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FEB 78 J R TRIPLET, M H RICE

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6 ANALYSIS OF LASER-SUPPORTED DETONATION WAVES AND LASER BEAM PROPAGATION IN TWO DIMENSIONS.

10 J. R. TRIPLET
M. H. RICE

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ABSTRACT

It is shown that the Flux-Corrected Transport (FCT) algorithm correctly computes the propagation velocity and Chapman-Jouquet pressure for a laser-supported detonation (LSD) wave, even for zone size large compared to the radiation absorption length. A two-dimensional FCT computer program for analysis of LSD wave propagation phenomena is presented. A trajectory method for analysis of two-dimensional laser beam propagation in the paraxial Fresnel approximation, with continuously varying refractive index, is described.

1. INTRODUCTION

The developments described below constitute the initial portion of an effort to develop and apply efficient, versatile analytic techniques for the analysis of laser beam propagation and laser-target interactions. The two problems addressed in the report are described below.

1.1 EVALUATION OF NON-ADIABATIC SHOCK PROPAGATION

A two-dimensional hydrodynamics computer code was written using the FCT (Flux-Corrected Transport) method developed at NRL [References 1-5]. The performance of this code in describing the propagation of laser-supported detonation waves was studied in some detail from the standpoint of thermodynamic validity for the case of one-dimensional wave propagation; initial testing of two-dimensional detonation wave propagation was also carried out. The results in both cases appear to be highly satisfactory. The code listing is presented in Appendix I.

1.2 LASER-BEAM PROPAGATION IN PLASMAS

Two-dimensional methods for computing refraction and Fresnel diffraction of laser beams in plasmas and partially-ionized gases were devised, using a trajectory approach of the general type suggested by Glass.^[6] A computer code employing these methods is under development. A code listing is presented in Appendix II, representing the implementation of the text formulation at an incomplete stage of testing.

2. FLUX-CORRECTED TRANSPORT (FCT) APPLIED TO ONE-DIMENSIONAL LASER-SUPPORTED DETONATION (LSD) WAVE PROPAGATION

In this section the results of a series of calculations using the FCT method to describe the propagation of one-dimensional LSD waves are presented. The object is to determine the accuracy with which the numerical method reproduces such details of a steady-state wave as the spike pressure, the Chapman-Jouguet (CJ) pressure, and the propagation velocity.

2.1 EQUATION OF STATE

The equation of state used for these calculations is that of an ideal gas modified to allow for single ionization. The specific internal energy is related to the temperature and specific volume by

$$E = \frac{1}{2} RT \left[f + 3x + \frac{2\epsilon_0}{kT} x \right], \quad (1)$$

where R is the gas constant (per gram), T is the temperature in kelvins, f is the number of degrees of freedom, k is the Boltzmann constant, ϵ_0 is the ionization potential, and x is the fraction of molecules which are ionized. It is related to the temperature and specific volume, V , by the Saha equation

$$\frac{x^2}{1-x} = AVT^{3/2} \exp(-\epsilon_0/kT) \quad (2)$$

where the constant A is given by

$$A = \frac{g_e g_i}{g_a} \frac{M}{N_0} \left[\frac{2\pi m_e k}{h^2} \right]^{3/2},$$

where M is the gram molecular weight, N_0 is Avogadro's number, m_e is the electronic mass, and h is Planck's constant. With $g_e = 2$ and $g_i/g_a = 1.9$ (the weight factor for ions relative to atoms), the numerical value for A corresponding to a molecular weight of $M = 28$ g/mole is

$$A = 4.2662 \times 10^{-7} \text{ g cm}^{-3} \text{ K}^{-3/2}.$$

Given values for the specific volume and internal energy (the calling arguments from the hydrodynamic subroutine), the temperature is obtained from Equations (1) and (2) by an iterative procedure. The pressure is then calculated from the ideal gas relation,

$$PV = R(1 + x)T. \quad (3)$$

The equation of state subroutine used for the above calculations also returns values of the sound speed for use in determining the time-step. A Fortran listing is given in Appendix I.

2.2 STRUCTURE OF A ONE-DIMENSIONAL LSD WAVE

A qualitative sketch of the structure of a steady-state, one-dimensional LSD wave is given in Figure 1. An initial shock at the spike pressure preheats and partially ionizes the gas, providing the free electrons necessary to initiate absorption from the incident beam. As the energy absorbed increases through the absorption front, the pressure decreases and the temperature and specific volume increase until the CJ point is reached, at which point essentially all of the incident beam energy has been absorbed by the gas.

The quantitative determination of the spike and CJ pressures for a given laser flux is indicated in Figure 2. The Hugoniot relation for conservation of energy for a steady

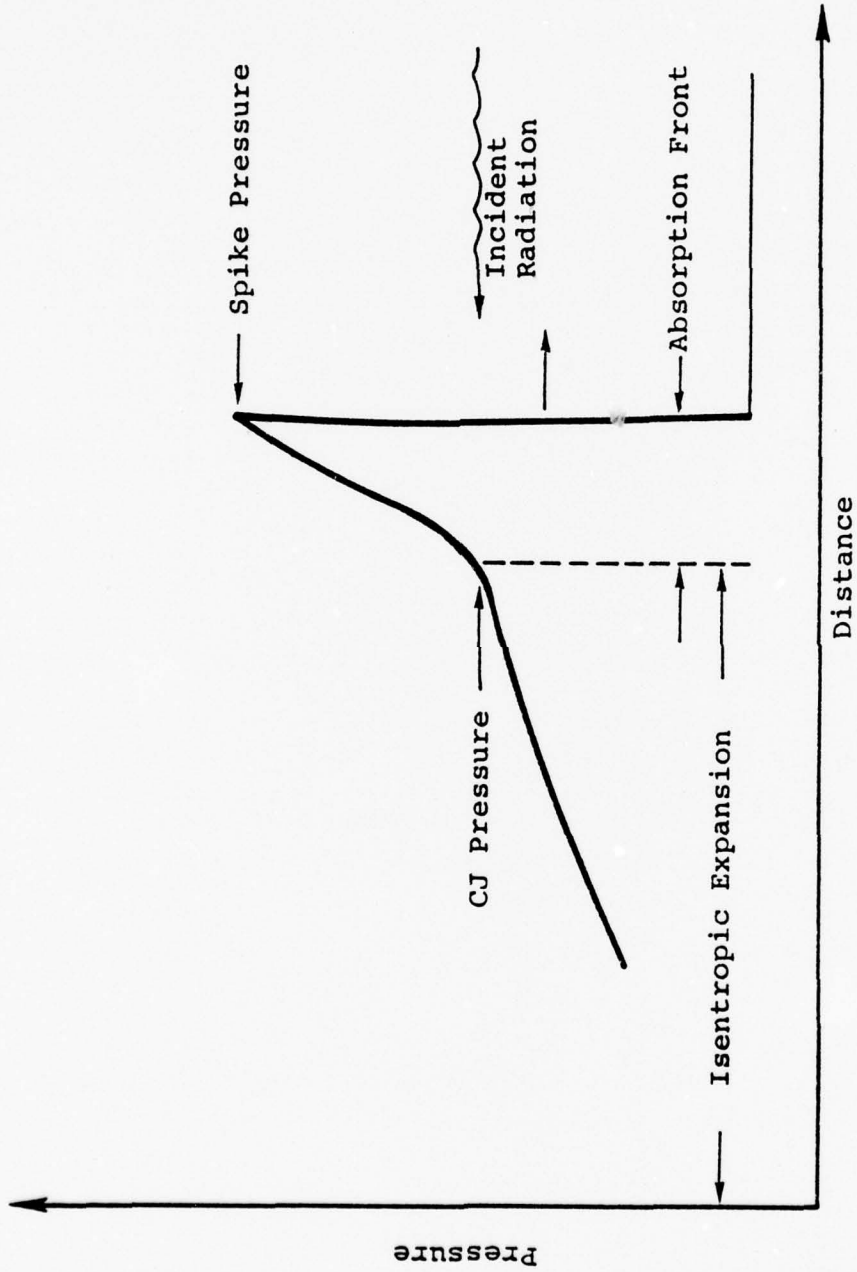


Figure 1. Structure of a LSD wave (schematic).

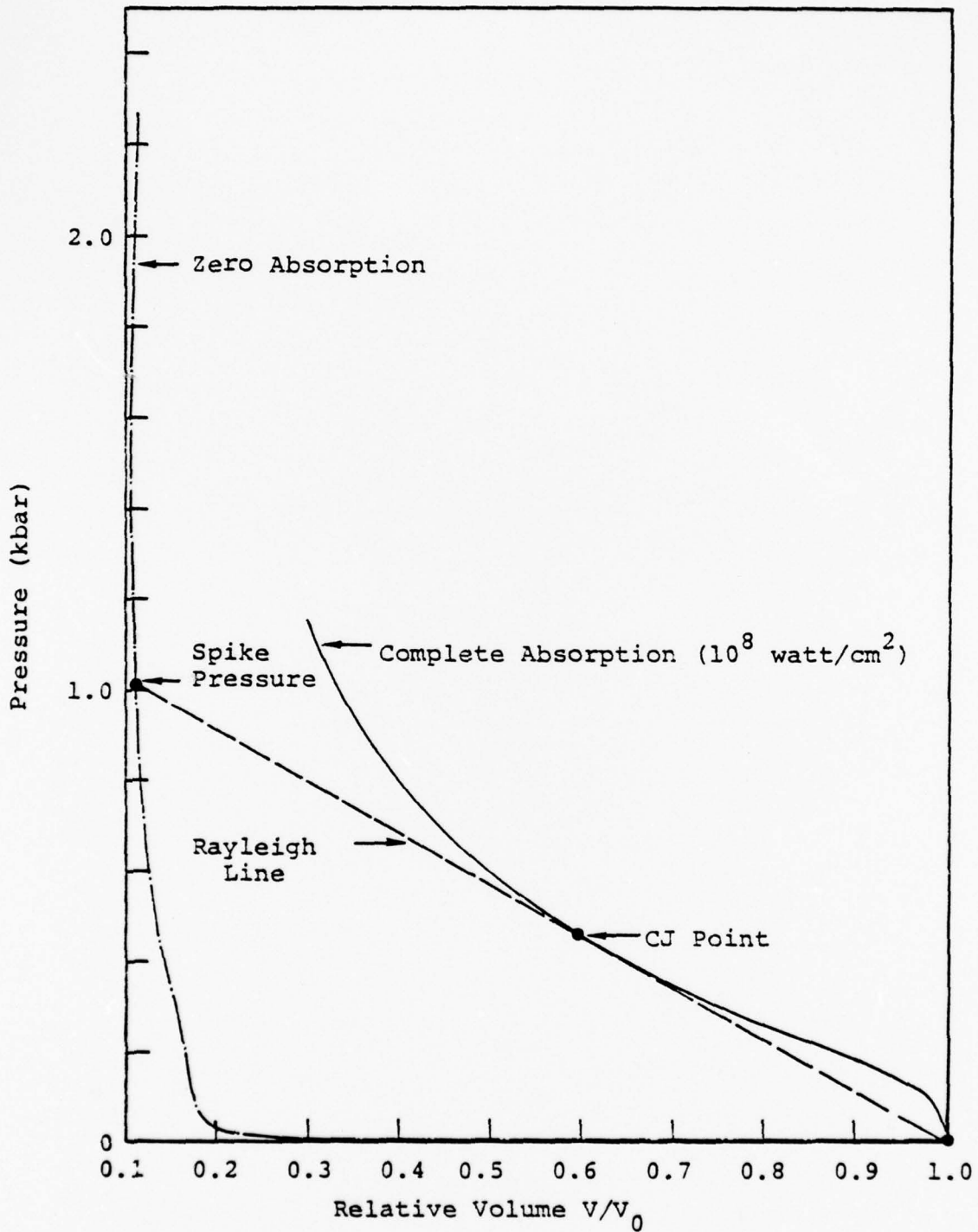


Figure 2. Hugoniot for an ionizable ideal gas corresponding to zero energy absorption and to complete energy absorption for a laser beam flux of 10^8 watt/cm².

state absorption wave connecting an initial state P_0, V_0, E_0 to a final state P, V, E (Figure 3) is

$$E - E_0 = \frac{1}{2} (P + P_0) (V_0 - V) + \frac{G}{\rho_0 D}, \quad (4)$$

where G is the laser flux (erg/cm²/sec) and D is the wave velocity, which for a steady-state wave is related to the pressure and volume by

$$D = V_0 \sqrt{\frac{P - P_0}{V_0 - V}}. \quad (5)$$

The curve labeled "Complete Absorption" in Figure 2 is the Hugoniot as calculated from Equation (4), the P, V, E equation of state as described in Section 2.1, and a laser flux G of 10^8 watt/cm². The initial state is $P_0 = 10^6$ dyne/cm², $T_0 = 298.16$ kelvins, $V_0 = 885.4$ cm³/g, and $E_0 = 2.213 \times 10^9$ erg/g. The parameters used in the equation of state are:

$$f = 5$$

$$R = 2.9694 \times 10^6 \text{ erg/g/K}$$

$$E_0 = 14.4 \text{ eV}$$

$$A = 4.2662 \times 10^{-7} \text{ g cm}^{-3} \text{ K}^{-3/2}$$

The CJ point is that point at which the Rayleigh line is tangent to the Hugoniot curve, as indicated in Figure 2. The spike pressure is given by the intersection of this same Rayleigh line with the Hugoniot corresponding to zero energy absorption (calculated from Equation (4) with $G = 0$). For this equation of state and a flux of 10^8 watt/cm², the spike pressure is 1.0 kbar, the CJ pressure is 0.45 kbar, and the wave speed is 10.0×10^5 cm/sec.

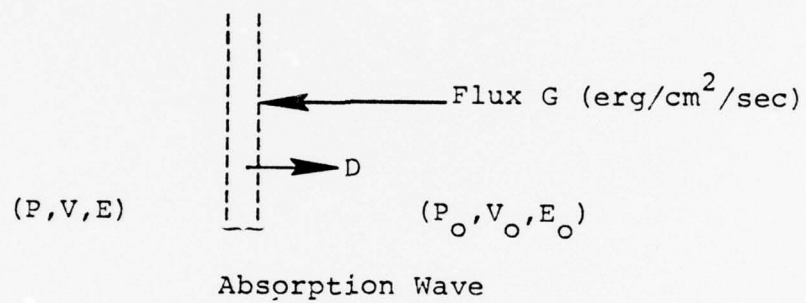


Figure 3. Steady-state absorption wave connecting initial state P_0, V_0, E_0 to final state P, V, E .

2.3 NUMERICAL METHOD

The Fortran listings of the one-dimensional FCT modules as given by Boris,^[1] modified where necessary to allow for running on the CDC-7600 and Univac 1108 computers, have been incorporated into a preliminary two-dimensional test code. A complete listing is given in Appendix I. The subroutine UPDATE is a realization of the two-dimensional time-splitting procedure as outlined in Reference [2]. The calculations reported here were done using the one-dimensional option, which is capable of operating in either the Eulerian or the Lagrangian mode.

The flux-corrected transport method has been discussed in a series of papers.^[1-5] Briefly, it solves the generalized continuity equation of the form

$$\frac{\partial \phi}{\partial t} + \frac{1}{r^m} \frac{\partial}{\partial r} (r^m \phi u) = \text{Source Terms} , \quad (6)$$

where the terms on the left are the one-dimensional equivalent of $(\partial \phi / \partial t) + \nabla \cdot (\phi \bar{u})$. Specifically, in the present case the algorithm is applied in succession to the three equations,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0, \quad (7)$$

$$\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2) = - \frac{\partial P}{\partial x} , \quad (8)$$

$$\frac{\partial \epsilon}{\partial t} + \frac{\partial}{\partial x} (\epsilon u) = - \frac{\partial}{\partial x} (P u) , \quad (9)$$

where

$$\epsilon \equiv \rho \left(E + \frac{1}{2} u^2 \right) . \quad (10)$$

An alternative form of the last equation is

$$\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x} (\rho E u) = - P \frac{\partial u}{\partial x} . \quad (11)$$

In the above equations, which represent the conservation of mass, momentum and energy, respectively, ρ is the density, u is the material velocity, P is the pressure, x is the Eulerian space coordinate, and E is the specific internal energy (erg/g).

