)$$

and

$$x_{i_b} = \left(\frac{A_b}{A} \frac{E}{kT_{i_b}} \right)^{1/2}. \quad (33)$$

Also, for $E_{r_e} \leq 5.442 \times 10^{-5} Z^2$ MeV (this assumes $\mu_e = m_e$)

$$\Lambda_e = \left(\frac{1}{\pi^{1/2} e^3} \right) \frac{kT_e^{1/2} E_{r_e} \gamma_c}{n_e^{1/2} Z} \equiv \Lambda_e \text{ (classical)}, \quad (34)$$

and for $E_{r_e} > 5.442 \times 10^{-5} Z^2$ MeV

$$\Lambda_e = \alpha \left(2m_e c^2 \right)^{1/2} \frac{Z}{E_{r_e}^{1/2}} \Lambda_e \text{ (classical)}. \quad (35)$$

For the ions,

$$\Lambda_{i_b} = \left(\frac{1}{\pi^{1/2} e^3} \right) \frac{kT_e^{1/2} E_{r_{i_b}} \gamma_c}{n_e^{1/2} Z Z_b} \quad (36)$$

With $j = e$ or i_b , $G(x_j)$ is as per Eq. (11) where the mass ratio can be replaced by the ratio of atomic weights. Similarly, E_{r_j} is as per Eq. (26) using the appropriate atomic weight ratios and temperatures.

C. Nuclear Scattering Energy Loss

The average instantaneous rate of energy loss by the test particle to the plasma ions is

$$-\left(\frac{\partial E}{\partial t}\right)_i^N = -\sum_b \left(\frac{\partial E}{\partial t}\right)_{i_b}^N = v n_i \sum_b \overline{\Delta E_b(E)} \sigma_b(E) N_{f_b} \quad (37)$$

with the latter result obtained by using the relationship between the energy loss per unit path length and the reaction rate,⁷ along with Eq. (7). We have

$$\overline{\Delta E_b(E)} \sigma_b(E) = \frac{2A_b A}{(A_b + A)^2} E \sigma_{E_b}(E) \quad (38)$$

where the energy loss cross section, $\sigma_{E_b}(E)$, is given by

$$\sigma_{E_b}(E) = 2\pi \int_{-1}^{+1} \sigma_b(E, \eta) (1 - \eta) d\eta \quad (39)$$

with η being the cosine of the scattering angle in the CM system. If scattering is isotropic in the CM system (an assumption only made in determining the spectra of knockons), the energy loss cross section is equal to the cross section for nuclear scattering, $\sigma_b(E)$. Furthermore, $\overline{\Delta E_b(E)}$, the average energy loss by the test particle or equivalently the average energy gained by the ion (per collision), including the first order correction for finite ion temperature⁴ becomes

$$\overline{\Delta E_b(E)} = \frac{2A_b A}{(A_b + A)^2} \left[E - \frac{3}{2} kT_i \right] \quad (40)$$

D. Spectra of Knockon Ions

In elastic ion scattering, the energy lost by the test particle is given up to the ions. Thus for either Coulomb or nuclear scattering, Eq. (37) is valid and for a specific reaction off of a given ion species, b ,

$$-\left(\frac{\partial E}{\partial t}\right)_b = \overline{\Delta E_b(E)} N_t(E) \quad , \quad (41)$$

where the collision frequency, $N_t(E)$, (collisions/unit time) is

$$N_t(E) = V \sigma_b(E) n_{i_b} \equiv \frac{1}{\tau(E)} \quad , \quad (42)$$

and $\tau(E)$ is the mean time to collision. Defining the normalized spectra of knockon ions for a given test particle energy E as $\pi(E \rightarrow E'_b)$, where E'_b is the ion energy, Eq. (41) can be rewritten as

$$-\left(\frac{\partial E}{\partial t}\right)_b = N_t(E) \int \Delta E'_b(E) \pi(E \rightarrow E'_b) dE'_b \quad . \quad (43)$$

Thus, the corresponding number of knockon ions scattered to E'_b is

$$N(E \rightarrow E'_b) = N_t(E) \pi(E \rightarrow E'_b) \quad ; \quad (\text{i.e., particles/MeV sh}) \quad . \quad (44)$$

