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Report

MEDUSA

A ONE-DIMENSIONAL NUMERICAL MODEL FOR LASER FUSION CALCULATIONS

J P CHRISTIANSEN
D E T F ASHBY
K V ROBERTS

CULHAM LABORATORY
Abingdon Berkshire
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ABSTRACT

This report describes the physics and mathematics used in MEDUSA, a computer code designed for calculating the compression of a plasma by laser radiation together with the thermonuclear reactions that take place. Sections 1-3 of this report deal with the physical processes and mathematical formulae used, whilst Sections 4-10 present the numerical techniques employed in the model. Sections 11-13 describe the code.

UKAEA Research Group
Culham Laboratory
Abingdon, Berkshire

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1. INTRODUCTION

The computer program MEDUSA 1 described in this report calculates the 1-dimensional hydrodynamic and thermodynamic behaviour of a plasma irradiated by an intense laser beam. The results are intended to assist in understanding the proposed Laser Fusion method for generating thermonuclear power [1,2,3,4,5].

The plasma is described by 4 main dependent variables ρ, u, T_i, T_e representing respectively the density, velocity, ion and electron temperatures. The equations are outlined in Section 2. Each variable is a function of a single space coordinate r which can be chosen to correspond to slab, cylindrical or spherical geometry as required. The motion of the plasma, the boundary conditions and the equations of state are treated in Section 3. All physical quantities are expressed at the points of a moving Lagrangian mesh which is described in Section 4, together with a summary of the integration scheme used. The details of the integration scheme and the method of solution are given in Section 5, and the timestep control in Section 6.

The structure of MEDUSA 1 is based on the OLYMPUS package [6,7]. Section 11 presents a diagram illustrating the organization of the calculation. The Appendix of [8] lists the subprograms of MEDUSA 1 and those common variables and arrays which can be set by the user. It should be read in conjunction with Section 12, which is meant as an 'instruction manual' for those wishing to run the program and also serves as a guide to the standard tests described in Section 9 of [8].

To facilitate the reading of this report as well as of the program listing we refer to subprograms by their identification numbers. Thus the notation ⟨2.9⟩ means subprogram 9 of Class 2, the decimal numbering being that explained in [6,7]. Conversely the program listing contains numbered references to the equations of this report as well as to those of ref.[8] which is a shortened version.* There is a similar correspondence for variable and array names. SI units are used throughout.

Complex computer programs often undergo a continuous process of development which sometimes makes it difficult for the reader to determine the precise assumptions that have been made in any particular calculation. To avoid such misunderstandings we shall therefore refer to the standard 'frozen' version presented here and in ref.[8] as MEDUSA 1. Published calculations then need only refer specifically to any ad hoc modifications that have been made to this standard version. We hope to describe further versions of MEDUSA in due course.

2. PHYSICAL MODEL

The plasma is assumed to consist of a charge-neutral mixture of electrons (e), and various species of ions and atoms or molecules which are collectively referred to as 'ions' (i), the individual species of heavy particles being distinguished where necessary by the subscript 'k'.

The thermodynamics of MEDUSA 1 treats the electrons as one subsystem, with internal energy U_e per unit total mass, temperature T_e, pressure p_e, specific heat ratio λ_e and so on, and the 'ions' as a second subsystem with a corresponding set of variables. Charge-neutrality requires that the two subsystems share the same velocity u. Electric fields are neglected in MEDUSA 1, and the two subsystems are coupled together by this common velocity and by the exchange of energy due to electron-ion or electron-atom collisions.

The 8 species considered in the published code are H (hydrogen), D (deuterium), T (tritium), ^{3}He (Helium 3), ^{4}He (Helium 4), N (an arbitrary neutral atom or molecule with mass number M_N), X (an arbitrary ion with charge number Z_X and mass number M_X), and n (neutrons). Species N and X play no role in the standard version, but are carried along in the hydrodynamics and in other parts of the code to facilitate ad hoc modifications using the EXPERT facility [6,7]. Neutrons are assumed to escape freely from the system without further interaction, thus leading to a loss of mass and a change in momentum; they are not included in the subscript 'k'. The standard version does not allow either for ionization or for the finite range of the charge reaction products so that the number of electrons in each Lagrangian fluid element remains invariant.

* Equation numbers followed by a letter, e.g.(86A), do not appear in ref.[8].

The local electron density is denoted by n_e and only changes with time because of the hydrodynamic expansion and contraction of the moving fluid element. The local 'ion' density is denoted by n_i and this may suffer a further change due to atomic or nuclear reactions. The instantaneous local chemical composition is described in the code by a set of fractions f_k such that

$$n_k = f_k \, n_i \tag{1}$$

is the number density of 'ions' of species k, the fractions being adjusted at each step to maintain the normalization

$$\sum_k f_k = 1 \quad . \tag{2}$$

A similar fraction f_n is used to describe the number of neutrons that have been produced by each element but this is not included in the normalization (2).