2.3.1 Absorption Coefficient

The laser beam intensity as a function of position for one-dimensional propagation in an absorbing medium is given by

$$I = I_0 \exp \left[- \int_{x_0}^x k_\nu dx \right] .$$

The resulting expression used to compute the increase in specific internal energy within a computational zone in time Δt is

$$\rho_m \Delta E_m = I_{m+1} \left[1 - \exp \left(- k_\nu |\Delta x| \right) \right] \frac{\Delta t}{\Delta x} \text{ erg/cm}^3 , \quad (12)$$

where I_{m+1} is the intensity (erg/cm²/sec) incident on the right interface of the zone. The absorption coefficient k_ν for a laser frequency ν is given by the sum of the absorption coefficients for free-free transitions in the ionic and atomic fields,

$$k = k_{\nu,i} + k_{\nu,a} , \quad (13)$$

which are given by the formulae^[7]

$$k_{v,i} = B_1 Z^2 \lambda^3 x^2 T^{-1/2} (\rho^2/M^2) x [1 - \exp(-hv/kT)] \quad (14)$$

$$k_{v,a} = B_2 \sigma \lambda^3 x(1-x) T^{3/2} (\rho^2/M^2) [1 - \exp(-hv/kT)] \quad (15)$$

where Z is the degree of ionization (equal to 1.0 for these calculations), λ is the laser wavelength in μm , x is the fraction of ionization from Equation (2), M is the gram molecular weight, and σ is the collisional cross-section between electrons and molecules, which was assigned the value 10^{-15} cm^2 . The expressions for the numerical coefficients in the above expressions are

$$\begin{aligned} B_1 &= \frac{4}{3} \left(\frac{2\pi}{3m_e k} \right)^{1/2} \frac{e^6 N_{av}^2}{m_e c^4} \times 10^{-12} \\ &= 4.97 \times 10^{12} \text{ microns}^3 \text{ K}^{1/2} \text{ cm}^5 \text{ mole}^{-2} \end{aligned}$$

$$\begin{aligned} B_2 &= \left(\frac{2k}{\pi m_e} \right)^{3/2} \frac{e^2 N_{av}^2}{hc^4} \times 10^{-12} \\ &= 4.69 \times 10^{17} \text{ micron}^{-3} \text{ K}^{-3/2} \text{ cm}^3 \text{ mole}^{-2} \end{aligned}$$

Actually, the precise form of the density and temperature dependence of the absorption coefficient was of little consequence for these calculations, since the detailed structure within the absorption wave was not of interest. For example, at the CJ point corresponding to a flux of 10^8 watt/cm^2 , the specific volume is $524 \text{ cm}^3/\text{gm}$, the temperature is 41,500 kelvins, and the absorption coefficient as calculated from Equations (14) and (15) for a 10.6 micron laser wavelength is 4100 cm^{-1} , i.e., the absorption front is of the order of 10^{-4} cm thick. Thus, extremely fine zoning

is required to resolve the structure of the absorption front itself.

2.3.2 Test Calculations

The ability of the FCT method to describe the development and propagation of an LSD wave using a zoning which is coarse with respect to the physical thickness of the absorption front is shown in Figure 4. The calculational configuration consists of 200 zones, each 0.01 cm thick, with a rigid wall for the left boundary. The wave was "ignited" by an initial heating of the first three computational zones. An initial energy in these zones of 3.96×10^{11} erg/g at the ambient density of 1.1295×10^{-3} g/cm³ results in an initial pressure of 96.8 bars, and an initial temperature of 20,360 kelvins, which produces sufficient initial absorption for wave development. The energy in this calculation was updated with Equation (9).

Since the zone width of 0.01 cm is approximately 40 times the absorption length at the CJ point, all of the beam energy is absorbed in one computational zone, and, as expected, such details as the 1.0 kbar spike pressure are not reproduced by the calculation. The other features of the wave profile are reproduced quite well, however. As shown in Figure 4, the wave profiles behind the "pseudo" spike correlate very well with the analytical value of 0.45 kbar at the CJ point and with the analytical values of the slopes at the CJ point as obtained with a simple rarefaction wave centered at $x = 0$:

$$\left(\frac{\partial P}{\partial x}\right)_{CJ} = \frac{\rho c^2}{\left[1 + \frac{\rho}{2} \frac{d(c^2)}{dP}\right] x} \quad (16)$$

where the square of the sound speed, c^2 , and the density, ρ ,

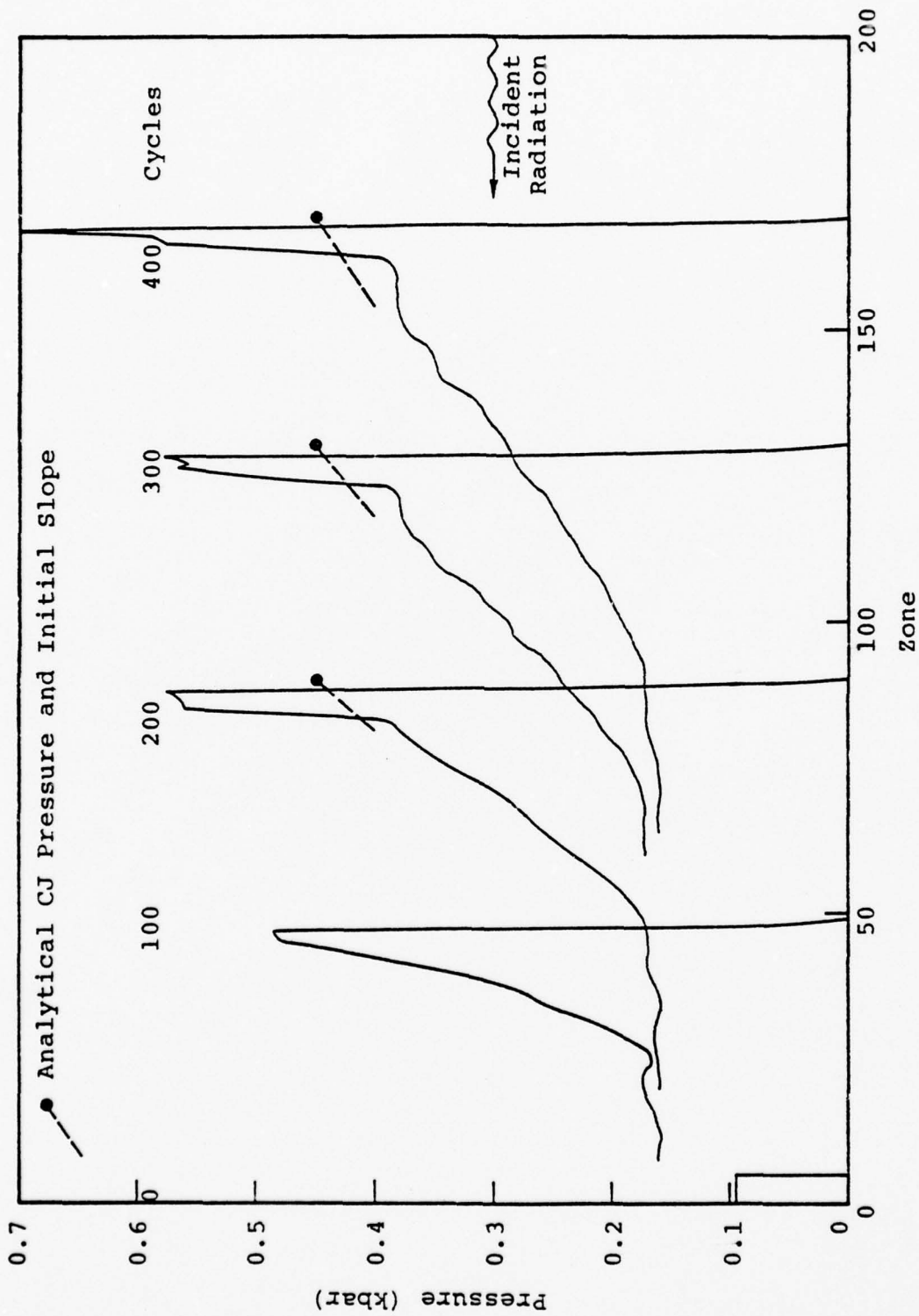


Figure 4. Eulerian FCT calculation of a LSD wave for a flux of 10^8 watt/cm². The zone width of 0.01 cm is coarse with respect to the absorption length.

are the values at the CJ point,

$$\begin{aligned} c^2 &= 3.56 \times 10^{11} \text{ cm}^2/\text{sec}^2 \\ &= 1.91 \times 10^{-3} \text{ g/cm}^3 \end{aligned}$$

$$\frac{d(c^2)}{dP} = 271 \text{ (cm}^2/\text{sec}^2)/(\text{dyne/cm}^2) .$$

In the interval between 100 cycles (0.466 μsec) and 400 cycles (1.668 μsec), the peak wave pressure progresses from zone 47 to zone 167. The corresponding average wave speed D is then 9.98×10^5 cm/sec, in agreement with the analytical value of 10.0×10^5 cm/sec. Finally, the steady-state pressure at the left boundary is about 0.16 kbar, also in agreement with the analytic value of ~ 0.159 kbar. The conclusion is that the FCT method can propagate an LSD wave properly even with zoning which is much too coarse to resolve the structure within the actual absorption front.

The results of a calculation identical to that described above except that the zone size has been decreased from 0.01 cm to 5.0×10^{-5} cm are given in Figure 5. For this calculation the energy absorption front is about five zones thick, and as a result, the calculated spike pressure of ~ 0.9 kbar is more nearly equal to the analytic value of 1.0 kbar. The ripples superimposed on the rarefaction following the spike are not physical, but are an example of a nonlinear numerical error called "terracing". This type of error, which occurs on the flanks of steep gradients, is discussed in Reference [2].

The two calculations described above were done using the FCT modules in the Eulerian mode, i.e., the zone boundaries were fixed in space. The results of a calculation using the Lagrangian mode are shown in Figure 6. The initial

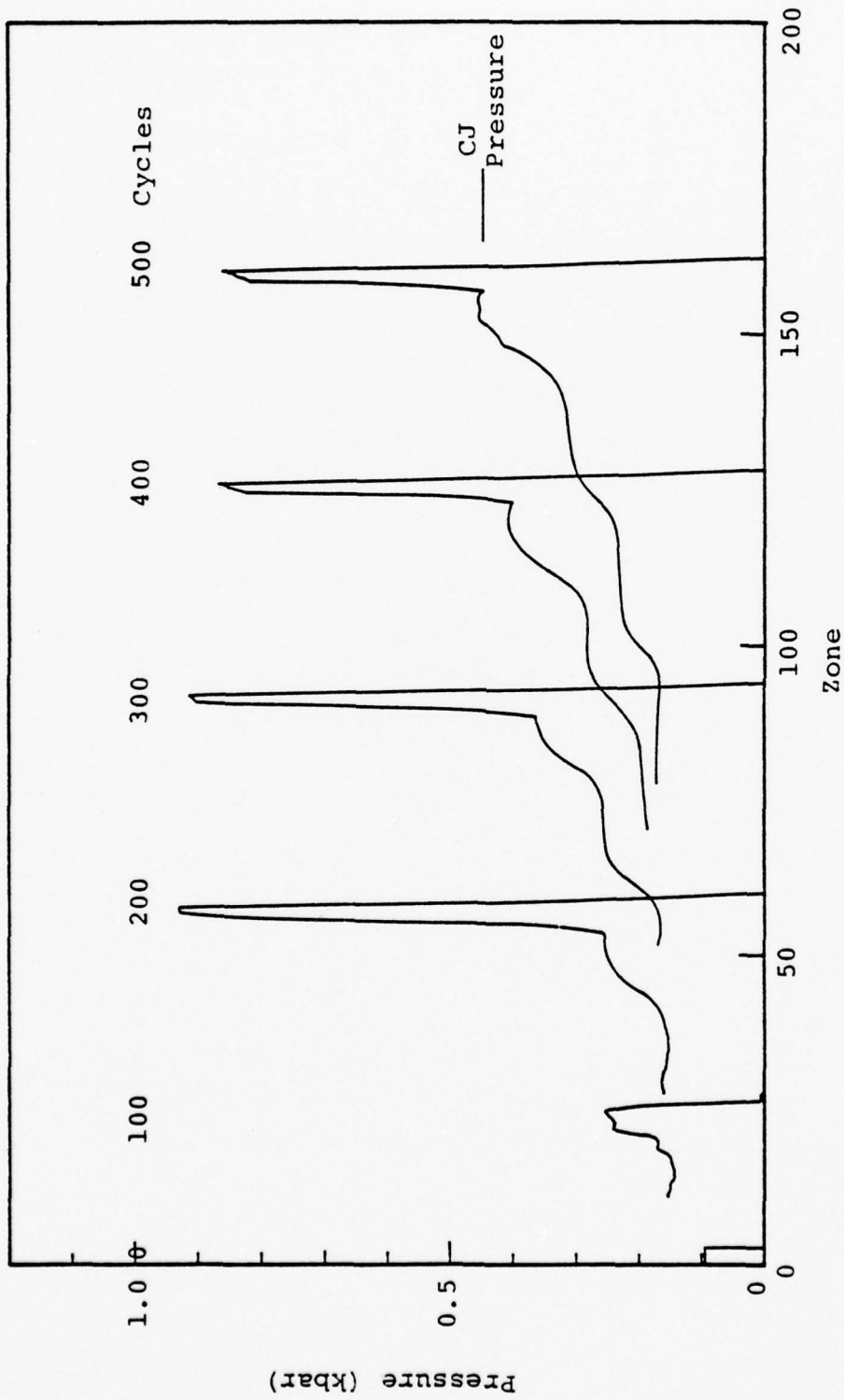


Figure 5. Eulerian FCT calculation of a LSD wave for a flux of 10^8 watt/cm². The zone width of 5.0×10^{-5} cm is of the order of the absorption length.

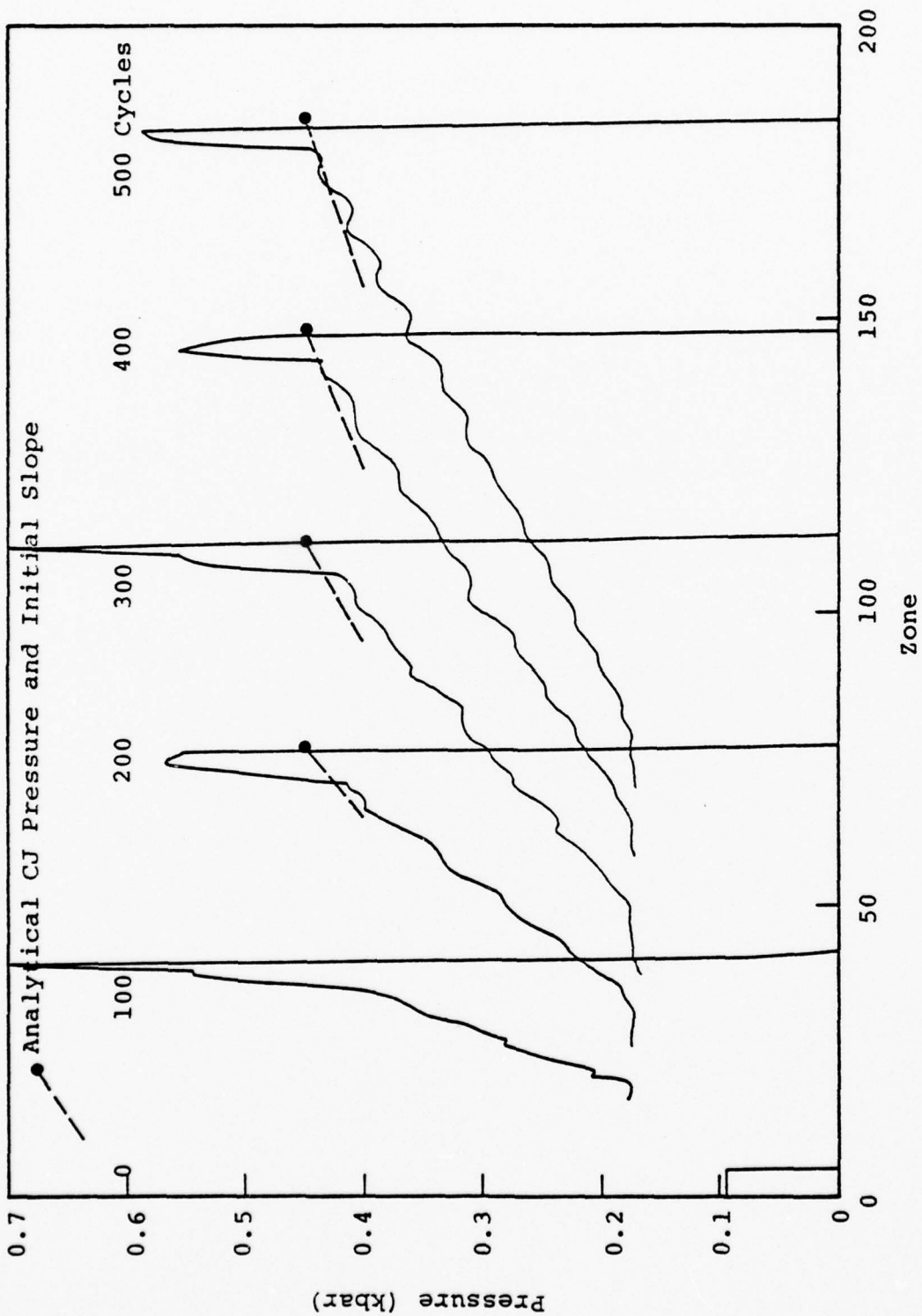


Figure 6. Lagrangian FCT calculation of a LSD wave for a flux of 10^8 watt/cm². The initial zone width of 0.01 cm is coarse with respect to the absorption length.

zone width was 0.01 cm, as in the first calculation, but the zone boundaries were allowed to move with the material velocity at each point. This calculation also reproduced the main features of the wave quite well, even though the initial zone width was very large compared with the absorption length. The average wave speed from cycle 100 (0.3999 μ sec) to cycle 500 (1.8182 μ sec) was 10.0×10^5 cm/sec, in agreement with the analytic value of 10.0×10^5 cm/sec for a flux of 10^8 watt/cm². The wave profiles also correlate well with the pressure and the initial slope at the CJ point. It will be noticed from Figure 6 that the peak pressure of the pseudo spike fluctuates considerably as the wave progresses. This fluctuation is a result of the coarse zoning, but it is not an instability; it arises because at times the conditions at the shock front are such that the energy absorption occurs across two computational zones instead of one. When this happens, the pressure in the first zone approaches more nearly the analytical spike pressure.