The total number scattered to E'_b from all E is equal to an integral over all time, or conversely using Eq. (4),

$$N(E'_b) = - \int_{E_{\min}(E'_b)}^{E_{\max}(E'_b)} \frac{N(E \rightarrow E'_b)}{(\partial E / \partial t)_{\text{tot}}} dE \quad . \quad (45)$$

Using Eq. (44) and (41), this may be rewritten as

$$N(E'_b) = \int_{E_{\min}(E'_b)}^{E_{\max}(E'_b)} \frac{(\partial E / \partial t)_b}{(\partial E / \partial t)_{\text{tot}}} \frac{\pi(E \rightarrow E'_b)}{\Delta E_b(E)} dE \quad (46)$$

Integrating Eq. (46) over all final energy, E'_b , yields

$$N = \int_{E_{\text{th}}}^{E_0} \frac{(\partial E / \partial t)_b}{(\partial E / \partial t)_{\text{tot}}} \frac{dE}{\Delta E_b(E)} \quad (47)$$

where N is the total number of collisions between the test particle and ion species, b , during the slowing down process.

In calculating the ion knockon spectra, it is desirous to define an energy cutoff, E_c , below which the knockon ions are considered to remain in the thermal sea. The two supplemental integrals which describe the number of ions which have undergone collisions with the test particle but which have remained in the thermal sea, and the energy given up to these ions, are respectively

$$\begin{aligned} & \int_{E'_{b\min}}^{E_c} N(E'_b) dE'_b \\ &= \int_{E_{\text{th}}}^{E_0} \frac{(\partial E / \partial t)_b}{(\partial E / \partial t)_{\text{tot}}} \frac{dE}{\Delta E_b(E)} \int_{E'_{b\min}}^{E_c} \pi(E \rightarrow E'_b) dE'_b \quad (48) \end{aligned}$$

and

$$\int_{E_{b\min}}^{E_c} \Delta E'_b(E) N(E'_b) dE'_b$$

$$= \int_{E_{th}}^{E_o} \frac{(\partial E / \partial t)_b}{(\partial E / \partial t)_{tot}} \frac{dE}{\Delta E_b(E)} \int_{E'_{b\min}}^{E_c} \Delta E'_b(E) \pi(E \rightarrow E'_b) dE'_b \quad (49)$$

If $E_c = E'_{b\max}$, these two equations reduce to Eq. (47) and (5), respectively. The corresponding properties for the knockon spectra, $E'_b \geq E_c$, may be obtained by replacing the limit on these two integrals, i.e., $E_c \leq E'_b \leq E'_{b\max}$. However, once the spectra, Eq. (46) has been obtained, it is easier to obtain these parameters by integrations over the spectra itself.

E. Spectra of Knockon Ions from Coulomb Interactions

It will be assumed that scattering is off of a cold media except the relative energy will be given by Eq. (26). The spectra of ions of species b being knocked up to energy E'_b by the test particle of energy E is given by⁹

$$\pi_b^C(E \rightarrow E'_b) \sim \frac{1}{E'^2_b} \quad (50)$$

Normalizing this probability to unity between its available energies,

$E'_{b\min}$ and $E'_{b\max}$, yields

$$\pi_b^C(E \rightarrow E'_b) = \frac{1}{\left[\frac{1}{E'_{b \min}} - \frac{1}{E'_{b \max}} \right]} \frac{1}{E'_b{}^2} . \quad (51)$$

The average energy gained by the ions per collision is then equal to

$$\overline{\Delta E_b(E)} = \overline{\Delta E'_b(E)} = \overline{E'_b} = \int_{E'_{b \min}}^{E'_{b \max}} E'_b \pi_b^C(E \rightarrow E'_b) dE'_b , \quad (52)$$

or

$$\overline{E'_b} = \frac{1}{\left[\frac{1}{E'_{b \min}} - \frac{1}{E'_{b \max}} \right]} \ln \left(\frac{E'_{b \max}}{E'_{b \min}} \right) . \quad (53)$$