The average mass and charge numbers associated with each 'ion' are denoted by

$$M = \sum_k f_k \, M_k \tag{3}$$

$$Z = \sum_k f_k \, Z_k \tag{4}$$

where M_k, Z_k are the mass and charge numbers of the individual species. The electron and ion densities are then related by

$$n_e = Z \, n_i \quad m^{-3} \tag{5}$$

and the physical density can be written as

$$\rho = n_i \, M \, m_H = \frac{1}{V} \quad kg/m^3 \tag{6}$$

where m_H is the proton mass and V is the specific volume; we neglect the electron mass, the neutron mass difference and all mass defects in formulating the hydrodynamics. Note that the specific volume V depends not only on the geometry of a moving element (as in an ordinary Lagrangian code) but also on any change in mass that has occurred; also that energy gain and loss processes are expressed in the code as rates/unit mass so that the coefficients depend on both the total mass and on the chemical composition.

Physical coefficients such as ion-electron energy exchange rate, thermal conductivity, bremsstrahlung etc. which involve encounters between 2 charged particles will employ averages such as (3) and (4) together with averages of other powers such as $\overline{M^p Z^q}$, although the formulae obtained in this simple way will not necessarily be accurate, particularly if species with large M_k, Z_k are involved. Ad hoc modifications must however be introduced if neutral atoms or molecules are taken into account, since the standard formulae in the code refer only to charged-particle collisions. Any average involving a non-zero power of Z_k always ignores the neutral species N so that division by zero is avoided.

The internal energies per unit mass are denoted by (we omit the subscripts e and i) :

$$U = \frac{pV}{\gamma - 1} \quad J/kg \tag{7}$$

and the two subsystems have independent equations of state

$$U = U(\rho, T), \quad p = p(\rho, T) \tag{8}$$

which may in general not be the same. The energy equation is written as

$$C_v \frac{dT}{dt} + B_T \frac{d\rho}{dt} + p \frac{dV}{dt} = S \quad W/kg \tag{9}$$

where S is the rate per unit mass at which energy enters each subsystem and

$$C_v = \left(\frac{\partial U}{\partial T}\right)_\rho \qquad B_T = \left(\frac{\partial U}{\partial \rho}\right)_T \quad . \tag{10}$$

The source terms S_i and S_e of equation (9) for ions and electrons respectively are written as

$$S_i = H_i - K + Y_i + Q, \qquad W/kg \tag{11}$$

$$S_e = H_e + K + Y_e + J + X, \quad W/kg \tag{12}$$

where H represents the flow of heat due to thermal conduction; K is the rate of exchange of energy between ions and electrons; Y is the rate of thermonuclear energy release; J is the rate of bremsstrahlung emission; X is the rate of absorption of laser light; Q is the rate of viscous shock heating (see Section 4). In the following we shall define the expressions used for the various terms in equations (11) and (12). These are all expressed in Watts/kg and if subscript i or e is omitted the expression concerned applies to both.

Thermal conductivity

The heat conduction term becomes

$$H = \frac{1}{\rho} \nabla . \varkappa \nabla T \tag{13}$$

where $\varkappa$ is the thermal conductivity. The expressions for $\varkappa$ (2.13) are adapted from [9] to be

$$\varkappa_i = 4.3 \times 10^{-12} \, T_i^{5/2} (\log \Lambda)^{-1} \, \overline{M^{-\frac{1}{2}} Z^{-2}} \left(\overline{Z^2}\right)^{-1} \quad W/m \; K \tag{14}$$

$$\varkappa_e = 1.83 \times 10^{-10} \, T_e^{5/2} (\log \Lambda)^{-1} \, Z \left(\overline{Z^2}\right)^{-1} \quad W/m \; K \tag{15}$$

where $\log \Lambda$ (2.8) is the Coulomb logarithm given by [9] as

$$\Lambda = 1.24 \times 10^6 \, T_e^{3/2} \, n_e^{-\frac{1}{2}} / Z \tag{16}$$

Free-streaming limit

A limit in ⟨2.13⟩ is imposed on the electron thermal flux $F_e = \kappa_e \nabla T_e$, the so-called free-streaming limit [8]

$$(F_e)_{max} = \frac{1}{a}\frac{1}{4} n_e \overline{v_e} k T_e \qquad W/m^2$$

where a is an adjustable numerical constant.

The flux is limited according to

$$\frac{1}{F_e'} = \frac{1}{F_e} + \frac{1}{(F_e)_{max}} \qquad (17)$$

by using a modified expression for the thermal conductivity

$$\kappa_e' = \kappa_e \left(1 + a \frac{\lambda_e}{T_e}\frac{dT_e}{dx}\right)^{-1} \qquad (18)$$

where λ_e is the electron mean free path

$$\lambda_e = 5.7 \times 10^7 \, T_e^2/n_i \overline{Z^2} \quad m. \qquad (19)$$

Energy exchange

The exchange of energy between ions and electrons ⟨2.11⟩ occurs at the rate [10]

$$\omega = \frac{M^{-1} Z^2 e^4 n_i \log\Lambda \, m_e^{\frac{1}{2}}}{32\sqrt{2\pi}\,\epsilon_o^2 m_H} (k T_e)^{-3/2} \qquad s^{-1}. \qquad (20)$$