The results of a calculation to check the use of an artificially long absorption length are shown in Figure 7. The zone width for this Eulerian calculation was 0.01 cm; but if the value of k_ν as calculated from Equations (14) and (15) was such that $k_\nu |\Delta x| > 1.0$, it was reset to 1.0 for that zone. In other words, the beam intensity was not allowed to decrease by more than a factor of e^{-1} across any computational zone. The result of this numerical limiting is an absorption-front thickness of four or five computational zones; and, as expected, the peak spike pressure is close to the analytical value of 1.0 kbar for a flux of 10^8 watt/cm². A disadvantage of artificially limiting the absorption coefficient is that the time required to attain steady state is unrealistically long. From Figure 7 it is seen that even after 400 computational cycles, or a travel of 1.4 cm, the pressure behind the spike has still not reached the steady-state CJ value of 0.45 kbar.

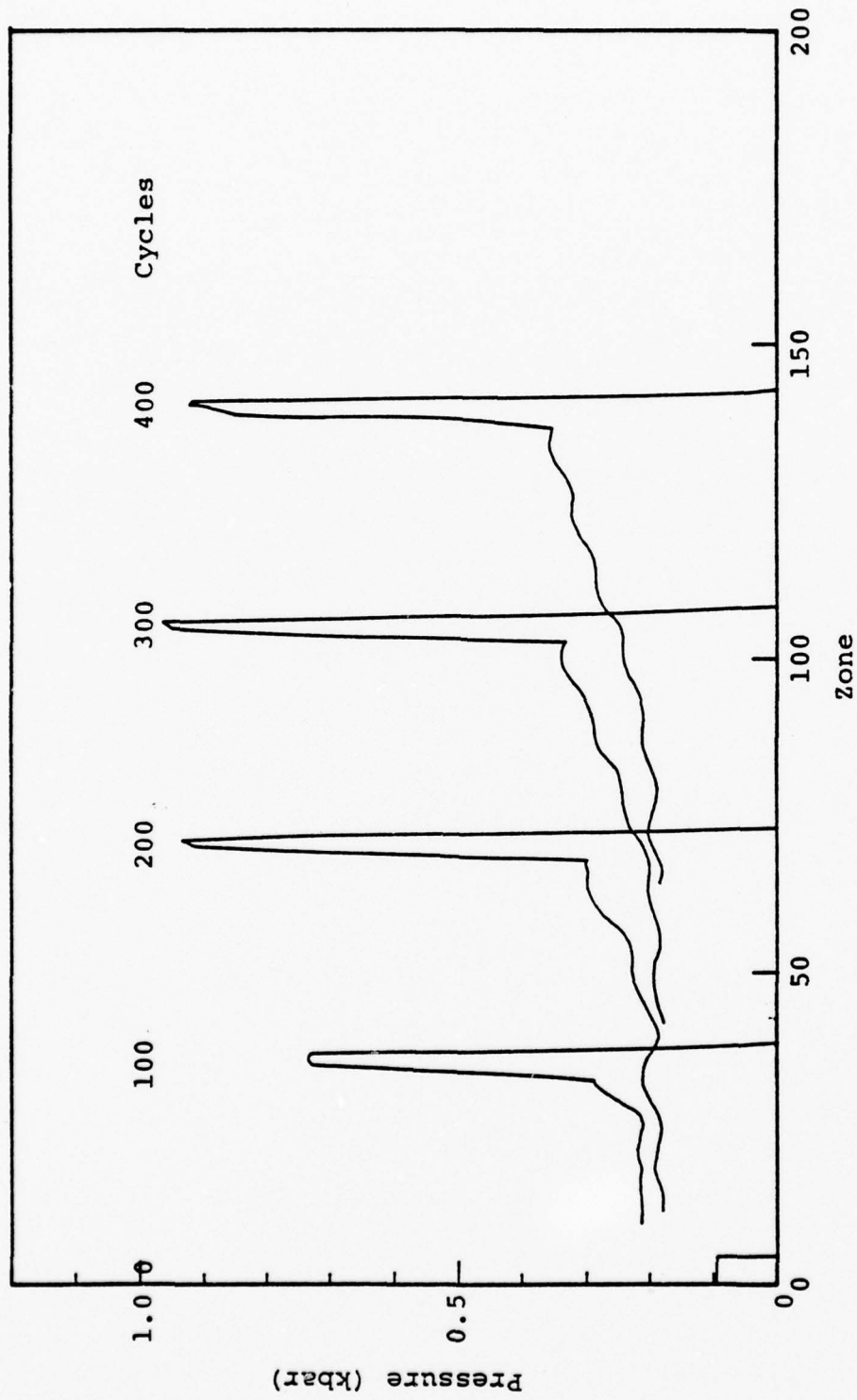


Figure 7. Eulerian FCT calculation of a LSD wave for a flux of 10^8 watt/cm². The absorption length has been artificially forced to be of the same order as the zone width of 0.01 cm.

2.4 CONCLUSIONS

The FCT method is a convenient and satisfactory numerical procedure for describing the propagation of one-dimensional LSD waves. In particular, the method yields satisfactory results even for zoning which is much too coarse to resolve the structure within the energy absorption front.

3. LASER BEAM PROPAGATION IN GASES AND PLASMAS

The propagation of a laser beam is a highly specialized problem from the standpoint of radiation transport in general, since the radiation field is very sharply peaked with respect to both angular distribution and frequency distribution. These characteristics can only be maintained in a material medium whose properties vary continuously and slowly over finite intervals of space and time, so that the variations may be considered as perturbations within these intervals. At the boundaries of such intervals, discontinuous material properties may be taken into account in the beam model by introducing additional beams; such may also originate in the interior of an interval by means of stimulated Raman scattering and similar processes. In this section the propagation of a single beam within a continuous medium will be discussed. The properties of the medium will be assumed given, although they may depend in various ways upon the radiation field itself.

For a beam with axis in the z direction in a medium with complex refractive index, n , the amplitude E satisfies the scalar wave equation

$$\nabla^2 E + \frac{\partial^2 E}{\partial z^2} - \frac{n^2}{c^2} \frac{\partial^2 E}{\partial t^2} = 0 \quad (17)$$

where the ∇ operator is restricted to the x - y plane. The perturbation formulation discussed above suggests that the amplitude be written as the product of a slowly-varying envelope and a fast unperturbed part:

$$E(x, y, z, t) = \psi(x, y, z, t) e^{i(k_0 z - \omega_0 t)} \quad (18)$$

where ω_0 is the central laser beam frequency and $k_0 = n_0 \omega_0 / c$,

with n_0 being a constant real index of refraction assumed as a base of reference. Let

$$\alpha = 2 \frac{\omega_0}{c} \text{Im } n = \text{Im } k \quad (19)$$

$$\mu = \frac{\text{Re } n - n_0}{n_0} = \frac{\text{Re } k - k_0}{k_0} \quad (20)$$

represent the local absorption coefficient and index perturbation, respectively, then on dropping terms of second order in $\partial/\partial z$, $\partial/\partial t$, α , μ , and $\omega - \omega_0$ there results the time-dependent paraxial wave equation

$$\nabla^2 \psi + 2ik_0 \left(\frac{\partial \psi}{\partial z} + \frac{1}{v} \frac{\partial \psi}{\partial t} \right) + \left(ik_0 \alpha + 2k_0^2 \mu \right) \psi = 0 \quad (21)$$

where v is the group velocity. Fleck^[8] solved this equation directly for the real and imaginary parts of ψ in the time-independent, axially symmetric case. Glass^[6] followed the alternative approach of separating ψ into amplitude and phase parts. The latter method leads, as will be shown, to a formulation in terms of variables which have simple geometrical interpretations and are well suited to calculations with adaptive coordinate grids. We have adopted this latter approach in the present effort.

Following Reference [6] we introduce real intensity and inclination variables I and \underline{u} by the relations

$$\psi = \sqrt{I} e^{i\phi} \quad (22)$$

$$\underline{u} = \frac{1}{k_0} \nabla \phi \quad (23)$$

With these definitions, the real and imaginary parts of (21) yield the pair of equations

$$\left(\frac{\partial}{\partial z} + \frac{1}{v} \frac{\partial}{\partial t} + \underline{u} \cdot \nabla \right) I = - (\alpha + \nabla \cdot \underline{u}) I \quad (24)$$

$$\left(\frac{\partial}{\partial z} + \frac{1}{v} \frac{\partial}{\partial t} + \underline{u} \cdot \nabla \right) \underline{u} = \nabla(\mu + P) \quad (25)$$

where the diffraction potential P is defined as

$$P = \frac{1}{4k_0^2} \left(\frac{\nabla^2 I}{I} - \frac{1}{2} \left(\frac{\nabla I}{I} \right)^2 \right) \quad (26)$$

These equations may be integrated along characteristics, or trajectories, which are the analogs in Fresnel diffraction theory of the rays of geometric optics. These trajectories are defined by the pair of equations

$$\frac{d}{dz} \underline{r} = \underline{u} \quad (27)$$

$$\frac{d}{dz} t = \frac{1}{v} \quad (28)$$

where \underline{r} is the radius vector projection in the plane normal to the z axis and t is the time. Along such trajectories (24) and (25) take the form

$$\frac{d}{dz} I = - (\alpha + \nabla \cdot \underline{u}) I \quad (29)$$

$$\frac{d}{dz} \underline{u} = \nabla(\mu + P) \quad (30)$$

Let us consider an arbitrary portion of the beam cross-section for given z , t . This is a region R of the xy plane, bounded by a set of points \underline{r} at which (27) holds. On integrating (24) over this region, with boundary terms defined by (27), one finds

$$\iint_R \left(\alpha I + \frac{1}{v} \frac{\partial I}{\partial t} \right) dx dy + \frac{d}{dz} \iint_R I dx dy = 0 \quad (31)$$

which implies that energy flows only along, not across, trajectories. We may, in fact, replace (29) by (31) in order to have an explicit equation for energy conservation. Similarly, with the aid of (27) we may replace (30) by

$$\frac{d^2}{dz^2} \underline{r} = \nabla(\mu + P) \quad (32)$$

The time-dependence represented by (28) is a result of the finiteness of the group velocity. It requires an interpolation procedure, since the differentiations in the x and y directions require constancy of t as well as z , and unless the group velocity is constant, trajectories that are simultaneous at one value of z will not be simultaneous at other values. Time-dependence may be of considerable importance in some applications, but there are many in which the scale of the problem is such that finite propagation velocity effects are not of interest. When this is the case, we may set $v \rightarrow \infty$ in the above equations, and drop (28). Trajectories are then reinterpreted as space paths rather than space-time paths. If the material properties and boundary conditions are time-dependent, the trajectories will, of course, change with time, but no time derivatives will appear in the radiation propagation equations.

A second simplification which is worth introducing is the restriction to axial symmetry. This is particularly convenient in a developmental program, since it greatly reduces the number of trajectories required for a given spatial resolution. The time-independent axially symmetric forms of (31) and (32) may then be written

$$\frac{dW_i}{dz} + \alpha_i(z) W_i = 0 \quad (33)$$

$$\frac{d^2 r_i}{dz^2} = \frac{\partial}{\partial r} (\mu + P) \quad (34)$$

where

$$W_i(z) = \int_{r_i}^{r_{i+1}} 2\pi r I(r, z) dr \quad (35)$$

is the beam power in the ring $r_i < r < r_{i+1}$, and

$$\alpha_i(z) = \int_{r_i}^{r_{i+1}} 2\pi r \alpha(r, z) I(r, z) dr / W_i(z) \quad (36)$$

is the effective absorption coefficient in the ring.

It may be noted that (33) does not involve the radial variable r at all, and in (34) r appears as a dependent variable. This suggests that the right side of (34) be evaluated in terms of an independent variable which is related to W . It is also important to account properly for the radial boundary conditions, both at $r = 0$ and at the outer boundary. Fleck^[8] devised a method of cylindrical cubic spline representation specifically for the r variable. An alternative approach becomes possible with other variable choices, which may provide certain advantages.

For the evaluation of the right side of (34) we choose as dependent variable the cumulative area to radius r (per radian)

$$y = \frac{1}{2} r^2 \quad (37)$$

and as independent variable

$$x = -\log (1-S(r)/S_T) \quad (38)$$

where

$$S(r) = \int_0^r 2\pi r I(r) dr \quad (39)$$

is the beam power within radius r , and $S_T = S(\infty)$ is the total power. It is clear that a Gaussian beam profile

$$I(r) = \frac{2S_T}{\pi w^2} \exp (-2r^2/w^2) \quad (40)$$

is represented in these variables as the straight line

$$y = \frac{1}{4} w^2 x \quad (41)$$

Since in the absence of perturbations the Gaussian profile propagates without change of shape (except for changes in the scale radius w), it is natural to assume a Gaussian shape for the beam profile at the outer edge of the calculational mesh as a boundary condition which is not likely to propagate spurious information into the interior. Such a boundary condition, in view of (41), is easily imposed with the variable definitions chosen.

The derivative terms appearing in (26) and on the right side of (34) are easily evaluated. With derivatives by x denoted by dots, one finds from (37), (38) and (39)

$$I = S_T e^{-x/\dot{y}} \quad (42)$$

$$T_1 = \frac{1}{rI} \frac{dI}{dr} = \frac{1}{I} \frac{dI}{dy} = - \left(\frac{1}{\dot{y}} + \frac{\ddot{y}}{\dot{y}^2} \right) \quad (43)$$

$$T_2 = \frac{d}{dy} T_1 = (\ddot{y} - \ddot{y} + 2\ddot{y}^2/\dot{y})/\dot{y}^3 \quad (44)$$

$$T_3 = \frac{d}{dy} T_2 = (\ddot{y} - \ddot{y})/\dot{y}^4 + (7\ddot{y} \ddot{y} - 3\ddot{y}^2)/\dot{y}^5 - 8\ddot{y}^3/\dot{y}^6 \quad (45)$$

Then (26) may be written

$$\begin{aligned} P &= \frac{1}{4k_o^2} \left(\frac{1}{Ir} \frac{d}{dr} r \frac{dI}{dr} - \frac{1}{2} \left(\frac{1}{I} \frac{dI}{dr} \right)^2 \right) \\ &= \frac{1}{4k_o^2} \left(\frac{1}{I} \frac{d}{dy} (2yI T_1) - yT_1^2 \right) \\ &= \frac{1}{4k_o^2} \left(2T_1 + yT_1^2 + 2yT_2 \right) \end{aligned} \quad (46)$$

so that

$$\frac{\partial P}{\partial r} = \frac{r}{4k_o^2} \left(4T_2 + T_1^2 + 2yT_1T_2 + 2yT_3 \right) . \quad (47)$$

The refraction term in (34) is simply

$$\frac{\partial \mu}{\partial r} = r\dot{\mu}/\dot{y} \quad (48)$$

It may be noted that the right sides of (47), (48) and therefore of (34) vanish properly at $r = 0$.