To determine the energy limits on the spectra, we can write E'_b in terms of the impact parameter, x , as⁹

$$E'_b = \frac{2}{m_b} \left(\frac{ZZ_b e^2}{V} \right)^2 \frac{1}{x^2 + b_{0b}^2} , \quad (54)$$

and b_{0b} is given by Eq. (21). This may be reduced to the form

$$E'_b = \frac{4A}{A + A_b} E_{r_b} \frac{1}{\left(\frac{x}{b_{0b}} \right)^2 + 1} \quad (55)$$

with E_{r_b} from Eq. (26). The maximum energy exchange is for a headon collision, $x = 0$ ($\theta = 180^\circ$), from which

$$E'_{b_{\max}} = \frac{4A}{A + A_b} E_{r_b} \quad (56)$$

Thus, Eq. (55) may be rewritten as

$$E'_b = E'_{b_{\max}} \frac{1}{\left(\frac{x}{b_{ob}}\right)^2 + 1} \quad (57)$$

The minimum energy exchange is obtained when $x = \ell_D$ ($\theta \ll 90^\circ$), where ℓ_D is the Debye length given by Eq. (16),

$$E'_{b_{\min}} = E'_{b_{\max}} \frac{1}{\left(\frac{\ell_D}{b_{ob}}\right)^2 + 1} = E'_{b_{\max}} \frac{1}{\Lambda_b^2 + 1} \quad (58)$$

with the latter form coming from Eq. (15). Thus, our spectra, Eq. (51), may be rewritten as

$$\pi_b^C(E \rightarrow E'_b) = \frac{E'_{b_{\max}}}{\Lambda_b^2} \frac{1}{E_b'^2} \quad (59)$$

and the average energy gained per collision, Eq. (57), as

$$\overline{E'_b} = \frac{E'_{b_{\max}}}{\Lambda_b^2} \ln(\Lambda_b^2 + 1) \quad (60)$$

The domain of the knockon spectra is shown in Figure 1.

Figure 1 - Domain of the knockon spectra for Coulomb scattering in a cold media.

From this, the limits on the spectra calculation, Eq. (46) are determined as:

$$\begin{aligned}
 E'_{b,min}(E_0) \leq E'_b \leq E'_{b,min}(E_{th}) \quad , \quad E(E'_{b,min}) \leq E \leq E_0 \quad ; \\
 E'_{b,min}(E_{th}) \leq E'_b \leq E'_{b,max}(E_{th}) \quad , \quad E_{th} \leq E \leq E_0 \quad ; \\
 E'_{b,max}(E_{th}) \leq E'_b \leq E'_{b,max}(E_0) \quad , \quad E(E'_{b,max}) \leq E \leq E_0 \quad . \quad (61)
 \end{aligned}$$

To explicitly specify these limits, $E'_{b,min}(E)$ is given by Eq. (58), $E'_{b,max}(E)$ by Eq. (56), and $E_r(E)$ by Eq. (26). Inverting this latter expression,

$$E(E_r) = \left(\frac{A + A_b}{A_b} \right) \left[E_r - \left(\frac{A}{A + A_b} \right) \frac{3}{2} kT_i \right] \quad (62)$$

Similarly, inverting Eq. (56),

$$E_r(E'_{b_{\max}}) = \left(\frac{A + A_b}{4A} \right) E'_{b_{\max}} \quad (63)$$

with $E(E_r)$ then given by Eq. (62). Equation (58) is rewritten, with the help of Eq. (56), as

$$E'_{b_{\min}}(E) = \frac{4A}{A + A_b} \frac{E_r}{\left(\alpha^2 E_r^2 + 1 \right)} \quad (64)$$

where, from Eq. (36),

$$\alpha = \left(\frac{1}{\pi^{1/2} e^3} \right) \frac{kT_e^{1/2}}{n_e^{1/2} Z_b} \gamma_c \quad (65)$$

Inverting Eq. (64),

$$E_r(E'_{b_{\min}}) = \frac{1}{2\alpha^2 E'_{b_{\min}}} \left\{ \frac{4A}{A + A_b} + \sqrt{\left(\frac{4A}{A + A_b} \right)^2 - \left(2\alpha E'_{b_{\min}} \right)^2} \right\} \quad (66)$$

with $E(E_r)$ then given by Eq. (62).