The term K of equations (11) and (12) is

$$K = \frac{1}{\rho}\omega n_e k(T_i - T_e) \quad . \qquad (21)$$

Substituting for ω we get ⟨2.11⟩

$$K = 0.59 \times 10^{-8} n_e (T_i - T_e) T_e^{-3/2} \overline{M^{-1} Z^2} \log\Lambda \quad W/kg \quad . \qquad (22)$$

Bremsstrahlung

The quantity J represents the bremsstrahlung radiation emitted by the electrons. This is assumed to escape from the plasma and is thus an energy loss ($J < 0$). For a Maxwellian gas J is adapted from [10] to be

$$J = -\frac{\overline{Z^2} e^6 n_e \overline{v_e}}{24\pi\epsilon_o^3 c^3 m_e m_H Mh} \qquad W/kg \quad . \qquad (23)$$

Inserting for v_e etc we get ⟨2.10⟩

$$J = -8.5 \times 10^{-14} n_e T_e^{\frac{1}{2}} \overline{Z^2} M^{-1} \qquad W/kg \quad . \qquad (24)$$

The term J may be modified, see Section 3.

Absorption of laser light

Absorption ⟨2.9⟩ is assumed to occur via bremsstrahlung at densities below the critical density

$$\rho_C = \frac{\epsilon_o M m_H m_e}{Ze^2}\omega_L^2 \qquad kg/m^3 \qquad (25)$$

at which the plasma frequency equals the frequency ω_L of the laser light. The absorption coefficient is given in [11] as

$$\alpha = 13.51 \, \lambda^{-2}\beta^2(1-\beta)^{-\frac{1}{2}} T_e^{-3/2}(5.05 + \log\lambda T_e) \overline{Z^2} \, m^{-1} \qquad (26)$$

where $\beta = \rho/\rho_C < 1$ and λ is the wavelength of the laser light. If $P_L(R_o)$ is the laser power ⟨2.3⟩ incident on the plasma boundary at $r = R_o$ then

$$P_L(r,t) = e^{-\alpha(R_o - r)} P_L(R_o,t) \qquad (27)$$

and the term in equation (12) becomes (dM is an infinitesimal mass element)

$$X(r,t) = \frac{1}{dM} P_L(r,t) \qquad W/kg \quad . \qquad (28)$$

At $r = r_C$ we have $\rho = \rho_C$ and then the remaining laser power is all assumed to be absorbed at this density to simulate anomalous absorption, i.e. ⟨2.9⟩

$$X(r_C,t) = \frac{1}{dM} P_L(r_C,t) \qquad W/kg \quad . \qquad (29)$$

Thermonuclear reactions

The terms Y_i and Y_e represent the rate of energy released from the 4 thermonuclear reactions ⟨2.12⟩

$$\begin{aligned} D + T &\rightarrow {}^4He(3.6\ MeV) + n(14.1\ MeV) \\ D + D &\rightarrow T\ (1.0\ MeV) + H(3.0\ MeV) \\ D + D &\rightarrow {}^3He(0.8\ MeV) + n(2.45\ MeV) \\ D + {}^3He &\rightarrow {}^4He(3.6\ MeV) + H(14.7\ MeV) \quad . \end{aligned} \qquad (30)$$

The number of reactions taking place is

$$R_{DT} = (\sigma v)_{DT} f_D f_T n_i^2 \qquad m^{-3} sec^{-1} \qquad (31)$$

with similar expressions for the D-D and D-^{3}He reactions. $(\sigma v)_{DT}$ is the reaction rate [12] which is a function of T_i. The neutrons are assumed to escape from the plasma carrying off their energy and this represents a mass and momentum loss. The charged reaction products H, T, ^{3}He and ^{4}He are assumed to deposit their energy locally to the ions and electrons in ratios which we write for the D-T reaction as P_{DT} and $1-P_{DT}$ respectively, where P_{DT} is a function of T_e [4], with a similar notation for the other reactions. Let E_{DT}, E_{DD} and E_{D^3He} denote the energies of the charged reaction products of equation (30). Then ⟨2.12⟩

$$Y_i = (P_{DD}\, E_{DD}\, R_{DD} + P_{DT}\, E_{DT}\, R_{DT} + P_{D^3He}\, E_{D^3He}\, R_{D^3He}) \quad W/kg, \quad (32)$$

with a similar expression for Y_e where $1-P_{DT}$ replaces P_{DT} etc.

Chemical composition

The composition of the plasma changes due to the reactions (30). We calculate the fraction $f_T = n_T/n_i$ from ⟨2.28⟩

$$\frac{1}{n_i}\frac{d}{dt}\, n_T = (\tfrac{1}{2} R_{DD} - R_{DT})\frac{1}{n_i} \quad s^{-1} \quad (33)$$

subsequently renormalizing according to equation (2). Similar equations apply to the fractions f_D etc.

Shock heating

The quantity Q will be dealt with in Section 5.

3. HYDRODYNAMICS, BOUNDARY CONDITIONS, EQUATIONS OF STATE

Geometry

The plasma occupies a finite but variable region whose geometry described by the parameter g can be chosen as either

$g = 1$. A slab of unit cross-section

$g = 2$. A section of a cylinder of unit height and one radian in angle

$g = 3$. A section of a sphere, of one steradian in solid angle.