The derivatives of y and μ with respect to x may be evaluated from spline representations. In order to construct these, trajectory values of x , y are first set up. These are determined by (37) and (38) following each integration

step for (33) and (34):

$$x_j = -\log(1 - S_j/S_T), \quad j = 1, n \quad (49)$$

where

$$S_1 = 0 \quad (50)$$

$$S_{j+1} = \sum_{i=1}^j W_i, \quad j = 1, n \quad (51)$$

$$S_T = S_{n+1} \quad (52)$$

$$y_i = \frac{1}{2} r_j^2 \quad (53)$$

According to (45) derivatives of y up to fourth order are required. A quintic spline representation provides continuous derivatives through fourth order. A recently developed natural quintic spline code, QUINAT^[9] was therefore modified for the purpose. The procedure consists of two steps:

1. After an integration step for the W_j , Equation (33), and calculation of new values of x_j , Equation (49), the first part of the spline calculation is done. This consists of setting up a matrix of coefficients and decomposing it into triangular and diagonal factors, using a Cholesky method. The results of this step depend only on the x_j and can be used repeatedly for calculation of spline representation of other trajectory variables in step (2).
2. The second step is done for each new or modified set of trajectory values of α , μ and y . It yields coefficients B_j , C_j , D_j , E_j , and F_j for the natural spline polynomials

$$\begin{aligned}
 A(x) = & A_j + B_j (x-x_j) + C_j (x-x_j)^3 \\
 & + E_j (x-x_j)^4 + F_j (x-x_j)^5, \quad x_j \leq x < x_{j+1}, \\
 & j = 1, n
 \end{aligned} \tag{54}$$

where the A_j are the prescribed values of some functions at the points x_j . The representation $A(x)$ and its first four derivatives are continuous at the interior nodes x_j , $j = 2, n - 1$. At the end-points x_1 and x_n the third, fourth and fifth derivatives of A vanish automatically.

In the original QUINAT program^[9] it was not possible to separate these two steps. By explicitly factorizing the coefficient matrix in step (1) this separation is made possible. Since the operations in step (2) must be carried out many times compared to the more time-consuming ones in step (1), the gain in efficiency is large.

It remains to specify integration methods for (33) and (34). The coefficients α_j defined by (33) are evaluated from the spline representations of $\alpha(x)$ and $y(x)$. With $I(x)$ defined by (42) the integration in (36) can be done analytically. If the α_i vary slowly with z , they may be taken as constant within each increment of the z variable, in which case (33) may be integrated directly:

$$W_j(z + \Delta z) = W_i(z) \exp(-\alpha_j \Delta z) \tag{55}$$

For x_j strongly dependent on z it may be preferable to integrate the equivalent form

$$\frac{d}{dz} \log W_i = -\alpha(z) \tag{56}$$

using a higher-order numerical procedure.

For integration of Equation (34) a predictor-corrector method is used. The method chosen is a generalization to nonuniform meshes of Störmer's method for solving second-order equations of the form

$$\frac{d^2 r}{dz^2} = G(r, z) . \quad (57)$$

Specifically, let

$$h = z_{n+1} - z_n$$

$$g = z_n - z_{n-1}$$

The corrector, or closed, formula is then

$$\begin{aligned} gr_{n+1} = & (h + g) r_n - h r_{n-1} + \frac{1}{12} h (g^2 + gh - h^2) r_{n-1}'' \\ & + \frac{1}{12} (g + h) (g^2 + 3gh + h^2) r_n'' + \frac{1}{12} g (h^2 + gh \\ & - g^2) r_{n+1}'' + \frac{1}{360} hg (g^2 - h^2) (2g^2 + 5gh + 2h^2) r^{iv}(z_n + \epsilon) \end{aligned} \quad (58)$$

where the last term indicates the order of error incurred by dropping it. The predictor, or open formula chosen is

$$\begin{aligned} gr_{n+1} = & (h + g) r_n - h r_{n-1} + \frac{1}{6} h (g^2 - h^2) r_{n-1}'' \\ & + \frac{1}{6} h (h + g) (h + 2g) r_n'' + \frac{1}{24} (3g^4 h - 2h^3 g^2 \\ & + h^4 g) r^{iv}(z_n + \epsilon) \end{aligned} \quad (59)$$

Following an initial estimate of r_{n+1} by (59), the right side of (34) is evaluated as described above to provide an estimate of r_{n+1}'' . The process is then iterated to convergence using the corrector (58).

The initialization of the trajectories does not present any particular problem. It is useful to record some relations characterizing Gaussian beams, in which the intensity varies as in (40) or (41). The scale radius w of such a beam has a z -dependence given by the hyperbola^[10]

$$w(z)^2 = w_0^2 + \frac{4}{k_0^2 w_0^2} (z - z_0)^2 \quad (60)$$

where z_0 , w_0 are the values of z and w at the waist of the beam. Each trajectory is a similar hyperbola

$$r_j(z) = \frac{r_j(z_0)}{w_0} w(z) \quad (61)$$

so that

$$\frac{d^2}{dz^2} r_j = \frac{4r_j}{k_0^2 w(z)^4} \quad (62)$$

The result (62) is also derivable from (34), (41) and (47) with the added assumptions $\alpha = \mu = 0$. The values of r and r'' needed to initialize trajectories in a Gaussian beam may be determined very simply by these relations.

Material properties k_0 , $\alpha(r,z)$ and $\mu(r,z)$ may be specified in a variety of ways. A dispersion relation for partially ionized gas,

$$k^2 = k_0^2 - \frac{\omega_p^2}{c^2} \frac{\omega}{\omega + i(\nu_i + \nu_n)} \quad (63)$$

where ω_p is the electron plasma frequency and ν_i , ν_n are the electron collision frequencies with ions and neutrals respectively, is being used in test calculations. The

quantities α and μ are obtained from (63) by extracting the complex square root and applying (19) and (20).

A Fortran listing of the routines which perform the operations discussed above is presented in Appendix II.

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APPENDIX I

LISTING OF LSD WAVE PROPAGATION ROUTINES

***** MAINC *****

```
1. PROGRAM MAINC(INPUT,OUTPUT,TAPES=INPUT,TAPES=OUTPUT)
2.
3. C
4. C TWO-D DRIVER FOR ETBFCT
5. C
6. REAL RNEW(202,12),VZNEW(202,12),VRNEW(202,12),ENEW(202,12)
7. REAL PNEW(202,12),F(202,12),TOLD(202,12),SNDSPD(202,12)
8. REAL FLUX(202,12),RADZ(202),RADR(12),RBC(2.4),LBC(2.4)
9. REAL ZERO(202),UNIT(202)
10. C
11. COMMON/UPDT/ RNEW, VZNEW, VRNEW, ENEW, PNEW, F, TOLD, SNDSPD, FLUX
12. COMMON/UPDT/ RADZ, RADR, RADZR, RADZL, RADZL, RADRR, RADRL, NZ, NR, RBC
13. COMMON/UPDT/LBC, ZERO, UNIT, DELTAZ, DELTAR, DELTAT, COUR, ENRGMN
14. COMMON/UPDT/FLAG
15. COMMON/DELZ/DELZ(202)
16. C
17. COMMON/EDITC/NREDIT, IDELTR, ISTEPX, LPRINT, TIME
18. COMMON/EOSC/ ENRG, RHO, P, T, FRAC, A, B, DEGF, RM, SND
19. COMMON/FLXC/ FZERO, XLAMDA, Z, GMUT, CUTOFF
20. C
21. READ EOS CONSTANTS, ETC
22. READ(5,100) XLAMDA,A,B,DEGF,GASCON,GMUT,Z,COUR,CUTOFF
23. 100 FORMAT(4E20,14)
24. C
25. READ(5,100) FZERO, RZERO, ENRGL, ENRGR, DELTAZ, DELTAR, ENRGMN
26. READ(5,100) FLAG
27. C
28. READ(5,101) MAXSTP, IPRINT, NZ, NR, LPRINT, MZ, MR, NREDIT, IDELTR
29. 101 FORMAT(8I10)
30. C
31. READ(5,103) RBC
32. READ(5,103) LBC
33. 103 FORMAT(8F10,0)
34. C
35. RM=GASCON
36. RINV=1./RZERO
37. ELEFT=RZERO*ENRGL
38. ERIGHT=RZERO*ENRGR
39. C
40. RHO=RZERO
41. ENRG=ENRGL
42. CALL EOS
43. TLEFT=T
44. PLEFT=P
45. FLEFT=FRAC
46. SNDL=SND
47. C
48. ENRG=ENRGR
49. CALL EOS
50. TRIGHT=T
51. PRIGHT=P
52. FRIGHT=FRAC
53. SNDR=SND
```

```

***** MAINC *****
53.          C
54.          VZRIGHT=0.
55.          VZLEFT=0.
56.          VRRIGHT=0.
57.          VRLEFT=0.
58.
59.          WRITE(6,102) XLAMDA,A,B,DEGF,GASCON,GMWT,Z,COUR,FZERO,RZERO,
60.          ENRGL,ENRGR,DELTAZ,DELTA,MAXSTP,IPRINT,NZ,NR,LPRINT,MZ,MR,
61.          NREDIT,NDELTR
62.          102 FORMAT(1,'//',XLAMDA=,'E14.8//',A=,'E14.8//',B=,'E14.8//',DEGF=,'E14.
63.          8//',GASCON=,'E14.8//',GMWT=,'E14.8//',7=,'E14.8//',COUR=,'E14.8//',FZE
64.          RO=,'E14.8//',RZERO=,'E14.8//',ENRGL=,'E14.8//',ENRGR=,'E14.8//',DELTA
65.          Z=,'E14.8//',DELTAZ=,'E14.8//',MAXSTP=,'15//',IPRINT=,'15//',NZ=,'15//',
66.          NR=,'15//',LPRINT=,'15//',MZ=,'15//',MR=,'15//',NREDIT=,'15//',NDELTR=
67.          ',15)
68.
69.          C
70.          WRITE(6,104) CUTOFF,RBC,LBC
71.          104 FORMAT(1X,'CUTOFF=,'E14.8//',RBC(1,1)=,'F5.0//',RBC(2,1)=,'F5.0//',RB
72.          C(1,2)=,'F5.0//',RBC(2,2)=,'F5.0//',RBC(1,3)=,'F5.0//',RBC(2,3)=,'F5.
73.          0//',RBC(1,4)=,'F5.0//',RBC(2,4)=,'F5.0//',LBC(1,1)=,'F5.0//',LBC(2,1)
74.          =,'F5.0//',LBC(1,2)=,'F5.0//',LBC(2,2)=,'F5.0//',LBC(1,3)=,'F5.0//',LB
75.          C(2,3)=,'F5.0//',LBC(1,4)=,'F5.0//',LBC(2,4)=,'F5.0)
76.          WRITE(6,105) ENRGMN
77.          105 FORMAT(1X,'ENRGMN=,'E14.8)
78.          WRITE(6,106) FLAG
79.          106 FORMAT(1X,'FLAG=,'F5.0)
80.          C
81.          SET UP THE GRID
82.          DO 10 I=1,NZ
83.          RADZ(1)=FLOAT(1-1)*DELTAZ
84.          RADZR=RADZ(NZ) + 0.5*DELTAZ
85.          RADZL=RADZ(1) - 0.5*DELTAZ
86.          DO 11 J=1,NR
87.          RADR(J)=FLOAT(J-1) + 5*DELTAR
88.          RADRR=RADR(NR) + 0.5*DELTAR
89.          RADRL=RADR(1) - 0.5*DELTAR
90.          C
91.          INITIALIZE THE MESH
92.          DO 12 J=1,NR
93.          DO 12 I=1,NZ
94.          FNEW(I,J)=RZERO
95.          VNEW(I,J)=0.
96.          FNEW(I,J)=FRIGHT
97.          TOLD(I,J)=TRIGHT
98.          F(I,J)=FRIGHT
99.          ENEM(I,J)=ERIGHT
100.          SINDSPD(I,J)=SNDR
101.          CONTINUE
102.          C
103.          DO 17 I=1,NZ
104.          DELZL(I)=DELTAZ
105.          MM=MAX0(NZ,NR)
106.          DO 115 I=1,MM

```


***** EDIT *****

```
1 SUBROUTINE EDIT
2
3 C
4 REAL RNEW(202,12),VZNEW(202,12),VRNEW(202,12),ENEW(202,12)
5 REAL PNEW(202,12),F(202,12),TOLD(202,12),SNDSPD(202,12)
6 REAL FLUX(202,12),RADZ(202),RADR(12),RBC(2,4),LBC(2,4)
7 REAL ZERO(202),UNIT(202)
8
9 C
10 COMMON/UPDT/ RNEW, VZNEW, VRNEW, ENEW, PNEW, F, TOLD, SNDSPD, FLUX
11 COMMON/UPDT/ RADZ, RADR, RADZR, RADZL, RADRR, RADRL, NZ, NR, RBC
12 COMMON/UPDT/ LBC, ZERO, UNIT, DELTAZ, DELTAR, DELTAT, COUR, ENRGMN
13 COMMON/UPDT/ FLAG
14
15 C
16 COMMON/EOSC/ENRG,RHO,P,T,FRAC,A,B,DEGF,RM
17
18 C
19 COMMON/EDITC/NREDIT, NDELTR, ISTEP, LPRINT, TIME
20
21 C
22 1000 FORMAT('1',// ' AFTER STEP NO.',I5,' DZ=',E14.8,' AND DT=',E14.8,
23 , TIME=',E14.8,' J=',I5,/)
24 1001 FORMAT(2X,I3,1P9E12.4)
25 1002 FORMAT(7X,'DENSITY',7X,'TEMP',6X,'PRESSURE',5X,'VELOCZ',6X,'VELOCR
26 ,6X,'ENRGTOT',5X,'ZCOORD',6X,'RCOORD',5X,'HTNGRATE',/)
27
28 C
29 JSTEP=ISTEP - 1
30 DO 10 K=1,NREDIT
31 J=1 + NDELTR*(K-1)
32 WRITE(6,1000) JSTEP,DELTAZ,DELTAT,TIME,J
33 WRITE(6,1002)
34 WRITE(6,1001) (I,RNEW(I,J),TOLD(I,J),PNEW(I,J),VZNEW(I,J),
35 VRNEW(I,J),ENEW(I,J),RADZ(I),RADR(J),FLUX(I,J), I=1,LPRINT)
36
37 10 CONTINUE
38 RETURN
39 END
```

***** EOS *****

```
1  SURROUTINE EOS
2  IDEAL GAS EQUATION OF STATE
3  OUTPUT VARIABLES
4  T IS TEMP IN KELVINS
5  P IS PRESSURE IN DYNE/CM**2
6  FRAC IS FRACTION IONIZATION, N-/NZERO
7  C IS SOUND SPEED(CM/SEC)
8  DPDE IS ENRG DERIV OF PRES AT CONST VOL
9  DPDV IS VOL DERIV OF PRES AT CONST ENRG
10
11
12
13
14 INPUT
15 E IS INTERNAL ENERGY, ERG/GM
16 V IS SPECIFIC VOLUME IN CC/GM
17 A = (G*KG/GA)*((MOLWT/AVAGNO)*(2*PI*EELECMASS*BOLTZ/PLANCK**2)**1.5
18 B = IONIZATION POT/BOLTZ
19 F IS DEGREES OF FREEDOM (=3 FOR MONATOMIC GAS)
20 RM IS GAS CONSTANT IN ERG/GM/DEG
21
22 COMMON/EOSC/ E, RHO, P, T, FRAC, A, B, F, RM, C
23 V=1./RHO
24 IF(E.GT.0.) GO TO 40
25 E=2
26 WRITE(6,50)
27 FORMAT(IX,'NEG ENERGY INPUT TO EOSIG')
28 INEGE=INEGE+1
29 CONTINUE
30
31 AV=AKV
32 E2OVRM=2.*E/RM
33 B2=2.*B
34
35 C
36 THI=E2OVRM/F
37 TLO=AMAX1(0.,(E2OVRM-B2)/(F+3.))
38 IF(TLO.GT.0.) GO TO 100
39 FUNC1=-E2OVRM
40 GO TO 110
41 XX=AMAX1(-80.,-B/TLO)
42 Y=AV*TL0*SQRT(TLO)*EXP(XX)
43 X=0.5*(SQRT(Y*(Y+4.))-Y)
44 FUNC1=TL0*(F+3.*X) + B2*X - E2OVRM
45 XX=AMAX1(-80.,-B/THI)
46 Y=AV*THI*SQRT(THI)*EXP(XX)
47 X=0.5*(SQRT(Y*(Y+4.))-Y)
48 FUNC2=THI*(F+3.*X) + B2*X - E2OVRM
49 TOLD=TLO - FUNC1*(THI-TLO)/(FUNC2-FUNC1)
50 THEM=TOLD
51
52 DO 10 K=1,30
53 ICOUNT=K
54 XX=AMAX1(-80.,-B/TOLD)
```