The two inner integrals in Eq. (48) and (49) may be analytically performed to yield:

for $E_c \leq E'_{b\min}(E)$, both integrals are zero;

for $E'_{b\min}(E) < E_c < E'_{b\max}(E)$

$$\int_{E'_{b\min}}^{E_c} \pi_b^C(E \rightarrow E'_b) dE'_b = \frac{\Lambda_b^2 + 1}{\Lambda_b^2} \left[1 - \frac{E'_{b\min}}{E_c} \right] , \quad (67)$$

$$\int_{E'_{b\min}}^{E_c} E'_b \pi_b^C(E \rightarrow E'_b) dE'_b = \frac{E'_{b\max}}{\Lambda_b^2} \ln \left(\frac{E_c}{E'_{b\min}} \right) ; \quad (68)$$

and using Eq. (58) and replacing E_c by $E'_{b\max}$ here, it is obvious that for $E'_{b\max}(E) \leq E_c$, these last two integrals reduce to unity and $\bar{E}'_b$ [Eq. (60)], respectively.

F. Spectra of Knockon Ions from Nuclear Scattering

It will again be assumed that scattering is off of a cold media. Additionally, it will be assumed that nuclear scattering is isotropic in the center of mass system, i.e., a constant energy spectra,

$$\pi_b^N(E \rightarrow E'_b) = K . \quad (69)$$

Normalizing this spectra to unity between its available energies,

$0 \leq E'_b \leq E'_{b \max}$, yields

$$\pi_b^N(E \rightarrow E'_b) = \frac{1}{E'_{b \max}} \quad (70)$$

The average energy gained by the ions per collision is then

$$\overline{\Delta E_b(E)} = \overline{\Delta E'_b(E)} = \overline{E'_b} = \frac{E'_{b \max}}{2} \quad (71)$$

or

$$E'_{b \max} = 2\overline{E'_b} \quad (72)$$

with $\overline{E'_b}$ from Eq. (40).

The domain of the knockon spectra is shown in Figure 2.

Figure 2 - Domain of the knockon spectra for nuclear scattering in a cold media.

From this, the limits on the spectra calculation, Eq. (46), are determined as

$$E(E'_{b\max}) \leq E \leq E_0, \quad (73)$$

where using Eq. (40) and (72),

$$E(E'_{b\max}) = \frac{(A'_b + A)^2}{4A'_b A} E'_{b\max} + \frac{3}{2} kT_i. \quad (74)$$

The two inner integrals in Eq. (48) and (49) may be analytically performed to yield:

$$\text{for } 0 < E_c < E'_{b\max}(E)$$

$$\int_{E'_{b\min}}^{E_c} \pi_b^N(E \rightarrow E'_b) dE'_b = \frac{E_c}{2E'_b}, \quad (75)$$

$$\int_{E'_{b\min}}^{E_c} E'_b \pi_b^N(E \rightarrow E'_b) dE'_b = \left(\frac{E_c}{2}\right)^2 \frac{1}{E'_b}; \quad (76)$$

and replacing E_c by $E'_{b\max}$ in these last two integrals, it is obvious that for $E'_{b\max} \leq E_c$, these two integrals reduce to unity and $\bar{E}_b^T$ [Eq. (71)], respectively.

G. Like Particle Scattering - Coulomb

For test particle and ion b identical, the higher energy particle from the scattering event will be considered to still be the test particle. This limits its angular domain to $0 \leq \eta \leq 1$, where η is the CM cosine of the scattering angle. Now, Evans¹⁰ has shown (for DD scattering) that over this domain $(\partial E / \partial t)^C$ is very well approximated by using Rutherford scattering as an approximation to the Coulomb cross section. Thus, Eqs. (30) - (36) will still be considered valid for the energy loss but the knockon spectra description will be changed.