Only the coordinate r is used in each case, the cross-sections being needed only for normalization purposes.

Equations of motion

The motion of the plasma is governed by the Navier-Stokes equation ⟨2.17⟩,

$$\rho \frac{du}{dt} = -\nabla p . \quad (34)$$

Here u is the velocity of the plasma which defines the motion of the Lagrangian coordinates ⟨2.19⟩ according to

$$\frac{dr}{dt} = u(r,t) . \quad (35)$$

p is the hydrodynamic pressure ⟨2.24⟩ defined as

$$p = p_i + p_e \quad N/m^2 \quad (36)$$

together with an artificial viscous pressure discussed in Section 5.

Boundary conditions

It is necessary to specify both hydrodynamic and thermodynamic boundary conditions at the inner and outer boundaries. MEDUSA 1 does not specifically allow for hollow shells [2], and for the inner boundary we simply choose

$$u(r = o) \equiv 0 , \quad (37)$$

and zero thermal flux. At a moving outer boundary point $r = R_o$, we distinguish between the following 4 cases ⟨2.25⟩ :

1. $p(R_o) = 0$; Zero thermal flux
2. $u(R_o) = 0$; $T_i(R_o) = T_i(t)$; $T_e(R_o) = T_e(t)$
3. $p(R_o) = p(t)$; Zero thermal flux
4. $u(R_o) = u(t)$; Zero thermal flux

(38)

Case 1 is used for general problems involving the absorption of laser light, Case 2 is used to study simplified thermal conduction problems, e.g. compression and expansion of a plasma. The standard expressions used in the published version for the functions $p(t)$ etc. will be described in Section 8.

Equations of state

The equations of state (8) used in MEDUSA 1 assume the ions to behave as a non-degenerate perfect gas ⟨2.6⟩ and the electrons to behave as a perfect gas which may either be non-degenerate or partially or fully degenerate ⟨2.7⟩. For the ions this simply means

$$(C_v)_i = \frac{1}{\gamma_i - 1}\frac{k}{m_H M} ; \quad (B_T)_i = 0 ; \quad p_i = \frac{k}{m_H}\frac{1}{M}\rho\, T_i . \quad (39)$$

If the electrons are assumed to behave as a non-degenerate gas we use equation (39). In such a case we can however simulate degeneracy effects by choosing an initial electron temperature T_e^{σ} which yields the same pressure as the Fermi pressure of a fully degenerate gas at zero temperature, provided that we also change the expression (24) for the bremsstrahlung rate to ⟨2.10⟩

$$J = -8.5 \times 10^{-14}\, n_e\, \delta T_e^{\frac{1}{2}}\, \overline{Z^2}\, M^{-1} \quad W/kg \quad (40)$$

where

$$\delta T_e = T_e - \left(\frac{n_e}{n_e^o}\right)^{\gamma_e - 1} T_e^o \quad (41)$$

is the departure from the initial adiabat. This prevents an unphysical cooling of the electron gas to an energy density below the Fermi minimum.

If however the electrons are assumed to behave as a degenerate gas we introduce the quantity

$$\xi = T_e/T_F , \quad (42)$$

where

$$k\,T_F = \frac{h^2}{8M}\left(\frac{3}{\pi}\right)^{2/3}\left(\frac{Z}{Mm_H}\right)^{2/3}\rho^{2/3} \qquad (43)$$

is the Fermi energy [13]. ξ measures the degree of degeneracy and is used to obtain p_e, $(C_v)_e$ and $(B_T)_e$ from expansions of the Fermi-Dirac functions given in [1] and [13]. Different expressions are used in three ranges of ξ as follows

$$p_e = \frac{k}{m_H}\frac{Z}{M}\rho\,T_e \begin{cases} \frac{2}{5}\xi^{-1} + \frac{\pi^2}{6}\xi - \frac{\pi^4}{40}\xi^3 & \xi < \xi_{min} \\ 1 + (3\sqrt{2\pi})^{-1}\,\xi^{-3/2} & \xi_{min} \leqslant \xi < \xi_{max} \\ 1 & \xi_{max} \leqslant \xi \end{cases} \qquad (44)$$

$$(C_v)_e = \frac{1}{\gamma_e - 1}\frac{k}{m_H}\frac{Z}{M} \begin{cases} \frac{\pi^2}{3}\xi - \frac{\pi^4}{10}\xi^3 & \xi < \xi_{min} \\ 1 - (6\sqrt{2\pi})^{-1}\,\xi^{-3/2} & \xi_{min} \leqslant \xi < \xi_{max} \\ 1 & \xi_{max} \leqslant \xi \end{cases} \qquad (45)$$

$$(B_T)_e = \frac{1}{\gamma_e - 1}\,p_F\,\rho^{-2} \begin{cases} \frac{2}{3} - \frac{5\pi^2}{18}\xi^2 + \frac{\pi^4}{8}\xi^4 & \xi < \xi_{min} \\ 5\,(6\sqrt{2\pi})^{-1}\,\xi^{-1/2} & \xi_{min} \leqslant \xi < \xi_{max} \\ 0 & \xi_{max} < \xi \end{cases} \qquad (46)$$

p_F is the pressure of a completely degenerate gas [13]

$$p_F = \frac{h^2}{20m}\left(\frac{3}{\pi}\right)^{2/3}\left(\frac{Z}{Mm_H}\right)^{5/3}\rho^{5/3} \qquad (47)$$