***** EOS *****

```
53 Y=AV*TOLD*SQRT(TOLD)*EXP(XX)
54 X=0.5*(SQRT(Y*(Y+4.))-Y)
55 FUNC=TOLD*(F + 3.*X) + B2*X - E20VRM
56 IF (FUNC)4,20,5
57 THI=AMINI(TOLD,THI)
58 GO TO 6
59 4 TLO=AMAX1(TOLD,TLO)
60 6 DXDT=(1.5 + B/TOLD)*X*(1.-X)/((2.-X)*TOLD)
61 FUNC=F + 3.*X + (3.*TOLD + B2)*DXDT
62 TNEW=TOLD - FUNC/FUNC
63 IF (ABS((TNEW-TOLD)/TOLD) .LT. 1.E-07) GO TO 20
64 IF (TNEW .GE. THI .OR. TNEW .LE. TLO) TNEW=0.5*(THI+TLO)
65 TOLD=TNEW
66 10 CONTINUE
67 WRITE(6,30) E,V
68 30 FORMAT(IX,'EOS FAILED AT E=',E14.8,2X,'V=',E14.8)
69 C
70 20 CONTINUE
71 T=TNEW
72 XX=AMAX1(-80.,-B/T)
73 Y=AV*T*SQRT(T)*EXP(XX)
74 FRAC=0.5*(SQRT(Y*(Y+4.))-Y)
75 X=FRAC
76 DXDV=XX*(1.-X)/(V*(2.-X))
77 C
78 CALCULATE THE PRESSURE
79 C
80 F=RMK(1.,+FRAC)*T/V
81 C
82 PRESSURE DERIVATIVES
83 C
84 DPDT=RMK(T)*DXDT + (1. + X)/V
85 DPDV=RMK(T)*DXDV-(1. + X)/V/V
86 DEDT=RMK((F+3.*X)*.5+(1.5*T+B)*DXDT)
87 DEDV=RMKDXDV*(1.5*T+B)
88 C
89 DPDE=DPDT/DEDT
90 DPDV=DPDV - DPDT*DEDV/DEDT
91 C
92 CSQ=(V**2)*(P*DPDE-DP*DV)
93 C=SQRT(CSQ)
94 RETURN
95 END
96
```

***** FLX *****

```
1 SUBROUTINE FLX
2
3 C
4 C
5 C
6 C
7 C
8 C
9 C
10 C
11 C
12 C
13 C
14 C
15 C
16 C
17 C
18 C
19 C
20 C
21 C
22 C
23 C
24 C
25 C
26 C
27 C
28 C
29 C
30 C
31 C
32 C
33 C
34 C
35 C
36 C
37 C
38 C
39 C
40 C
41 C
42 C
43 C
44 C
45 C
46 C
47 C
48 C
49 C
50 C
51 C
52 C

TEMPORARY SUBROUTINE FOR 2-D CHECKOUT
CALCULATES HEATING RATE AT CELL CENTERS IN ERG/CM**3

REAL RNEW(202,12),VZNEW(202,12),VRNEW(202,12),ENEW(202,12)
REAL FNEW(202,12),F(202,12),TOLD(202,12),SNDSPD(202,12)
REAL FLUX(202,12),RADZ(202),RADR(12),RBC(2,4),LBC(2,4)
REAL ZERO(202),UNIT(202)

COMMON/UPDT/ RNEW, VZNEW, VRNEW, ENNEW, FNEW, F, TOLD, SNDSPD, FLUX
COMMON/UPDT/ RADZ, RADR, RADZR, RADZL, RADRR, RADRL, NZ, NR, RBC
COMMON/UPDT/ LBC, ZERO, UNIT, DELTAZ, DELTAR, DELTAT, COUR, ENRGMN
COMMON/UPDT/ FLAG
COMMON/DELZ/ DELZ(202)

COMMON/FLXC/ FZERO, XLAMDA, Z, GMJLT, CUTOFF

NRR=NR+1
DO 20 J=2,NRR
FIN=FZERO
FLUX(NZ,J)=FIN
JM=J-1
NN=NZ-1
DO 10 K=1,NN
L=NZ+1-K
TX=TOLD(L,JM)
VX=1./RNEW(L,JM)
FRAC=F(L,JM)
XKAPA=ABSORB(TX,VX,XLAMDA,Z,FRAC,GMJLT)
IF(FIN) 2,2,3
IF (FLUX(L-1,J)=0.
2 FLUX(L-1,J)=0.
GO TO 10
3 TERMX=AMAX1(-CUTOFF,-XKAPA*DELZ(L))
FLUX(L-1,J)=FIN*EXP(-TERMX)
FIN=FLUX(L-1,J)
IF((FIN/FZERO).LT.1.E-08) FIN=0.
10 CONTINUE
TX=TOLD(1,JM)
VX=1./RNEW(1,JM)
FRAC=F(1,JM)
XKAPA=ABSORB(TX,VX,XLAMDA,Z,FRAC,GMJLT)
TERMX=AMAX1(-CUTOFF,-XKAPA*DELZ(1))
FL=FLUX(1,J)*EXP(-TERMX)

DO 30 I=2,NZ
FLUX(I,JM)=(FLUX(I,J) - FLUX(I-1,J))/DELZ(I)
30 CONTINUE
FLUX(1,JM)=(FLUX(1,J) - FL)/DELZ(1)
20 CONTINUE
RETURN
END
```

***** FLX *****

***** TDEL T *****

```
1 SUBROUTINE TDEL T
2 C
3 C TWO-D, EULERIAN, CYLINDRICAL COORDINATES
4 C FLAG = 1.0 FOR 1-D LAGRANGE
5 C
6 C REAL RNEW(202,12), VZNEW(202,12), VRNEW(202,12), ENEW(202,12)
7 C REAL PNEW(202,12), F(202,12), TOLD(202,12), SNDSPD(202,12)
8 C REAL FLUX(202,12), RADZ(202), RADR(12), RBC(2,4), LBC(2,4)
9 C REAL ZERO(202), UNIT(202)
10 C
11 C COMMON/UFDT/ RNEW, VZNEW, VRNEW, ENEW, PNEW, F, TOLD, SNDSPD, FLUX
12 C COMMON/UPDT/ RADZ, RADR, RADZR, RADZL, RADRL, RADRR, RADRL, NZ, NR, RBC
13 C COMMON/UPDT/LBC, ZERO, UNIT, DELTAZ, DELTAR, DELTAT, COUR, ENRGMN
14 C COMMON/UFDT/FLAG
15 C COMMON/DELZ/DELZL(202)
16 C
17 C FACTOR=1. - FLAG
18 C TMIN=1.E+06
19 C DO 10 J=1,NR
20 C DO 10 I=1,NZ
21 C TRT=DELZL(I)/(SNDSPD(I,J) + FACTOR*ABS(VZNEW(I,J)))
22 C IF (TRT GE. TMIN) GO TO 10
23 C TMIN=TRT
24 C 10 CONTINUE
25 C DELTAT=COUR*TMIN
26 C RETURN
27 C END
```

***** UPDATE *****

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SUBROUTINE UPDATE
C
C ONE TIME-CYCLE UPDATE FOR TWO-D.CYL.INDRICAL COORDINATES
C (EULERIAN) FCT TIME-SPLITTING
C MAY BE USED FOR 1-D LAGRANGE IF FLAG IS SET TO 1.0
C
C
C REAL RADZOL(202)
C REAL SAVE0(202), SAVEN(202), ROLD(202), VZOLD(202), VROLDD(202)
C REAL POLD(202), EOLD(202), PVZ(202), PVR(202), SCR1(202)
C REAL SCR2(202), SCR3(202), RVZOLD(202), RVZNEW(202)
C REAL RVROLDD(202), RVNEW(202)
C
C REAL RNEW(202,12), VZNEW(202,12), VRNEW(202,12), ENEW(202,12)
C REAL PNEW(202,12), F(202,12), TOLD(202,12), SNDSPD(202,12)
C REAL FLUX(202,12), RADZ(202), RADR(12), RBC(2,4), LBC(2,4)
C REAL ZERO(202), UNIT(202)
C
C COMMON/UPDT/ RNEW, VZNEW, VRNEW, ENEW, PNEW, F, TOLD, SNDSPD, FLUX
C COMMON/UPDT/ RADZ, RADR, RADZR, RADZL, RADRL, RADRR, RADRL, NZ, NR, RBC
C COMMON/UPDT/LBC, ZERO, UNIT, DELTAT, DELTAR, DELTAT, COUR, ENRGMN
C COMMON/DELZ/DELZL(202)
C
C COMMON/EOSC/ ENRG, RHO, P, T, FRAC, A, B, DEGF, RM, SND
C
C EQUIVALENCE (SAVE0(1),SAVEN(1)), (PVZ(1),PVR(1))
C
C INITIALIZE QUANTITIES FOR CYCLE
C
C CALL NGRIDE(RADZ,NZ,RADZR,RADZL,1)
C CALL OGRIDE(NZ)
C IF(FLAG.LT.0.5) GO TO 3
C DO 4 I=1,NZ
C RADZOL(I)=RADZ(I)
C DTGRID=0.5*DELTAT*FLAG
C DO 2 I=1,NZ
C RADZ(I)=RADZOL(I) + DTGRID*VZNEW(I,1)
C RADZR=RADZR + DTGRID*VZR
C RADZL=RADZL + DTGRID*VZL
C CONTINUE
C CALL NGRIDE(RADZ,NZ,RADZR,RADZL,1)
C
C DO 20 J=1,NR
C
C DO 10 I=1,NZ
C ROLD(I)=RNEW(I,J)
C VZOLD(I)=VZNEW(I,J)
C VROLDD(I)=VRNEW(I,J)
C RVZOLD(I)=ROLD(I)*VZOLD(I)
C RVROLDD(I)=ROLD(I)*VROLDD(I)
C EOLD(I)=ENEW(I,J)
C POLD(I)=PNEW(I,J)
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***** UPDATE *****
53. PVZ(I)=POLD(I)*VZOLD(I)
54. 10 CONTINUE
55. C
56. C HALF STEP FOR Z
57. C
58. C VZR=0.5*VZOLD(NZ)*(1.+RBC(1,2))
59. C VZL=0.5*VZOLD(1)*(1.+LBC(1,2))
60. C
61. C CALL VELOCE(VZOLD,NZ,VZR,VZL,.0.5*DELTA)
62. C
63. C DO 21 I=1,NZ
64. C SCR1(I)=-POLD(I)
65. C SCR2(I)=-PVZ(I)
66. C SCR3(I)=FLUX(I,J)
67. C 21 CONTINUE
68. C
69. C CALL ETBFCT(ROLD,SAVEN,NZ,RBC(1,1),LBC(1,1))
70. C
71. C DO 221 I=1,NZ
72. C RNEW(I,J)=SAVEN(I)
73. C 221
74. C PLEFT=LBC(1,1)*POLD(I)
75. C PRIGHT=RBC(1,1)*POLD(NZ)
76. C
77. C CALL SORC(NZ,.0.5*DELTA,2,UNIT,SCR1,-FRIGHT,-PLEFT)
78. C
79. C CALL ETBFCT(RVZOLD,RVZNEW,NZ,RBC(1,2),LBC(1,2))
80. C
81. C IF(NR.GT.1) GO TO 116
82. C DO 130 I=1,NZ
83. C RVRNEW(I)=0.
84. C GO TO 117
85. C 130
86. C 116 CONTINUE
87. C
88. C CALL ETBFCT(RVROLD,RVRNEW,NZ,RBC(1,3),LBC(1,3))
89. C
90. C 117 CONTINUE
91. C
92. C VLEFT=LBC(1,2)*VZOLD(1)
93. C VRIGHT=RBC(1,2)*VZOLD(NZ)
94. C
95. C CALL SORC(NZ,.0.5*DELTA,1,ZERO,SCR2,-PRIGHT*VRIGHT,-PLEFT*VLEFT)
96. C
97. C CALL SORC(NZ,.0.5*DELTA,3,ZERO,SCR3,.0.)
98. C
99. C CALL ETBFCT(EOLD,SAVEN,NZ,RBC(1,4),LBC(1,4))
100. C
101. C DO 222 I=1,NZ
102. C ENEM(I,J)=SAVEN(I)
103. C
104. C CALCULATE INTERMEDIATE QUANTITIES
105. C
106. C DO 24 I=1,NZ
107. C VZNEW(I,J)=RVZNEW(I)/RNEW(I,J)

```

***** UPDATE *****

```
107 VRNEW(I,J)=RVRNEW(I)/RNEW(I,J)
108 ENRG=ENW(I,J)/RNEW(I,J) - 0.5*(VZNEW(I,J)*VZNEW(I,J) +
109 VRNEW(I,J)*VRNEW(I,J))
110 IF (ENRG.LT.ENRGMN) ENRG=ENRGMN
111 RHO=RNEW(I,J)
112 C
113 CALL EOS
114 C
115 PNEW(I,J)=P
116 PVZ(I)=PNEW(I,J)*VZNEW(I,J)
117 CONTINUE
118 24
119 VZR=0.5*(VZNEW(NZ,J)*(1.+RBC(1,2))
120 VZL=0.5*(VZNEW(1,J)*(1.+LBC(1,2))
121 C
122 DO 223 I=1,NZ
123 SAVE0(I)=VZNEW(I,J)
124 C
125 IF (FLAG.LT.0.5) GO TO 5
126 DTGRID=DELTA*FLAG
127 DO 6 I=1,NZ
128 RADZ(I)=RADZOL(I) + DTGRID*VZNEW(I,1)
129 RADZR=RADZR + 0.5*DTGRID*VZR
130 RADZL=RADZL + 0.5*DTGRID*VZL
131 CALL NGRID(RADZ,NZ,RADZR,RADZL,1)
132 CONTINUE
133 C
134 CALL VELOC(SAVE0,NZ,VZR,VZL,DELTA)
135 C
136 FULL STEP FOR Z
137 C
138 DO 25 I=1,NZ
139 SCR1(I)=-PNEW(I,J)
140 SCR2(I)=-PVZ(I)
141 CONTINUE
142 C
143 CALL ETBFCT(ROLD,SAVEN,NZ,RBC(1,1),LBC(1,1))
144 C
145 DO 224 I=1,NZ
146 RNEW(I,J)=SAVEN(I)
147 PLEFT=LBC(1,1)*PNEW(I,J)
148 FRIGHT=RBC(1,1)*PNEW(NZ,J)
149 C
150 CALL SORC(NZ,DELTA,2,UNIT,SCR1,-FRIGHT,-PLEFT)
151 C
152 CALL ETBFCT(RVZOLD,RVZNEW,NZ,RBC(1,2),LBC(1,2))
153 C
154 IF (NR.EQ.1) GO TO 118
155 CALL ETBFCT(RVROL,D,RVRNEW,NZ,RBC(1,3),LBC(1,3))
156 CONTINUE
157 118
158 VLEFT=LBC(1,2)*VZNEW(1,J)
159 VRIGHT=RBC(1,2)*VZNEW(NZ,J)
160 C
```

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***** UPDATE *****
161. CALL SORC(NZ, DELTAT, 1, ZERO, SCR2, -PRIGHT*VRIGHT, -PLEFT*VLEFT)
162. C
163. C ADD THE TOTAL EXTERNAL SOURCE ENERGY HERE (OMIT EXTERNAL SOURCE
164. C IN THE R-INTEGRATIONS)
165. C
166. C CALL SORC(NZ, DELTAT, 3, ZERO, SCR3, 0., 0.)
167. C
168. C CALL ETBFCT(EOLD, SAVEN, NZ, RBC(1,4), LRC(1,4))
169. C
170. C DO 225 I=1, NZ
171. C 225 ENEW(I, J)=SAVEN(I)
172. C
173. C DO 110 I=1, NZ
174. C VZNEW(I, J)=RVZNEW(I)/RNEW(I, J)
175. C 110 VRNEW(I, J)=RVRNEW(I)/RNEW(I, J)
176. C 20 CONTINUE
177. C
178. C IF (NR.GT.1) GO TO 115
179. C J=1
180. C DO 119 I=1, NZ
181. C ENRG=ENEM(I, J)/RNEW(I, J) - 0.5*VZNEW(I, J)*VZNEW(I, J)
182. C IF (ENRG.LT.ENRGMN) ENRG=ENRGMN
183. C RHO=RNEW(I, J)
184. C CALL EOS
185. C PNEW(I, J)=P
186. C TOLD(I, J)=T
187. C SNDSFD(I, J)=SND
188. C F(I, J)=FRAC
189. C 119 CONTINUE
190. C
191. C EXIT FOR ONE-DIMENSIONAL CARTESIAN CALCULATION
192. C
193. C RETURN
194. C
195. C 115 CONTINUE
196. C
197. C RESET VARIABLES FOR R-INTEGRATION
198. C
199. C CALL NGRID(RADR, NR, RADRR, RADRL, 2)
200. C CALL OGRID(NR)
201. C CALL NGRID(RADR, NR, RADRR, RADRL, 2)
202. C
203. C DO 30 I=1, NZ
204. C
205. C DO 30 J=1, NR
206. C ROLD(J)=RNEW(I, J)
207. C RVZOLD(J)=RVNEW(I, J)*VZNEW(I, J)
208. C VROLD(J)=VRNEW(I, J)*VRNEW(I, J)
209. C EOLD(J)=ENEM(I, J)
210. C VZOLD(J)=VZNEW(I, J)
211. C VROLD(J)=VRNEW(I, J)
212. C ENRG=EOLD(J)/ROLD(J) - 0.5*(VZOLD(J)*VZOLD(J) + VROLD(J)*VROLD(J))
213. C IF (ENRG.LT.ENRGMN) ENRG=ENRGMN
214. C RHO=ROLD(J)