The maximum energy exchange, is then, $x = b_{ob}$ ($\theta = 90^\circ$), from which with the aid of Eq. (54) yields

$$E'_{b \max} = \frac{2A}{A + A_b} E_{r_b}, \quad (77)$$

rather than that from Eq. (56). The minimum energy exchange remains unchanged and thus $E'_{b \min}$ is still as per Eq. (58). Thus, our spectra, Eq. (51) may be written, rather than Eq. (59), as

$$\pi_b^C(E \rightarrow E'_b) = \frac{2E'_{b \max}}{(A_b^2 - 1)} \frac{1}{E_b'} \quad (78)$$

The average energy, gained per collision then becomes

$$\overline{E}_b' = \frac{2E'_{b \max}}{(A_b^2 - 1)} \ln \left(\frac{A_b^2 + 1}{2} \right), \quad (79)$$

which replaces Eq. (60).

The domain of the knockon spectra is still as per Eqs. (61) - (66) with the exception that inverting Eq. (77) leads, rather than Eq. (63), to

$$E_r(E'_{b_{\max}}) = \left(\frac{A + A_b}{2A} \right) E'_{b_{\max}} \quad (80)$$

The two inner integrals in Eq. (48) and (49) may still be analytically performed to yield

$$\int_{E'_{b_{\min}}}^{E_c} \pi_b^C(E \rightarrow E'_b) dE'_b = \left(\frac{\Lambda_b^2 + 1}{\Lambda_b^2 - 1} \right) \left[1 - \frac{E'_{b_{\min}}}{E_c} \right] \quad (81)$$

$$\int_{E'_{b_{\min}}}^{E_c} E'_b \pi_b^C(E \rightarrow E'_b) dE'_b = \frac{2E'_{b_{\max}}}{(\Lambda_b^2 - 1)} \ln \left(\frac{E_c}{E'_{b_{\min}}} \right) \quad (82)$$

which replace Eq. (67) and (68).

H. Like Particle Scattering - Nuclear

As for Coulomb scattering, the high energy particle from the scattering event will be considered to be the test particle. Eq. (39) is then replaced by

$$\sigma_{E_b}(E) = 2\pi \int_0^1 \sigma_b(E, \eta) (1 - \eta) d\eta \quad (83)$$

If scattering is assumed to be isotropic in the CM system, one obtains

$$\sigma_b(E) = 2\sigma_{E_b}(E) \quad , \quad (84)$$

where the nuclear scattering cross section is defined over this same angular domain. Substituting this result into Eq. (38) and introducing the first order ion temperature correction yield,

$$\overline{\Delta E}_b(E) = -\frac{A_b A}{(A_b + A)^2} \left[E - \frac{3}{2} kT_i \right] , \quad (85)$$

which is one half the value obtained previously in Eq. (40).

With the new definitions of Eqs. (83) - (85), $(\partial E / \partial t)_i^N$ is still given by Eq. (37) and the knockon spectra description by Eqs. (69) - (76) with the exception that Eq. (74) is replaced by

$$E(E'_{b \max}) = \frac{(A_b + A)^2}{2A_b A} E'_{b \max} + \frac{3}{2} kT_i . \quad (86)$$

I. Reaction Energy Loss and In-flight Reaction Probability

Consider now a nuclear reaction in which the test particle is completely removed. Analogous to Eq. (37), the average instantaneous rate of energy loss by the test particle is

$$-\left(\frac{\partial E}{\partial t}\right)^R = -\sum_b \left(\frac{\partial E}{\partial t}\right)_b^R = v n_i \sum_b E \sigma_{R_b}(E) N_{f_b} , \quad (87)$$

where $\sigma_{R_b}(E)$ is the reaction cross section. This result is to be added to the right hand side of Eq. (1) to obtain $(\partial E / \partial t)_{\text{tot}}$. The energy loss by the test particle by reactions is then obtained as per Eqs. (3) - (5).