4. MESH AND INTEGRATION SCHEME

The region extending from the fixed point r = 0 to the moving point $r = R_o$ is divided into N cells as indicated in Figure 1. The cell centres are

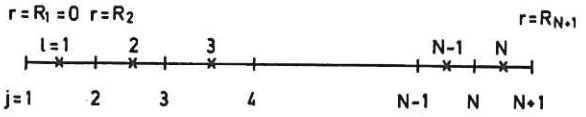

Fig.1. The arrangement of the mesh

marked by X and labelled ℓ. The cell boundaries labelled j are free to move thereby altering the volume of a cell. Each cell carries a mass dM_ℓ so that the specific volume is ⟨2.20⟩

$$V_\ell = \frac{1}{g}\,(R_{j+1}^g - R_j^g)\,\frac{1}{dM_\ell} \quad . \qquad (48)$$

The mass dM_ℓ can only change if a cell undergoes thermonuclear burning. From equation (48) ρ_ℓ can be found. Knowing M and Z we find the number densities ⟨2.20⟩

$$n_i = \rho\,\frac{1}{m_H M} \quad ; \quad n_e = Z\,n_i \quad . \qquad (49)$$

A quantity given at cell centres can be evaluated at a cell boundary by a simple average and vice versa, for example

$$R_\ell = \tfrac{1}{2}(R_j + R_{j+1}) \qquad (50)$$

A superscript n attached to any quantity indicates its value at the time

$$t^n = \sum_{i=1}^{n} \Delta t^i \quad ,$$

where Δt^i is the i^{th} step in a series of discrete

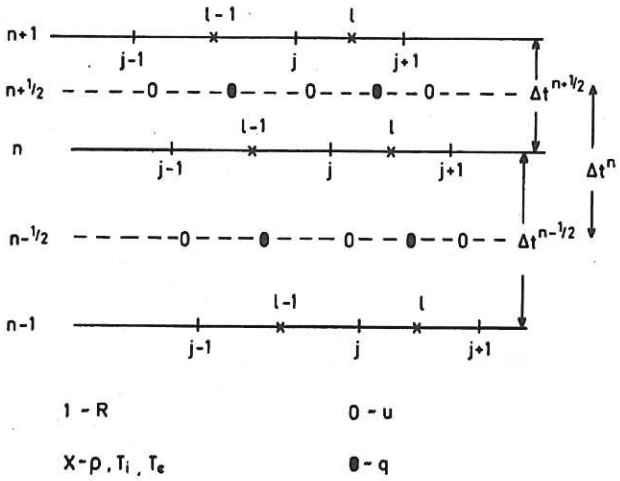

Fig.2. The 5 time levels indicating where the basic quantities are known

times. Suppose we are given (see Figure 2)

R_j , ρ_ℓ , T_ℓ, f_k	at level n-1
u_j	at level n-½
R_j , ρ_ℓ	at level n

where T stands for both T_i and T_e. The time integration scheme to be described in detail in Section 4 constructs from the above-written quantities

T_ℓ, f_k	at level n
u_j	at level n+½
R_j , ρ_ℓ	at level n+1

thereby advancing all basic quantities one step in time. Because the physical coefficients of the terms H, K, Y, J and X depend in a non-linear fashion on the temperatures T_i and T_e we perform several iterations on a single step n-1 → n. At

iteration m the value of T_i^n and T_e^n from iteration m-1 are used in order to get as accurate values of the phsyical coefficients as possible.

5. DIFFERENCE SCHEME

This section describes how equations (9)-(12) for the ions and electrons and equation (34) are expressed in finite difference form. We use subscripts ℓ and j, but omit for brevity subscripts i and e and superscript n where necessary

Energy equation

First we write out equation (9):

$$C_v^{n-\frac{1}{2}} \frac{T^n - T^{n-1}}{\Delta t^{n-\frac{1}{2}}} + B_T^{n-\frac{1}{2}} \frac{\rho^n - \rho^{n-1}}{\Delta t^{n-\frac{1}{2}}} + p^{n-\frac{1}{2}} \frac{V^n - V^{n-1}}{\Delta t^{n-\frac{1}{2}}} + S^{n-\frac{1}{2}} \quad . \tag{51}$$

All quantities in equation (51) are evaluated in cell ℓ. The quantities X_ℓ, Y_ℓ, J_ℓ and H_ℓ of equations (11) and (12) are worked out at level $n-\frac{1}{2}$ by

$$X_\ell^{n-\frac{1}{2}} = \tfrac{1}{2}(X_\ell^n + X_\ell^{n-1}) \quad , \tag{52}$$

a rule also applying to C_v, B_T and p.