```

***** UPDATE *****

```
215 C CALL EOS
216 C
217 C
218 C POLD(J)=P
219 C PVR(J)=POLD(J)*VROLD(J)
220 C CONTINUE
221 C 30
222 C
223 C HALF STEP FOR R
224 C
225 C VRR=0.5*KVROLD(NR)*(1.+RBC(2,2))
226 C VRL=0.
227 C
228 C CALL VELOCE(VROLD,NR,VRR,VRI,0.5*DELTA T)
229 C
230 C DO 33 J=1,NR
231 C SCR1(J)=-POLD(J)
232 C SCR2(J)=-PVR(J)
233 C CONTINUE
234 C 33
235 C
236 C CALL ETBFCT(ROLD,SAVEN,NR,RBC(2,1),LBC(2,1))
237 C
238 C DO 35 J=1,NR
239 C RNEW(I,J)=SAVEN(J)
240 C
241 C PLEFT=LBC(2,1)*POLD(1)
242 C PRIGHT=RBC(2,1)*POLD(NR)
243 C
244 C CALL SORC(NR,0.5*DELTA T,2,UNIT,SCR1,-PRIGHT,-PLEFT)
245 C
246 C CALL ETBFCT(RVROLD,RVNEW,NR,RBC(2,2),LBC(2,2))
247 C
248 C CALL ETBFCT(RVZOLD,RVZNEW,NR,RBC(2,3),LBC(2,3))
249 C
250 C VLEFT=LBC(2,2)*VROLD(1)
251 C VRIGHT=RBC(2,2)*VROLD(NR)
252 C
253 C CALL SORC(NR,0.5*DELTA T,1,ZERO,SCR2,-PRIGHT*VRIGHT,-PLEFT*VLEFT)
254 C
255 C CALL ETBFCT(EOLD,SAVEN,NR,RBC(2,4),LBC(2,4))
256 C
257 C DO 40 J=1,NR
258 C ENEW(I,J)=SAVEN(J)
259 C
260 C CALCULATE INTERMEDIATE QUANTITIES
261 C
262 C DO 41 J=1,NR
263 C VRNEW(I,J)=RVNEW(J)/RNEW(I,J)
264 C VZNEW(I,J)=RVZNEW(J)/RNEW(I,J)
265 C ENRG=ENEM(I,J)/RNEW(I,J) - 0.5*(VZNEW(I,J)*VZNEW(I,J) + VRNEW(I,J)
266 C *VRNEW(I,J))
267 C IF (ENRG.LT.ENRGMN) ENRG=ENRGMN
268 C RHO=RNEW(I,J)
269 C CALL EOS
```

***** UPDATE *****

```
269. C PNEW(I,J)=P
270. PVR(J)=PNEW(I,J)*VRNEW(I,J)
271. 41 CONTINUE
272. C
273. DO 42 J=1,NR
274. 42 SAVE(J)=VRNEW(I,J)
275. VRR=0.5*VRNEW(I,NR)*(1.+RBC(2,2))
276. VRL=0.
277. C
278. CALL VELOCE(SAVEO,NR,VRR,VRL,DELTAT)
279. C
280. FULL STEP FOR R
281. C
282. DO 43 J=1,NR
283. 43 SCR1(J)=-PNEW(I,J)
284. SCR2(J)=-PVR(J)
285. 43 CONTINUE
286. C
287. CALL ETBFCT(ROLD,SAVEO,NR,RBC(2,1),LBC(2,1))
288. C
289. DO 45 J=1,NR
290. 45 RNEW(I,J)=SAVEO(J)
291. FLETT=LBC(2,1)*PNEW(I,1)
292. PRIGHT=RBC(2,1)*PNEW(I,NR)
293. C
294. CALL SORC(NR,DELTAT,2,UNIT,SCR1,-PRIGHT,-PLEFT)
295. C
296. CALL ETBFCT(RVROL,D,RVRNEW,NR,RBC(2,2),LBC(2,2))
297. C
298. CALL ETBFCT(RVZOLD,RVZNEW,NR,RBC(2,3),LBC(2,3))
299. C
300. VLEFT=LBC(2,2)*VRNEW(I,1)
301. VRIGHT=RBC(2,2)*VRNEW(I,NR)
302. C
303. CALL SORC(NR,DELTAT,1,ZERO,SCR2,-PRIGHT*VRIGHT,-PLEFT*VLEFT)
304. C
305. CALL ETBFCT(EOLD,SAVEO,NR,RBC(2,4),LBC(2,4))
306. C
307. DO 50 J=1,NR
308. 50 ENEM(I,J)=SAVEO(J)
309. C
310. DO 70 J=1,NR
311. 70 VZNEW(I,J)=RVZNEW(J)/RNEW(I,J)
312. VRNEW(I,J)=RVRNEW(J)/RNEW(I,J)
313. RHO=RNEW(I,J)
314. ENRG=ENEM(I,J)/RNEW(I,J) - 0.5*(VZNEW(I,J)*VZNEW(I,J) + VRNEW(I,J)
315. *VRNEW(I,J))
316. IF(ENRG.LT.ENRGIN) ENRG=ENRGIN
317. C
318. CALL EOS
319. C
320. PNEW(I,J)=P
321. 322.
```

***** UPDATE *****

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323. TOLD(I,J)=T
324. F(I,J)=FRAC
325. SINDSPD(I,J)=SIND
326. 70 CONTINUE
327. C
328. 31 CONTINUE
329. C
330. RETURN
331. END
```

***** CONGRE *****

```
1. SUBROUTINE CONGRE (RHO, N, CSUM)
2. REAL RHO(N)
3.
4. COMPUTE VOLUME INTEGRAL OF DENSITY OVER GRID
5. ARGUMENTS
6. RHO          (1)
7. N            (1)
8. CSUM        (0)
9.
10. LOGICAL LSOURC
11. REAL SOURCE(202), SCRH(202), RHOT(202), DIFF(202)
12. REAL ADUGTH(202), FLXH(202), NULH(202), MULH(202)
13. REAL LNRHOT(202), FSGN(202), FABS(202), EPSH(202)
14. REAL LORHOT(202), TERP(202), TERM(202), ADUDTH(202)
15. REAL LO(202), LN(202), LH(202), RLO(202), RLN(202)
16. REAL RNH(202), ROH(202), RLH(202), AH(202)
17. COMMON /COM1/ SOURCE, SCRH, RHOT, DIFF, ADUGTH, NULH, MULH
18. COMMON /COM1/ LORHOT, ADUDTH, LO, LN, LH, RLO, RLN, RNH, ROH
19. COMMON /COM1/ RLH, AH, LSOURC
20. EQUIVALENCE (EPSH(1), SCRH(1)), (LNRHOT(1), LORHOT(1))
21. EQUIVALENCE (FLXH(1), SCRH(1)), (FSGN(1), RHOT(1))
22. EQUIVALENCE (FABS(1), SCRH(1)), (TERP(1), SOURCE(1))
23. EQUIVALENCE (TERM(1), SOURCE(1))
24.
25. CSUM = 0.0
26. DO 501 I = 1, N
27. CSUM = CSUM + LN(I) * RHO(I)
28.
29. RETURN
30.
31. END
32.
```

***** ETBFCT *****

```
1. SUBROUTINE ETBFCT (RHOO, RHON, N, RBC, LBC)
2. REAL RHOO(N), RHON(N), RBC, LBC
3.
4. FLUX-CORRECTED TRANSPORT FOR NONPERIODIC B. C.
5. SOLVE CONTINUITY EQUATION
6. (D/DT) RHO = -(1/A)*(D/DR) (AKV*RH0) + (1/A)*(D/DR) (A*DI)
7. + C*(D/DR) D2 + D3 WHERE A = R*(ALPHA-1)
8.
9. ARGUMENTS
10. RHOO GRID POINT DENSITIES AT START OF STEP (1)
11. RHON GRID POINT DENSITIES AT END OF STEP (0)
12. N NUMBER OF INTERIOR GRID POINTS (1)
13. RBC RIGHT BOUNDARY FACTOR (1)
14. LBC LEFT BOUNDARY FACTOR (1)
15.
16. LOGICAL LSOURC
17.
18. REAL SOURCE(202), SCRH(202), RHOT(202), DIFF(202)
19. REAL ADUGTH(202), FLXH(202), MULH(202), MULH(202)
20. REAL LNRHOT(202), FSGN(202), FABS(202), EPSH(202)
21. REAL LORHOT(202), TERP(202), TERM(202), ADUDTH(202)
22. REAL LO(202), LN(202), LH(202), RLO(202), RLN(202)
23. REAL RNH(202), ROH(202), RLH(202), AH(202)
24. COMMON /COM1/ SOURCE, SCRH, RHOT, DIFF, ADUGTH, MULH, MULH
25. COMMON /COM1/ LORHOT, ADUDTH, LO, LN, LH, RLO, RLN, RNH, ROH
26. COMMON /COM1/ RLH, AH, LSOURC
27. EQUIVALENCE (EPSH(1), SCRH(1)), (LNRHOT(1), LORHOT(1))
28. EQUIVALENCE (FLXH(1), SCRH(1)), (FSGN(1), RHOT(1))
29. EQUIVALENCE (FABS(1), SCRH(1)), (TERP(1), SOURCE(1))
30. EQUIVALENCE (TERM(1), SOURCE(1))
31.
32. CALCULATE CONNECTIVE AND DIFFUSIVE FLUXES
33. NP = N + 1
34.
35. DO 11 I = 2, N
36. FLXH(I) = 0.5 * ADUDTH(I) * (RHOO(I) + RHOO(I-1))
37. DIFF(I) = MULH(I) * (RHOO(I) - RHOO(I-1))
38.
39. RHOL = RHOO(1) * LBC
40. RHOR = RHOO(N) * RBC
41. DIFF(1) = MULH(1) * (RHOO(1) - RHOL)
42. DIFF(NP) = MULH(NP) * (RHOR - RHOO(N))
43. FLXH(1) = 0.5 * ADUDTH(1) * (RHOO(1) + RHOL)
44. FLXH(NP) = 0.5 * ADUDTH(NP) * (RHOR + RHOO(N))
45.
46. CALCULATE LAMBDA*RHOT, THE TRANSPORTED MASS ELEMENTS
47. DO 12 I = 1, N
48. LORHOT(I) = LO(I) * RHOO(I) - FLXH(I+1) + FLXH(I)
49.
50. ADD SOURCE TERMS
51. IF (.NOT. LSOURC) GO TO 14
52. DO 13 I = 1, N
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53 ***** ETBFCT *****
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13 LORHOT(I) = LORHOT(I) + SOURCE(I)
C
C
CALCULATE ANTIDIFFUSIVE FLUXES
DO 16 I = 1, N
14 RHOT(I) = LORHOT(I) * RLO(I)
DO 17 I = 2, N
16 FLXH(I) = MULH(I) * (RHOT(I) - RHOT(I-1))
17 FLXH(I) = MULH(I) * (RHOT(I) - LBC * RHOT(I))
18 FLXH(NP) = MULH(NP) * (RBC * RHOT(N) - RHOT(N))
C
C
CALCULATE DIFFUSED MASS ELEMENTS
DO 18 I = 1, N
18 LNRHOT(I) = LORHOT(I) + DIFF(I+1) - DIFF(I)
C
C
CALCULATE TRANSPORTED/DIFFUSED DENSITY AND FLUX
DO 19 I = 1, N
19 RHOT(I) = LNRHOT(I) * RLN(I)
DO 20 I = 2, N
20 DIFF(I) = RHOT(I) - RHOT(I-1)
21 DIFF(I) = RHOT(I) - LBC * RHOT(I)
22 DIFF(NP) = RBC * RHOT(N) - RHOT(N)
C
C
CALCULATE SIGN OF DIFFUSED/TRANSPORTED FLUX
DO 21 I = 1, NP
21 FSGN(I) = SIGN (1.0, DIFF(I))
C
C
CALCULATE MAGNITUDE OF ANTIDIFFUSIVE FLUX
DO 22 I = 1, NP
22 FABS(I) = ABS(FLXH(I))
C
C
CALCULATE FLUX LIMITS ON RIGHT AND LEFT
DO 23 I = 1, N
23 TERP(I) = FSGN(I) * LN(I) * DIFF(I+1)
TERP(NP) = 1.0E+30
DO 24 I = 1, NP
24 FABS(I) = AMIN1 (TERP(I), FABS(I))
DO 25 I = 2, NP
25 TERM(I) = FSGN(I) * LN(I-1) * DIFF(I-1)
26 TERM(1) = 1.0E+30
C
CORRECT FLUXES
DO 35 I = 1, NP
35 DIFF(I) = AMIN1 (FABS(I), TERM(I))
DO 36 I = 1, NP
36 FLXH(I) = AMAX1 (0.0, DIFF(I))
DO 37 I = 1, NP
37 FLXH(I) = FSGN(I) * FLXH(I)
C
C
CALCULATE FLUX-CORRECTED DENSITIES
DO 40 I = 1, N
40 LNRHOT(I) = LNRHOT(I) - FLXH(I+1) + FLXH(I)
DO 41 I = 1, N
41 SOURCE(I) = 0.0
RHOT(I) = LNRHOT(I) * RLN(I)
LSOURC = .FALSE.

```

***** ETBFCT *****

107.
108.

RETURN
END

***** NGRIDE *****

```
1. SUBROUTINE NGRIDE (RADN, N, RADR, RADL, ALPHA)
2.
3. INTEGER ALPHA
4. REAL RADN(N)
5.
6. SETUP FOR NEW GEOMETRY VARIABLES
7. ARGUMENTS
8. RADN NEW GRID-POINT POSITIONS
9. N NUMBER OF INTERIOR GRID POINTS
10. RADR POSITION OF RIGHT BOUNDARY
11. RADL POSITION OF LEFT BOUNDARY
12. ALPHA = 1 FOR CARTESIAN GEOMETRY
13. = 2 FOR CYLINDRICAL GEOMETRY
14. = 3 FOR SPHERICAL GEOMETRY
15.
16.
17.
18. LOGICAL L$SOURC
19. REAL SOURCE(202), SCRH(202), RHOT(202), DIFF(202),
20. REAL ADUGTH(202), FLXH(202), NULH(202), MULH(202)
21. REAL LNRHOT(202), FSGN(202), FABS(202), EPSH(202)
22. REAL LORHOT(202), TERP(202), TERM(202), ADUDTH(202)
23. REAL LO(202), LN(202), LH(202), RLO(202), RLN(202)
24. REAL RNRH(202), ROH(202), RLH(202), AH(202)
25. COMMON /COM1/ SOURCE, SCRH, RHOT, DIFF, ADUGTH, NULH, MULH
26. COMMON /COM1/ LORHOT, ADUDTH, LO, LN, LH, RLO, RLN, RNH, ROH
27. COMMON /COM1/ RLH, AH, L$SOURC
28. EQUIVALENCE (EPSH(1), SCRH(1)), (LNRHOT(1), LORHOT(1))
29. EQUIVALENCE (FLXH(1), SCRH(1)), (FSGN(1), RHOT(1))
30. EQUIVALENCE (FABS(1), SCRH(1)), (TERP(1), SOURCE(1))
31. EQUIVALENCE (TERM(1), SOURCE(1))
32.
33. COMMON/DELZ/DELZL(202)
34. DATA PI, FTPI /3.1415927, 4.1887902/
35.
36. NP = N + 1
37. CALCULATE NEW INTERFACE POSITIONS
38. DO 202 I = 2, N
39. RNI(I) = 0.5 * (RADN(I) + RADN(I-1))
40. RPI(I) = PADL
41. RII(NP) = RADR
42.
43. SELECT COORDINATE SYSTEM
44. GO TO (203, 206, 209), ALPHA
45.
46. CARTESIAN COORDINATES
47. DO 204 I = 1, NP
48. AH(I) = 1.0
49. DO 205 I = 1, N
50. LN(I) = RNI(I+1) - RNI(I)
51. DELZL(I) = LN(I)
52. GO TO 213
```

***** NGRIDE *****