The probability that the test particle undergo no reaction with ion species b while slowing down to thermal is given by¹¹

$$P_{\text{no reaction}_b} = e^{-\int_0^{R(E_{th})} n_i N_{fb} \sigma_{R_b}(s) ds} \quad (88)$$

Note that this is entirely similar to a neutron traversing an inhomogeneous media. Utilizing Eq. (4) and (7),

$$P_{\text{no reaction}_b} = e^{-\int_{E_0}^{E_{th}} n_i N_{fb} \sigma_{R_b}(E) \frac{V dE}{(\partial E / \partial t)_{\text{tot}}} } \quad (89)$$

Finally, employing Eq. (87),

$$P_{\text{no reaction}_b} = e^{-\int_{E_0}^{E_{th}} \frac{(\partial E / \partial t)_b^R}{(\partial E / \partial t)_{\text{tot}}} \frac{dE}{E}} \quad (90)$$

The probability of a reaction in slowing down from E_0 to E_{th} is then

$$P_{\text{reaction}_b} = 1 - P_{\text{no reaction}_b} \quad (91)$$

J. Parametric Scaling Variables

Consider a test particle slowing down predominantly by Coulomb scattering in a plasma in which the ion constituents are replaced by an average. If it is assumed that (see Eq. (13)) $x_e \ll 1$ and $x_i \gg 1$, Eq. (30) and (31) become¹²

$$-\left(\frac{\partial E}{\partial t}\right)_e^C = \frac{E}{t_E} \quad (92)$$

and

$$-\left(\frac{\partial E}{\partial t}\right)_i^C = \frac{\gamma}{E^{1/2}} \quad , \quad (93)$$

where t_E is the energy relaxation time for scattering from electrons,

$$\frac{1}{t_E} = \left(\frac{4\pi e^4}{m_e}\right) \frac{Z_E^2 E^{1/2}}{V} n_i L_e \frac{4}{3\sqrt{\pi}} \left(\frac{A_e}{A}\right)^{3/2} \frac{\bar{Z}}{(kT_e)^{3/2}} \quad (94)$$

and γ being equal to

$$\gamma = \left(\frac{4\pi e^4}{m_e}\right) \frac{A_e Z_E^2 E^{1/2}}{V} n_i \bar{L}_i \left(\frac{\bar{Z}_i^2}{A}\right) \quad (95)$$

The arguments of the Coulomb log follow from Eqs. (34) - (36) with Z_b being replaced by $\bar{Z}$ and the relative energies by $(3kT/2)$. Using Eq. (92) and (93), Eq. (4) may be expressed as

$$\frac{dE}{(\partial E/\partial t)_{\text{tot}}} = t_E \frac{U^{1/2} dU}{1 + U^{3/2}} \quad , \quad (96)$$

where

$$U = \frac{E}{(\gamma t_E)^{2/3}} \quad . \quad (97)$$

The integrals for the thermalization time, energy partitions, and range may now be carried through analytically. Of course, in the general case of a multiconstituent plasma in which nuclear scattering and reactions are considered, Eq. (92) and (93) are not valid. The parameter U however still may be useful as a convenient fitting variable.

One final parameter of interest is the energy dependent 90° deflection time, defined as¹².

$$t_D(E) = t_D(1)E^{3/2}, \quad (98)$$

where

$$t_D(1) = \frac{1}{2\pi Z^2 e^4 L_i n_i \overline{Z_i^2}} \frac{M^{1/2}}{2^{1/2}}. \quad (99)$$

III. GENERAL CODE COMMENTS

Some general comments are as follows:

1. The code is setup to operate on the LLL CDC 7600 computers.
2. Up to five ion constituents may be specified in the plasma.
3. Linear-linear interpolation is used with all input cross sections. These cross sections are identically zero outside the energy bounds on input.
4. A single disc file, INPUT, is required. This file contains the parameter cards for the run and its format is described in the next section. There is both HSP output (described in the OUTPUT section) as well as a BCD dump file, EDOTOUT. This latter file contains essentially the same information as the HSP file but in a more compact form suitable for additional processing. Any one interested in this file's format should contact the author. All units are MeV, cm, gm, shake, and barn (cross sections).
5. The technique of performing integrations is as follows: On input, the linearity convergence criteria, DIE, is specified. A general mesh is setup on test particle energy by calculating and thinning $(\partial E/\partial t)_{\text{tot}}$ so that it is linear-linear interpolable¹³ to a criteria specified by DIE/20. All input energies in the cross section tables are also given within this mesh. The thermalization time and range integrations are then carried out analytically. Furthermore, assuming that all partial $\partial E/\partial t$'s are also linear-linear interpolable on this mesh allows the energy partition integrals to be carried through analytically. All other integrals

are carried through by thinning the integrand so that it is linear-linear interpolable¹³ to a criteria specified by DIE and then analytically performing the integrations. Finally, the number of points in the knockon spectra is obtained by thinning the spectra so that it is linear-linear interpolable¹³ to a criteria specified by 10*DIE.