Heat conduction

The heat conduction term H becomes

$$H_\ell^n = \frac{1}{dM_\ell} (F_{j+1}^n - F_j^n) \tag{53}$$

where the flux through cell boundary j is

$$F_j^n = (R_j^n)^{g-1} \kappa_j^n \frac{T_\ell^n - T_{\ell-1}^n}{R_\ell^n - R_{\ell-1}^n} \tag{54}$$

Thermal conductivity ⟨2.13⟩

The conductivity κ_j^n is taken as $\frac{1}{2}(\kappa_{\ell-1}^n + \kappa_\ell^n)$ where κ_ℓ^n is obtained from equations (14) and (15). The electron thermal conductivity is then modified according to equation (18) which in finite difference is written as (subscript e omitted)

$$\kappa'^n_{j+1} = \kappa_{j+1}^n \left(1 + \frac{2\, a\, \lambda_\ell^n}{T_{\ell+1}^n + T_\ell^n} \frac{T_{\ell+1}^n - T_\ell^n}{R_{\ell+1}^n - R_\ell^n}\right) \tag{54A}$$

where a is a constant larger than 1 and λ_ℓ^n is expressed by equation (19).

Energy exchange ⟨2.11⟩

The heat exchange term K of equation (22) is evaluated in a different way in order to treat very rapid rates of energy exchange. We set ⟨2.11⟩

$$\begin{aligned} \omega^{n-\frac{1}{2}} &= \tfrac{1}{2}(\omega^n + \omega^{n-1}) \quad , \\ \theta &= \frac{1}{\gamma - 1} \frac{k}{M m_H} (T_i - T_e) \quad , \\ \theta^{n-\frac{1}{2}} &= \tfrac{1}{2}(\theta^n + \theta^{n-1}) \end{aligned} \tag{55}$$

$$\text{and} \quad \delta W^{n-\frac{1}{2}} = W_i^{n-\frac{1}{2}} - W_e^{n-\frac{1}{2}} \quad .$$

We write equation (9) as $C_v \frac{dT}{dt} = W \pm K$ (+ for electrons, - for ions), where W includes the terms $B_T \frac{d\rho}{dt}$, $p \frac{dv}{dt}$ and S without K, and subtract this equation for the electrons from that for the ions. With $\epsilon = 1 + (C_v)_i / (C_v)_e$ this yields

$$\frac{d\theta}{dt} = \delta W - \epsilon K \quad ,$$

which in finite difference form has the solution

$$\omega^{n-\frac{1}{2}}\, \theta^{n-\frac{1}{2}} = \frac{1}{\epsilon \Delta t^{n-\frac{1}{2}}} \left(\theta^{n-1} - \frac{\delta W^{n-\frac{1}{2}}}{\epsilon\, \omega^{n-\frac{1}{2}}}\right)\left(1 - e^{-\epsilon\, \omega^{n-\frac{1}{2}} \Delta t^{n-\frac{1}{2}}}\right) + \frac{1}{\epsilon} \delta W^{n-\frac{1}{2}} \quad . \tag{56}$$

The term $e^{-\epsilon\, \omega^{n-\frac{1}{2}} t}$ has been averaged as

$$\frac{1}{\Delta t^{n-\frac{1}{2}}} \int_0^{\Delta t^{n-\frac{1}{2}}} e^{-\epsilon\, \omega^{n-\frac{1}{2}}} dt = \frac{1 - e^{-\epsilon \omega^{n-\frac{1}{2}} \Delta t^{n-\frac{1}{2}}}}{\epsilon \omega^{n-\frac{1}{2}}\, \Delta t^{n-\frac{1}{2}}} \tag{57}$$

and the term $\delta W^{n-\frac{1}{2}}$ is

$$\delta W^{n-\frac{1}{2}} = \frac{1}{\Delta t^{n-\frac{1}{2}}} (\theta^n - \theta^{n-1}) + \epsilon\, \omega^{n-\frac{1}{2}} \theta^{n-\frac{1}{2}} \quad . \tag{58}$$

The heat exchange term can then be written as ⟨2.11⟩

$$K^{n-\frac{1}{2}} = \omega^{n-\frac{1}{2}}\, \theta^{n-\frac{1}{2}} \quad . \tag{59}$$

During the iterations on a single timestep we first evaluate the rate constant at level n from (see equations (20) and (22))

$$\omega = 0.59 \times 10^{-8}\, \overline{M^{-1} Z^2}\, n_i\, T_e^{-3/2} \log \Lambda \quad . \tag{59A}$$

The quantities $\omega^{n-\frac{1}{2}}$ and $\theta^{n-\frac{1}{2}}$ are found from equation (55) and $\delta W^{n-\frac{1}{2}}$ from equation (58) using the values of θ^n and $(\omega\theta)^{n-\frac{1}{2}}$ from a previous iteration. Equation (56) is then evaluated using

$$\epsilon = 1 + (C_v^n + C_v^{n-1})_i / (C_v^n + C_v^{n-1})_e \quad . \tag{59B}$$

If perfect gas laws are imposed we have $\epsilon = 2$.

Bremsstrahlung ⟨2.10⟩

Equations (40) and (41) are used to evaluate J_ℓ^n. If electron degeneracy is present we use equation (24) when $\xi_\ell^n \geq \xi_{min}$ (see eqn.(42)).