```
53 C
54 C
55 C
56 C
57 C
58 C
59 C
60 C
61 C
62 C
63 C
64 C
65 C
66 C
67 C
68 C
69 C
70 C
71 C
72 C
73 C
74 C
75 C
76 C
77 C
78 C
79 C
80 C
81 C
82 C
83 C
84 C
85 C

CYLINDRICAL COORDINATES
DO 207 I = 1, NP
DIFF(I) = RHH(I) * RHH(I)
207 AH(I) = PI * (ROH(I) + RHH(I))
DO 208 I = 1, N
LN(I) = PI * (DIFF(I+1) - DIFF(I))
GO TO 213

SPHERICAL COORDINATES
DO 210 I = 1, NP
DIFF(I) = RHH(I) * RHH(I) * RHH(I)
210 SCRH(I) = (ROH(I) + RHH(I)) * ROH(I)
DO 211 I = 1, NP
AH(I) = FTP1 * (SCRH(I) + RHH(I) * RHH(I))
DO 212 I = 1, N
LN(I) = FTP1 * (DIFF(I+1) - DIFF(I))

REMAINING GEOMETRIC VARIABLES
DO 214 I = 2, N
LH(I) = 0.5 * (LN(I) + LN(I-1))
LH(1) = LN(1)
LH(NP) = LN(N)
DO 215 I = 1, N
RLN(I) = 1.0 / LN(I)
DO 216 I = 1, NP
ADJGTH(I) = AH(I) * (RHH(I) - ROH(I))
DO 217 I = 2, N
RLH(I) = 0.5 * (RLN(I) + RLN(I-1))
RLH(1) = RLN(1)
RLH(NP) = RLN(N)
RETURN
END
```

***** OGRIDE *****

```
1 SUBROUTINE OGRIDE (N)
2
3 SETUP FOR OLD GEOMETRY VARIABLES
4 ARGUMENTS
5 N NUMBER OF INTERIOR GRID POINTS (1)
6
7
8 LOGICAL LSOURC
9 REAL SOURCE(202), SCRH(202), RHOT(202), DIFF(202)
10 REAL ADUGTH(202), FLXH(202), NULH(202), MULH(202)
11 REAL LNRHOT(202), FSGN(202), FABS(202), EPSH(202)
12 REAL LORHOT(202), TERP(202), TERM(202), ADUDTH(202)
13 REAL LO(202), LN(202), LH(202), RLO(202), RLN(202)
14 REAL RNH(202), ROH(202), RLH(202), AH(202)
15 COMMON /COM1/ SOURCE, SCRH, RHOT, DIFF, ADUGTH, NULH, MULH
16 COMMON /COM1/ LORHOT, ADUDTH, LO, LN, LH, RLO, RLN, RNH, ROH
17 COMMON /COM1/ RLH, AH, LSOURC
18 EQUIVALENCE (EPSH(1), SCRH(1)), (LNRHOT(1), LORHOT(1))
19 EQUIVALENCE (FLXH(1), SCRH(1)), (FSGN(1), RHOT(1))
20 EQUIVALENCE (FABS(1), SCRH(1)), (TERM(1), SOURCE(1))
21 EQUIVALENCE (TERM(1), SOURCE(1))
22
23
24 DATA ROH /202*1 0/
25
26 NP = N + 1
27 DO 401 I = 1, N
28 LO(I) = LN(I)
29 RLO(I) = RLN(I)
30 DO 402 I = 1, NP
31 ROH(I) = RNH(I)
32 RETURN
33 END
```

***** SORC *****

```
1 SUBROUTINE SORC (N, DT, MODES, C, D, DR, DL)
2 REAL C(N), D(N)
3
4 CALCULATE SOURCE CONTRIBUTIONS
5 ARGUMENTS
6 N NUMBER OF INTERIOR GRID POINTS
7 DT STEP SIZE FOR TIME INTEGRATION
8 MODES =1 ADDS + DIV(D)
9 =2 ADDS + C * GRAD(D)
10 =3 ADDS + D
11 C SOURCE VARIABLE AT GRID POINTS
12 D SOURCE VARIABLE AT GRID POINTS
13 DR D AT RIGHT BOUNDARY
14 DL D AT LEFT BOUNDARY
15
16 LOGICAL L_SOURC
17 REAL SOURCE(202), SCRH(202), RHOT(202), DIFF(202)
18 REAL ADUGTH(202), FLXH(202), NULH(202), MULH(202)
19 REAL LNRHOT(202), FSGN(202), FABS(202), EPSH(202)
20 REAL LORHOT(202), TERP(202), TERM(202), ADUDTH(202)
21 REAL LO(202), LI(202), LH(202), RLO(202), RLN(202)
22 REAL RINH(202), ROH(202), FLH(202), AH(202)
23 COMMON /COM1/ LORHOT, ADUDTH, LO, LI, LH, RLO, RLN, RINH, ROH
24 COMMON /COM1/ RLH, AH, L_SOURC
25 EQUIVALENCE (EPSH(1), SCRH(1)), (LNRHOT(1), LORHOT(1))
26 EQUIVALENCE (FLXH(1), SCRH(1)), (FSGN(1), RHOT(1))
27 EQUIVALENCE (FABS(1), SCRH(1)), (TERP(1), SOURCE(1))
28 EQUIVALENCE (TERM(1), SOURCE(1))
29
30 DATA L_SOURC, SOURCE / .FALSE., 202*0.0 /
31 NP = N + 1
32 DTH = 0.5 * DT
33 DTQ = 0.25 * DT
34 GO TO (310,320,330,340) MODES
35
36 ADD DIV(D)
37 DO 311 I = 2, N
38 SCRH(I) = DTH * AH(I) * (D(I) + D(I-1))
39 SCRH(I) = DT * AH(I) * DL
40 SCRH(IP) = DT * AH(IP) * DR
41 DO 312 I = 1, N
42 SOURCE(I) = SOURCE(I) + SCRH(I+1) - SCRH(I)
43 L_SOURC = .TRUE.
44 RETURN
45
46 ADD C * GRAD(D)
47 DO 321 I = 2, N
```

```

***** SORC *****
53 SCRH(I) = DTQ * D(I) + D(I-1)
54 SCRH(I) = DTH * DL
55 SCRH(NP) = DTH * DR
56 DO 322 I = 1, N
57   DIFF(I) = SCRH(I+1) - SCRH(I)
58 DO 323 I = 1, N
59   SOURCE(I) = SOURCE(I) + C(I) * (AH(I+1) + AH(I)) * DIFF(I)
60   LSOURC = .TRUE.
61 RETURN
62
63 C ADD D
64 DO 331 I = 1, N
65   SOURCE(I) = SOURCE(I) + DT * LQ(I) * D(I)
66   LSOURC = .TRUE.
67 RETURN
68
69 C FLUX SOURCE USING VALUES AT ZONE INTERFACES
70 C
71 DO 341 I=2,N
72   SOURCE(I)=(D(I) - D(I-1))*DT
73 CONTINUE
74 SOURCE(1)=(D(1) - DL)*DT
75 RETURN
76 END

```

***** VELOCE *****

```
1 SUBROUTINE VELOCE (U, N, UR, UL, DT)
2 REAL U(N)
3 VELOCITY DEPENDENT VARIABLE CALCULATION
4 ARGUMENTS
5 U
6 FLOW VELOCITY AT GRID POINTS
7 N NUMBER OF INTERIOR GRID POINTS
8 UR VELOCITY AT RIGHT BOUNDARY
9 UL VELOCITY AT LEFT BOUNDARY
10 DT STEPSIZE FOR TIME INTEGRATION
11
12
13 LOGICAL L,SOURCE
14 REAL SOURCE(202), SCRH(202), RHOT(202), DIFF(202)
15 REAL ADUGTH(202), FLXH(202), NULH(202), MULH(202)
16 REAL LNRHOT(202), FSGN(202), FABS(202), EPSH(202)
17 REAL LORHOT(202), TERP(202), TERM(202), ADUDTH(202)
18 REAL LO(202), LN(202), LH(202), RLO(202), RLN(202)
19 REAL RHH(202), ROH(202), RLH(202), AH(202)
20 COMMON /COM1/ SOURCE, SCRH, RHOT, DIFF, ADUGTH, NULH, MULH
21 COMMON /COM1/ LORHOT, ADUDTH, LO, LN, LH, RLO, RLN, RHH, ROH
22 COMMON /COM1/ RLH, AH, LSOURCE
23 EQUIVALENCE (EPSH(1), SCRH(1)), (LNRHOT(1), LORHOT(1))
24 EQUIVALENCE (FLXH(1), SCRH(1)), (FSGN(1), RHOT(1))
25 EQUIVALENCE (FABS(1), SCRH(1)), (TERP(1), SOURCE(1))
26 EQUIVALENCE (TERM(1), SOURCE(1))
27
28 NP = N + 1
29 DTH = 0.5 * DT
30
31 CALCULATE INTERFACE AREA * VELOCITY DIFFERENCE * DT
32 DO 101 I = 2, N
33 ADUDTH(I) = AH(I) * DTH * (U(I) + U(I-1)) - ADUGTH(I)
34 ADUDTH(1) = AH(1) * DT * UL - ADUGTH(1)
35 ADUDTH(NP) = AH(NP) * DT * UR - ADUGTH(NP)
36
37 CALCULATE HALF-CELL EPSILON = V*DT/DX
38 DO 102 I = 1, NP
39 EPSH(I) = ADUDTH(I) * RLH(I)
40
41 CALCULATE DIFFUSION AND ANTIDIFFUSION COEFFICIENTS
42 DO 103 I = 1, NP
43 MULH(I) = 0.166666667 + 0.333333333 * EPSH(I) * EPSH(I)
44 MULH(1) = 0.25 - 0.5 * NULH(I)
45 DO 104 I = 1, NP
46 NULH(I) = LH(I) * NULH(I)
47 MULH(I) = LH(I) * MULH(I)
48 RETURN
49 END
50
```

***** VELOCE *****

APPENDIX II

LISTING OF LASER BEAM PROPAGATION ROUTINES

***** ALPHA *****

```
1. SUBROUTINE ALPHA
2. COMMON A(30,50)
3. COMMON /N1/ N,MIND,IH,IA,IB,IC,ID,IE,IF,IJ
4. COMMON /N2/ IW,IX,IGP,IGM,IGBB,IGB,IG,IRBB,IRB,IR,IRP,IMU,IAB,
5.     IALPHA,IYP,II
6.
7. C
8. C
9. C
10. GIVEN ABSORPTION COEFFICIENT AB AT TRAJECTORY POINTS R(J)
11. COMPUTE ALPHA=INTENSITY-WEIGHTED MEAN BETWEEN R(J) AND R(J+1)
12.
13. DO 5 J=1,N
14.   A(IA,J)=A(IAB,J)
15.   CALL SPLNSB
16.   DO 30 J=1,N
17.     H=A(IH,J)
18.     IF (H LT .1E-3) GO TO 10
19.     EXPMH=EXP(-H)
20.     D=1.-EXPMH
21.     GO TO 20
22.   D=H*(1.-H/2.*(1.-H/3.*(1.-H/4.*(1.-H/5.))))
23.   EXPMH=1.-D
24.   SUMA=A(IF,J)
25.   SUMB=SUMA**X5
26.   SUMA=5.*SUMA+(IE,J)
27.   SUMB=SUMB+SUMA**X4
28.   SUMA=4.*SUMA+(ID,J)
29.   SUMB=SUMB+SUMA**X3
30.   SUMA=3.*SUMA+(IC,J)
31.   SUMB=SUMB+SUMA**X2
32.   SUMA=2.*SUMA+(IB,J)
33.   SUMB=SUMB+SUMA**X
34.   SUMA=SUMA+A(IA,J)
35.   A(ALPHA,J)=SUMA-SUMB*EXPMH/D
36. CONTINUE
37. RETURN
38. END
```

***** DIFS *****

```
1. SUBROUTINE DIFS (HB, HF, YPPB, YPP, YPPF, YB, Y, YF, ITER)
2. EVALUATES PREDICTOR AND CORRECTOR FORMULAS FOR INTEGRATION OF
3. (D/DZ)**2 Y = G(Z, Y)
4. WITH YPP=G(Z, Y), YPPB=G(Z-HB, YB), ETC. OUTPUT IS YF=Y(Z+HF).
5. HBF=HB+HF
6. HBHF=HB*HF
7. HB2=HB*HB
8. HF2=HF*HF
9. HBYF = HBF*Y - HF*YB
10. IF (ITER.GT.0) GO TO 10
11. PREDICTOR
12. T1=0.5*HB*HF*HRF
13. T2=HF/6.*(HF2-HB2)
14. HBYF=HBYF + T1*YPP + T2*(YPP-YPPB)
15. GO TO 20
16. CORRECTOR
17. T3 = HF*(HB*HBF - HF2)
18. T4 = HBF*(HBF*HBF + HBHF)
19. T5 = HB*(HF*HBF - HB2)
20. HBYF = HBYF + (T3*YPPB + T4*YPP + T5*YPPF)/12.
21. RETURN
22. END
23.
```

***** EDIS *****

1. SUBROUTINE EDIS (RHO,AWT,TEK,ZBAR,ZINDX,WL,EABS,EMU)
2. COMMON /C/ Z,HB,HF,T,AKZ,AKZ2
3. FOR MASS DENSITY RHO (GRAMS/CM**3), ATOMIC WEIGHT AWT (AMU),
4. ELECTRON TEMPERATURE TEK (KELVINS), IONIZATION ZBAR (FREE
5. ELECTRONS PER ATOM), UNPERTURBED REFRACTIVE INDEX ZINDX,
6. RADIATION WAVELENGTH WL (CM), COMPUTE ABSORPTION COEFFICIENT
7. EABS (CM**1) AND INDEX PERTURBATION EMU DUE TO FREE ELECTRONS.
8. COMPLEX KSG, KSTAR
9. C
10. C
11. DATA TUOPT /6.283185/
12. DATA C /2.9979E10/
13. C
14. OPCON = 4*PI*E**2/M (SEC**2 * CM**3, FOR ELECTRONS)
15. DATA OFCON /3.1826E9/
16. C
17. DATA VEV /6.592349E07/
18. C
19. RVEV = MEAN RECIPROCAL VELOCITY OF 1 EV ELECTRONS
20. DATA RVEV /1.9025296E-08/
21. C
22. ATOMIC MASS UNIT (GRAMS)
23. DATA AWTU /1.66053E-24/
24. C
25. KELVINS PER EV
26. DATA EVK /11604.5/
27. C
28. WAVELENGTH FOR 1 EV
29. DATA WLEV /1.23985E-04/
30. C
31. ELECTRON CHARGE SQUARED, CM**EV
32. DATA EQ /1.439978E-07/
33. C
34. PI/SQRT(27)
35. DATA PIOR27 / .6045997/
36. C
37. PHOTON ENERGY, EV
38. HNU=MLEV/WL
39. C
40. VACUUM WAVE NUMBER
41. WOC = TUOPT/WL
42. C
43. CIRCULAR FREQUENCY
44. WJ = WOC * C
45. C
46. UNPERTURBED WAVE NUMBER
47. AKZ = ZINDX * WOC
48. AKZ2 = AKZ**AKZ
49. C
50. ATOM DENSITY
51. ANA = RHO/(AWT*AWT)
52. C
53. ELECTRON DENSITY
54. ANE = ZBAR * ANA
55. C
56. ION DENSITY
57. ANI = ANA*(ANA,ANE)
58. C
59. Z SQUARED AVERAGE, APPROX.
60. ZSQ = ANA**2 (1.,ZBAR**2)
61. C
62. NEUTRAL DENSITY
63. ANN = ANA - ANI
64. C
65. ELECTRON TEMPERATURE, VELOCITY, RECIPROCAL VELOCITY
66. TEV = TEK / EVK
67. SQRTT = SQRT(TEV)
68. VE = VEV * SQRTT