IV. INPUT

The input description for the disc file, INPUT, is described in Table I below.

TABLE I
EDOT Input Data (Disc File INPUT)

Card Type	Column(Format)	Parameter	Description
Problem	1-3 (i3)	ITOT	No. problems in run.
	4-8 (F5.4)	DIE	Linearity convergence criteria; usually 0.001.
	9 (i1)	IPOPT	Printout option: = 0 is normal printout; = 1 is detailed printout.
	10 (i1)	IPARA	Problem input type parameter: = 0 each problem is completely independent; = 1 first problem is base calculation with consecutive problems only reading in RHO, TE, TI, GAMMAI, and IGAMC.
	11 (i1)	ISAME	Particle type parameter: = 0 particles are treated as both like and unlike (normal operation); = 1 all particles treated as unlike.
Test Particle	1-11 (E11.4)	E0	Incident energy (MeV).
	12-22 (E11.4)	A	Atomic weight (amu).
	23-33 (E11.4)	AA	Charge number, $Z = AA \cdot V + BB$ where V is particle speed (cm/sh).
	34-44 (E11.4)	BB	See AA above.
	45-55 (E11.4)	GAMMAI	Test particle floor energy (MeV). If GAMMAI = 0., it is set internally to $1.5 \cdot TI$.

TABLE I (continued)

Card Type	Column(Format)	Parameter	Description
Total Plasma	1-11 (E11.4)	RHO	Density (gm/cm^3).
	12-22 (E11.4)	TE	Electron temperature (MeV).
	23-33 (E11.4)	TI	Ion temperature (MeV).
	34-36 (i3)	JTOT	No. of materials in plasma (≤ 5).
	37-38 (i2)	IGAMC	Ion screening option. If IGAMC = 0, γ calculated by code (see Eq. (18)). If IGAMC = 1, $\gamma \equiv 1$.
Plasma Material	1-11 (E11.4)	AF	Atom fraction (sum of atom fractions does not need to total unity as it is normalized in the code).
	12-22 (E11.4)	ZI	Charge number.
	23-33 (E11.4)	AI	Atomic weight (amu).
	34-36 (i3)	JNUC	No. of ES, SIG (energy, cross section) pairs for nuclear scattering. = 0 is no nuclear scattering. (≤ 50).
	37-47 (E11.4)	ECUT	Knockon spectra floor (MeV). = 0. is no knockon spectra calculation.
	48-50 (i3)	IGPTN	No. of groups for knockon spectra. Only used when ECUT>0. = 0 is no group calculation. Same group structure is used for all materials. (≤ 100).
	51-53 (i3)	JREA	No. of ER, SIGR (energy, cross section) pairs for reaction. = 0 is no reaction. (≤ 150).

TABLE I (continued)

Card Type	Column(Format)	Parameter	Description
Nuclear Scattering (JNUC cards)	1-11 (E11.4)	ES	Energy (test particle) for scattering cross section. The values of ES are in ascending energy. (MeV).
	12-22 (E11.4)	SIG	Corresponding cross section (barns).
Reaction (JREA cards)	1-11 (E11.4)	ER	Energy (test particle) for reaction cross section. The values of ER are in ascending energy. (MeV).
	12-22 (E11.4)	SIGR	Corresponding cross section (barns).

Repeat Plasma Material, Nuclear Scattering, and Reaction cards for second, etc. up to JTOT plasma constituents.

Group Boundaries	1-11 (6E11.4)	GPBND	Lower energy boundary of group. Must be in order of increasing energy with GPBND(1) = 0. (IGPTN values) (MeV).
	12-22		
	etc.		

Read input data for next problem. If IPARA (Problem card) = 0, start over again with Test Particle card and continue up through Group Boundaries cards. If IPARA = 1, read the following card.