The Coulomb logarithm ⟨2.8⟩

Λ_ℓ^n is evaluated from equation (16). If $\Lambda_\ell^n < 10$ (dense cold plasma) shielding theory breaks down [9] and the physics changes. No provisions are made to alter the expressions involving Λ, hence if $\Lambda_\ell^n < 10$ we set $\Lambda_\ell^n = 10$.

Absorption of laser light ⟨2.9⟩

For a cell with a density less than ρ_C (equation (25)) we evaluate equation (26) and work out

$$P_L^n(R_j^n) = P_L^n(R_{j+1}^n)\, e^{-\alpha_\ell^n (R_{j+1}^n - R_j^n)} \tag{59C}$$

and

$$X_\ell^n = \frac{1}{\rho_\ell^n} \left(P_L^n(R_{j+1}^n) - P_L^n(R_j^n)\right) \quad . \tag{59D}$$

At the first cell ℓ = NABS 1 with $\rho < \rho_C$ we apportion the remaining laser power $P_L^n(R_{NABS\,1}^n)$ between cell NABS 1 and cell NABS 1+1 according to

$$X_{NABS\,1}^n = (1 - \mu^n)\, P_L^n(R_{NABS\,1}^n) / d M_{NABS\,1} \tag{59E}$$

$$X_{NABS\,1+1}^n = \mu^n\, P_L^n(R_{NABS\,1}^n) / d M_{NABS\,1+1} \tag{59F}$$

where

$$\mu^n = \frac{\rho_{NABS\,1}^n - \rho_C}{\rho_{NABS\,1}^n - \rho_{NABS\,1+1}^n} \quad . \tag{59G}$$

The coordinate RABS of which $\rho = \rho_C$ is determined by a linear interpolation from

$$RABS = \tfrac{1}{2}(R_{NABS\,1}^n + R_{NABS\,1+1}^m) + \mu^n (R_{NABS\,1+2}^n - R_{NABS\,1}^n) \tag{59H}$$

Thermonuclear reactions

The number of reactions taking place at level n (equation (31)) is computed from

$$R_{DT}^{n} = (\sigma v)_{DT}^{n} \; f_D^n \; f_T^n \; (n_i^n)^2 \qquad (59I)$$

$$R_{DD}^{n} = (\sigma v)_{DD}^{n} \; \tfrac{1}{2}(f_D^n)^2 \; (n_i^n)^2 \qquad (59J)$$

$$R_{D^3He}^{n} = (\sigma v)_{D^3He}^{n} \; f_D^n \; F_{^3He}^n \; (n_i^n)^2 \qquad (59K)$$

The cross-sections are taken as [12] (T_i expressed in keV

$$(\sigma v)_{DT}^{n} = 3.68\times10^{-18} \; T_i^{-2/3} \; e^{-19.94 \; T_i^{-1/3}} \; m^3 \, sec^{-1} \, , \qquad (59L)$$

but

$$(\sigma v)_{DT}^{n} = 7.5\times10^{-22} \; m^3 \, sec^{-1} \; \text{if } T_i > 35 \text{ keV} \, , \qquad (59M)$$

$$(\sigma v)_{DD}^{n} = 2.33\times10^{-20} \; T_i^{-2/3} \; e^{-19.42 \; T_i^{-1/3}} \; m^3 \, sec^{-1} \, , \qquad (59N)$$

$$(\sigma v)_{D^3He}^{n} = 0 \, , \qquad (59O)$$

but

$$(\sigma v)_{D^3He}^{n} = 10^{-23} \; m^3 \, sec^{-1} \; \text{if } T_i > 50 \text{ keV} \, . \qquad (59P)$$

The apportionment factors are adapted from [4] and written as (Te expressed in K)

$$P_{DT}^{n} = \frac{T_e^n}{T_e^n + 3.71 \times 10^8} \qquad (59Q)$$

$$P_{DD}^{n} = \frac{T_e^n}{T_e^n + 1.2 \times 10^9} \qquad (59R)$$

$$P_{D^3He}^{n} = \frac{T_e^n}{T_e^n + 1.2 \times 10^9} \qquad (59S)$$

Y_i^n and Y_e^n are then calculated from equation (32).

The total rate of neutron production is calculated from

$$R_{neu}^{n} = \sum_{\ell=1}^{N} (R_{DT} + \tfrac{1}{2} \, RDD)_\ell^n \; v_\ell^n \; dM_\ell \qquad (59T)$$

and the rate of energy carried off by the escaping neutrons is obtained from

$$\dot{E}^{n} = \sum_{\ell=1}^{N} (R_{DT} \; \bar{E}_{DT} + \tfrac{1}{2} \; R_{DD} \; \overline{E_{DD}})_\ell^n \; v_\ell^n \; dM_\ell \, , \qquad (59U)$$

where $\bar{E}_{DT}$ = 14.1 MeV and $\bar{E}_{DD}$ = 2.45 MeV.