```

***** EDIS *****
53. RVE = RVEV / SQRTT
54. ELECTRON TRANSPORT CROSS SECTION OF NEUTRALS
55. ASSUME 10 * PI*AO**2
56. SIGM = 8.79735E-16
57. ELECTRON-NEUTRAL COLLISION FREQUENCY
58. ANUN = ANN * VE * SIGM
59. PLASMA FREQUENCY SQUARED
60. OP2 = OPCON * ANE
61. ION COLLISION FREQUENCY FOR TRANSFER OF HNU
62. ANUI = PI*OR27*RVE**250*KE50/HNU*OPCON*ANI*(1.-EXP(-HNU/TEV))
63. COMPLEX WAVE NUMBER, EABS, EMU
64. KSQ = AKZ2 - OP2/C**2 * W/CMPLX(W,ANUN+ANI)
65. KSTAR = CSQRT(KSQ)
66. EABS = 2.*AIMAG(KSTAR)
67. EMU = REAL(KSTAR)/AKZ - 1.
68. RETURN
69. END
70.

```

***** GRADM *****

```
1 SUBROUTINE GRADM
2 COMMON A(30,50)
3 COMMON /N1/ N,MIND,IH,IA,IB,IC,ID,IE,IF,IJ
4 COMMON /N2/ IW,IX,IGP,IGH,IGBB,IGB,IG,IRBB,IRB,IR,IRP,IMU,IAB,
5     IALPHA,IYP,II
6     DO 10 J=1,N
7     10 A(IR,J)=A(IMU,J)
8     CALL SPLNSB
9     DO 20 J=1,N
10    20 A(IGM,J)=A(IGB,J)*A(IR,J)/A(IYP,J)
11    RETURN
12    END
```

***** GRADP *****

```
1. SUBROUTINE GRADP
2. COMMON A(30,50)
3. COMMON /N1/ N,MIND,IH,IA,IB,IC,ID,IE,IF,IZ
4. COMMON /N2/ Iw,IX,IGP,IGM,IGBB,IGB,IG,IRBB,IRB,IR,IRP,IMJ,IAB,
5. ALPHA,IYP,II
6. COMMON /C/ Z,HB,HF,T,AKZ,AKZ2
7.
8. C
9. C
10. C
11. C
12. C
13. C
14. C
15. C
16. C
17. C
18. C
19. C
20. C
21. C
22. C
23. C
24. C
25. C
26. C
27. C
28. C
29. C
30. C
31. C
32. C
33. C
```

GIVEN TRAJECTORY RADIUS R(J), J=1..N, CALCULATE Y(J)=R(J)**2/2
AND ITS DERIVATIVES BY X, THEN EVALUATE GRADP, THE DERIVATIVE BY
R OF THE DIFFRACTION POTENTIAL
 $P = 1/(4**K2)*((LAPLACIAN I)/1 - 5*(GRAD I)/1)**2$

```
5 A(IA,J)=.5KA(IR,J)**2
DO 10 J=1,N
CALL SPLNSB
DO 10 J=1,N
Y=A(IA,J)
Y1P=A(IB,J)
Y2P=A(IC,J)**2
Y3P=A(ID,J)**6
Y4P=A(IE,J)**24.
T1=(DI/DY)/1
T2=DT1/DY
T3=DT2/DY
T1=-((1 +Y2P/Y1P)/Y1P
T2=(Y2P-Y3P+2.*Y2P**2/Y1P)/Y1P**3
T3=(Y3P-Y4P)/Y1P**3+(7.*Y2P*Y3P-4.*Y2P**2)/Y1P**5-8.*Y2P**3/Y1P**6
A(IP,J)=(2.*T1 + Y*T1**2 + 2.*Y*T2)/(4.*AKZ2)
A(IGP,J)=A(IR,J)/(4.*AKZ2)*(4.*T2+T1**2+2.*Y*(T1*T2+T3))
A(IYP,J)=Y1P
10 CONTINUE
RETURN
END
```


***** SPLINEA *****

***** SPLNSB *****

```
1 SUBROUTINE SPLNSB
2 COMMON A(30,50)
3 DATA NRDIM/30/
4 COMMON /N1/ N,MIND,IH,IA,IB,IC,ID,IE,IF,IJ,IZ
5 EQUIVALENCE (IB1,IB), (IC1,IC), (IZ1,IZ)
6
7 C GIVEN A(IH,I) = X(I+1)-X(I), A(IA,I) = Y(I), I=1,N,
8 CALCULATE B1 = BACKWARD FIRST DIVIDED DIFFERENCE OF Y,
9 C1 = SECOND DIVIDED DIFFERENCE OF Y,
10 Z1 = FORWARD DIFFERENCE OF C1
11
12 C
13 C
14 C
15 C
16 C
17 C
18 C
19 C
20 C
21 C
22 C
23 C
24 C
25 C
26 C
27 C
28 C
29 C
30 C
31 C
32 C
33 C
34 C
35 C
36 C
37 C
38 C
39 C
40 C
41 C
42 C
43 C
44 C
45 C
46 C
47 C
48 C
49 C
50 C
51 C
52 C
```

MAXD=MIND+2
NM=N-1
M=N-2
A(IB1,1) = 0
DO 10 I=2,N
10 A(IB1,I) = (A(IA,I)-A(IA,I-1))/A(IH,I-1)
A(IC1,1) = 0
DO 20 I=2,NM
20 A(IC1,I) = (A(IB1,I+1)-A(IB1,I))/(A(IH,I-1)+A(IH,I))
A(IZ1,1) = 0
DO 30 I=2,M
30 A(IZ1,I) = A(IC1,I+1)-A(IC1,I)
A(IZ1,N-1) = 0
A(IZ1,N) = 0
CALL SYMSOL (NRDIM,M,MIND,MAXD,IZ1,IZ,A)

GIVEN B-SPLINE COEFFICIENTS CALCULATED BY SYMSOL IN Z,
FIRST BACKWARD DIVIDED DIFFERENCE OF Y IN B1 AND
SECOND DIVIDED DIFFERENCE OF Y IN C1,
CALCULATE COEFFICIENTS B,C,D,E,F FOR THE QUINTIC SPLINE
S(I) = Y(I)+B(I)*T+C(I)*T**2+D(I)*T**3+E(I)*T**4+F(I)*T**5
FOR I=1,N, T=X-X(I), 0.LE.T.LT.A(IH,I)

A(IZ,1)=0
A(IZ,NM) = 0
A(IZ,N) = 0
0 = A(IH,1)
03 = Q**3
R = A(IH,2)
R3 = R**3
QR = Q**R
H=A(IZ,2)/QR
A(ID,1)=0
A(IE,1)=0
A(IF,1)=H/Q
DO 40 I=2,NM
F=0
P3=03
Q=R

***** SPLN5B *****

```
53. Q3=R3
54. P0=QR
55. R=A(IH,I+1)
56. R3=R*I*X3
57. QR=Q+R
58. G=H
59. H=(A(IZ,I+1) - A(IZ,I))/QR
60. A(ID,I)=10/PQ*(A(IZ,I-1)*Q + A(IZ,I)*P)
61. A(IE,I)=5.*G
62. A(IF,I) = (P*(A(IB1,I+1)+Q*(A(IB1,I)))/PQ-P*(Q*(A(ID,I)-(P-Q)*A(IE,I)
63. + (P3)*A(IF,I-1)+Q3*(A(IF,I))/PQ)
64. A(IC,I) = A(IC1,I)+A(ID,I)*(P-Q)-(A(IE,I)*(P3+Q3)-A(IF,I-1)*P3)*P
65. +A(IF,I)*Q3*Q)/PQ
66.
67. 40 CONTINUE
68. P=A(IH,I)
69. P3=P*X3
70. A(IC,1)=A(IC,2)-10.*A(IF,1)*P3
71. A(IB,1)=A(IB,2) - (A(IC,1)+A(IF,1)*P3)*P
72. A(IC,N)=A(IC,NM)+10.*A(IF,NM)*Q3
73. A(IB,N)=A(IB,N) - (A(IC,N)-A(IF,NM)*Q3)*Q
74. A(ID,N) = 0.
75. A(IE,N) = 0.
76. A(IF,N) = 0.
77. RETURN
78. END
```

***** SETX *****

```
1 SUBROUTINE SETX
2 COMMON A(30,50)
3 COMMON /N1/ N,MIND,IH,IA,IB,IC,ID,IE,IF,IJ
4 COMMON /N2/ IW,IX,IGP,IGM,IGBB,IG,IRBB,IRB,IR,IRP,IMU,IAB,
5     TALPHA,IYP,II
6
7 C
8 C GIVEN W(J)=BEAM POWER BETWEEN R(J) AND R(J+1), J=1,N
9 C CALCULATE X(J)=-LOG(1-S(J)/S(NH+1)) WHERE S(J)=SUM W(I), I=1,J-1
10 C AND H(J)=X(J+1)-X(J), J=1,N-1. SET UP AND FACTOR SPLINE MATRIX.
11 C A(I1,J)=DS/DX=STOT*EXP(-X)
12
13 REAL A(NRDIM,N)
14 STOT = 0
15 DO 10 J=1,N
16 STOT=STOT+A(IW,J)
17 A(IX,1)=0
18 S=A(IW,1)
19 DO 20 J=2,N
20 EXPMX=1.-S/STOT
21 A(IX,J)=-ALOG(EXPMX)
22 A(II,J)=STOT*EXPMX
23 A(IH,J-1)=A(IX,J)-A(IX,J-1)
24 S=S+A(IW,J)
25 CALL SPLNSA(NRDIM,N,MIND,IH,A)
26 RETURN
27 END
```

***** STEP *****

```
1 SUBROUTINE STEP
2 COMM N A(30,50)
3 COMM /N1/ N,MIND,IH,IA,IB,IC,JD,JE,IF,IJ
4 COMM /N2/ IW,IX,IGP,IGM,IGBB,IGB,IG,IRBB,IRB,IR,IRP,IMU,IAB,
5 ALPHA,IYP,II
6 COMMON /C/ Z,HB,HF,T,AKZ,AKZZ
7
8 CALL KVAL
9 CALL ALPHA
10 ADVANCE Z,GBB,GB,RBB,RB,W
11 DO 10 J=1,N
12 A(IRBB,J)=A(IRB,J)
13 A(IRB,J)=A(IR,J)
14 A(IGBB,J)=A(IGB,J)
15 A(IGB,J)=A(IG,J)
16 Z=Z*HF
17 A(IW,J)=A(IW,J) * EXP(-A(ALPHA,J)*HF)
18 CALL SETX
19 REPS=1.E-3
20 ITER=0
21 CALL GRADP
22 CALL GRADM
23 DO 20 J=1,N
24 A(IG,J)=A(IGP,J) + A(IGM,J)
25 A(IRP,J)=A(IR,J)
26 CALL DIFS (HB,HF,A(IGBB,J),A(IGB,J),A(IG,J),A(IRBB,J),A(IRB,J),
27 A(IR,J),ITER)
28 CONTINUE
29 DO 25 J=1,N
30 IF(ABS(A(IR,J)-A(IRP,J)).LT.REPS) GO TO 25
31 ITER=ITER+1
32 IF(ITER.LT.20) GO TO 15
33 WRITE(6,1000) J
34 FORMAT(' STEP NONCONVERGENCE, J=',I6)
35 CALL EDIT
36 STOP 'STEP'
37
38 CONTINUE
39 INTENSITY I=(DS/DY)/(DS/DX)/(DY/DX)
40 DO 30 J=1,N
41 A(II,J)=A(II,J)/A(IYP,J)
42 CONTINUE
43 CALL EDIT
44 RETURN
45 END
```

***** SYMFAC *****

```
1. SUBROUTINE SYMFAC (NRDIM, M, MIND, MAXD, A, R)
2. FACTORIZATION OF POSITIVE DEFINITE SYMMETRIC BANDED MATRIX
3. A = L*DXU WITH L UNIT LOWER TRIANGULAR, D DIAGONAL, U TRANSPOSE
4. OF L OF RALSTON, WILF MATHEMATICAL METHODS FOR DIGITAL
5. COMPUTERS, V2, P72. THIS IS A MODIFIED CHOLESKY METHOD.
6. THE INPUT MATRIX IS STORED IN A BLOCK WITH NC=M COLUMNS AND
7. MAXD-MIND+1 ROWS, THE LATTER CORRESPONDING TO THE LOWER MATRIX
8. DIAGONALS, WITH THE PRINCIPAL DIAGONAL IN ROW MIND. THE ELEMENT
9. IN ROW R, COLUMN C OF THE MATRIX IS THEREFORE IN ELEMENT ID, C
10. OF THE ARRAY, WHERE ID = MIND+R-C AND R GE C.
11. THE ROW INDEX R IS RETURNED AS ZERO ON NORMAL COMPLETION. IF A
12. ZERO DIAGONAL ELEMENT IS GENERATED THE ROUTINE RETURNS AT ONCE.
13. THE OUTPUT MATRICES L AND D ARE WRITTEN OVER THE INPUT MATRIX A.
14. IT IS ASSUMED THAT MAXD-MIND+1 IS AT LEAST 2 AND NC AT LEAST 2.
15.
16.
17. REAL A(NRDIM,M)
18. DOUBLE PRECISION S,SL
19. INTEGER R,C,CMIN,CMAX
20.
21. NC = M
22. R=1
23. IF (A(MIND,1) EQ 0.) RETURN
24. R=2
25. SL = A(MIND+1,1)/A(MIND,1)
26. S = A(MIND,2) - SL*A(MIND+1,1)
27. A(MIND+1,1) = SL
28. A(MIND,2) = S
29. IF (A(MIND,2) EQ 0.) RETURN
30. IF (NC.LT.3) GO TO 60
31. DO 50 N=3,NC
32. R=N
33. JMIN = MAX(1,R-MAXD+MIND)
34. CMIN = JMIN+1
35. CMAX = R-1
36. THE FOLLOWING STATEMENT ALLOWS APPLICATION TO TRIDIAGONAL MATRICES
37. IF (CMIN .GT. CMAX) GO TO 30
38. DO 20 C=CMIN,CMAX
39. JMAX = C-1
40. S = A(MIND+R-C,C)
41. DO 10 J=JMIN,JMAX
42. S = S-DBLE(A(MIND+R-J,J)) * DBLE(A(MIND+C-J,J))
43. S = A(MIND,R)
44. DO 40 J=JMIN,CMAX
45. SL = A(MIND+R-J,J)/A(MIND,J)
46. S = S - SL*A(MIND+R-J,J)
47. A(MIND,R) = S
48. IF (A(MIND,R) EQ 0.) RETURN
49. CONTINUE
50. R=0
51.
52.
```

***** SYMFAC *****

53.
54. RETURN
END

***** SYMSOL *****

```
1. SUBROUTINE SYMSOL (NRDIM, M, MIND, MAXD, IZ1, IZ, A)
2. ARRAY A CONTAINS ON INPUT AND OUTPUT A DIAGONAL MATRIX D IN ROW MIND,
3. SUBDIAGONALS OF A UNIT LOWER TRIANGULAR MATRIX L IN ROWS MIND+1 TO
4. MAXD, VECTOR Z1 IN ROW IZ1, AND ON OUTPUT A SOLUTION VECTOR Z IN
5. ROW IZ. THE SYSTEM SOLVED IS L*DXUKZ=Z1 WHERE U IS THE
6. TRANSPOSE OF L.
7.
8. REAL A(NRDIM,M)
9. DOUBLE PRECISION S
10. INTEGER R
11. NC=M
12. C SOLVE L * DUZ = Z1 FOR DUZ
13. A(IZ,1)=A(IZ1,1)
14. DO 20 R=2,NC
15. KMAX=R-MAX0(1,R-MAXD+MIND)
16. S = A(IZ1,R)
17. DO 10 K=1,KMAX
18. S=S-DBLE(A(MIND+K,R-K))*DBLE(A(IZ,R-K))
19. 20 A(IZ,R)=S
20. C SOLVE D * UZ = DUZ FOR UZ
21. DO 30 R=1,NC
22. A(IZ,R)=A(IZ,R)/A(MIND,R)
23. C SOLVE U * Z = UZ FOR Z
24. DO 50 I=2,NC
25. R=NC+1-I
26. KMAX=MIND-(NC-R,MAXD-MIND)
27. S=A(IZ,R)
28. DO 40 K=1,KMAX
29. S=S-DBLE(A(MIND+K,R))*DBLE(A(IZ,R+K))
30. 50 A(IZ,R)=S
31. RETURN
32. END
```

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approximation, with continuously varying refractive index, is described.

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