Short Input	1-11 (E11.4)	RHO	Density (gm/cm ³).
	12-22 (E11.4)	TE	Electron temperature (MeV).
	23-33 (E11.4)	TI	Ion temperature (MeV).

TABLE I (continued)

Card Type	Column(Format)	Parameter	Description
Short Input (continued)			
	34-44 (E11.4)	GAMMAI	Test particle floor energy (MeV). If GAMMAI = 0., it is set internally to $1.5 \cdot T_I$.
	45-46 (i2)	IGAMC	Ion screening option. If IGAMC = 0, γ calculated by code (see Eq. (18)). If IGAMC = 1, $\gamma \equiv 1$.

Repeat reading problem input for all TTOT problems in the run.

V. OUTPUT

The HSP output is in an abbreviated people readable form and is available in both a normal and a detailed printout, depending on the value of the input parameter, IPOPT. In both cases the index J is on the plasma constituent and the index K is on the energy mesh for the test particle. The detailed printout contains the normal printout plus supplemental information on the slowing down parameters (Coulomb logs, relative energies, cross sections, breakdown of $(\partial E/\partial t)_{\text{tot}}$ into type and plasma constituent, etc.) as well as on the knockon spectra (spectral limits, rate parameters and integral parameters, e.g., breakdown of number of collisions and energy depositions). Its usefulness is in interpretation of the results, i.e., what type of slowing down mechanism is domineering and on what plasma constituent and over what test particle energy range. Anyone desiring further information on the detailed printout should contact the author.

The tables in the normal printout are described below:

Initial and Boundary Conditions - test particle description, plasma properties and description of plasma constituents including both nuclear scattering and reaction cross sections.

Test Particle Integral Slowing Down Properties - energy, speed, charge, $(\partial E/\partial t)_{\text{tot}}$, time, $(\partial E/\partial s)_{\text{tot}}$, range, density times the range, and flux, i.e., $-1/(\partial E/\partial s)_{\text{tot}}$.

Energy losses and partitions - DEL is the energy loss, broken up as to TOT(total), E(electrons), IC(ion Coulomb), IN(ion nuclear), R(reaction) as well as the fraction into the electrons and ions.

Knockon Spectra above E cut - NTOT is the integral of the spectra, DEL is the energy in the spectra, and $ER-AVER = DEL/NTOT$ is its average energy. PI is the normalized spectra and INT is its cumulative distribution. Tables are presented for both ion Coulomb and nuclear scattering.

Group Integrated Spectra above ECUT - Group boundaries and integrated spectra (over the groups).

In-flight Reaction Probability - See Section II-I.

Parametric Scaling Variables - See Section II-J.

Total Energy and Particle Summary per Test Particle - Breakdown of all energy losses as well as total number of knockon ions for each plasma constituent.

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4. S. T. Perkins, "Approximate Material Temperature and Boundary Motion Corrections for Local Energy Deposition Due to Elastic Scattering," UCID-17533, Lawrence Livermore Laboratory (1977).
5. L. Spitzer, Jr., *Physics of Fully Ionized Gases*, (Interscience Publishers, 1962) 2nd revised edition.
6. With the conversion ratios:

$$\frac{4\pi e^4}{m_e} = 4.582 \times 10^{-20} \text{ MeV cm}^4/\text{sh}^2 ,$$

$$A_e = 0.5488 \times 10^{-3} \text{ amu} ,$$

$$\pi^{1/2} e^3 = 9.684 \times 10^{-20} \text{ MeV}^{3/2} \text{ cm}^{3/2} ,$$

$$\alpha(2m_e c^2)^{1/2} = 7.377 \times 10^{-3} \text{ MeV}^{1/2} ,$$

and with

$$V = 13.89 E^{1/2}/A^{1/2} ,$$

and E and kT in MeV, V in cm/sh, n in particles/cm³, ρ in gm/cm³, our units for $\partial E/\partial t$ are MeV/sh. Note that 1 sh = 1 shake = 10⁻⁸ seconds.

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8. This cross section also contains the Coulomb-nuclear scattering interference terms. See Ref. 7 for additional details on this point.
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