Shock heating

The shock heating term Q of equation (11) is a modification of the standard expression used in textbooks [14]. We write Q as

$$Q^{n-\frac{1}{2}} = - \, q^{n-\frac{1}{2}} \; \frac{V^n - V^{n-1}}{\Delta t^{n-\frac{1}{2}}} \qquad (60)$$

where q, the viscous pressure for a given cell ℓ is expressed as

$$q_\ell^{n-\frac{1}{2}} = b^2 \; \tfrac{1}{2}(\rho_\ell^{n-1} + \rho_\ell^n) \; (u_{j+1}^{n-\frac{1}{2}} - u_j^{n-\frac{1}{2}})^2 \; \eta_\ell^{n-\frac{1}{2}} \, . \qquad (61)$$

This expression differs from the standard expression [14] by the factor η which is

$$\eta = \frac{\partial r \nabla u}{\partial r \nabla . u} = (r^{g-1} \, \partial u)/(\partial \, r^{g-1} \, u) \qquad (61A)$$

where in finite difference form

$$\partial r \, \nabla u = u_{j+1}^{n-\frac{1}{2}} - u_j^{n-\frac{1}{2}} \, , \qquad (61B)$$

$$\partial r \, \nabla . u = \frac{\nu}{(R_{j+\frac{1}{2}}^{n-\frac{1}{2}}) \, g-1} \left(u_{j+1}^{n-\frac{1}{2}} \left((R_{j+1}^{n-1})^{g-1} + (R_{j+1}^{n})^{g-1} \right) \right. \qquad (61C)$$

$$\left. - \, u_j^{n-\frac{1}{2}} \left((R_j^{n-1})^{g-1} + (R_j^n)^{g-1} \right) \right) \, ,$$

with $R_{j+\frac{1}{2}}^{n-\frac{1}{2}} = R_{j+1}^{n} + R_{j+1}^{n-1} + R_j^n + R_j^{n-1}$, (61D)

and ν = 1,2,8 for g = 1,2,3 respectively.

The viscous pressure q given by equation (61) is only applied if $\nabla u < 0$ and $\nabla . u < 0$, i.e. if both righthand sides of equations (61B) and (61C) are negative. Otherwise q is 0. In plane geometry (g = 1) we notice that η = 1.

The reason for including η in the formula for q is to decrease the shock heating contributed by the standard expression for q [14] to cells which undergo strong but adiabatic compression.

6. SOLUTION OF THE ION TEMPERATURE EQUATION

The coefficients of $T_{\ell-1}^n$, T_ℓ^n and $T_{\ell+1}^n$ arising from the H_i term are grouped such that equation (51) for the ions can be written as a matrix equation

$$A_\ell^n \; T_{\ell-1}^n + B_\ell^n \; T_\ell^n + C_\ell^n \; T_{\ell+1}^n = D_\ell^n + G_\ell^{n-1} \, . \qquad (62)$$

The quantities A,B,C and D ⟨2.14⟩ are functions of $(T_i)_\ell^n$ and $(T_e)_\ell^n$ and for this reason we solve equation (62) iteratively as explained earlier. The quantity G_ℓ^{n-1} ⟨2.4⟩ contains all the known quantities and is thus unaffected by iterations.

We write out the expressions for A,B,C,D and G of the ion temperature equation assuming that the equations of state are those given by (39). Subscript i is omitted for brevity.

$$A_\ell^n = -\frac{1}{dM_\ell}\,\frac{(R_j^n)^{g-1}\,\nu_j^n}{R_{j+1}^n - R_{j-1}^n}\,\Delta t^{n-\frac{1}{2}} \qquad (63)$$

$$C_\ell^n = -\frac{1}{dM_\ell}\,\frac{(R_{j+1}^n)^{g-1}\,\nu_{j+1}^n}{R_{j+2}^n - R_j^n}\,\Delta t^{n-\frac{1}{2}} \qquad (64)$$

$$B_\ell^n = C_v - A_\ell^n - C_\ell^n + \frac{p_\ell^n}{2T_\ell^n}\,(V_\ell^n - V_\ell^{n-1}) \qquad (65)$$

$$D_\ell^n = \tfrac{1}{2}(Y_\ell^n - 2K_\ell^{n-\frac{1}{2}})\Delta t^{n-\frac{1}{2}} - \tfrac{1}{2}\,p^{n-1}(V_\ell^n - V_\ell^{n-1}) + C_v\,T_\ell^{n-1} \qquad (66)$$

$$G_\ell^n = \tfrac{1}{2}\,Y_\ell^{n-1}\,\Delta t^{n-\frac{1}{2}} - C_\ell^{n-1}(T_\ell^{n-1} - T_\ell^{n-1}) + A_\ell^{n-1}\,(T_\ell^{n-1} - T_{\ell-1}^{n-1}) + Q_\ell^{n-\frac{1}{2}} \qquad (67)$$

Equation (62) is solved by a Gauss elimination procedure [14] for all 4 cases of boundary conditions (equation (38)). For cases 1, 3 and 4 we have $A_1^n \equiv C_N^n \equiv 0$. For case 2 we set $A_1^n \equiv 0$ and $D_N^n = D_N^n - C_N^n\,T_{N+1}^n$, where T_{N+1}^n is a temperature applied at the outer boundary, i.e. $T_{N+1}^n = T_{N+1}^n(t)$.

Following [14] we set ⟨2.15⟩

$$E_1 = \frac{C_1}{B_1}\,, \qquad F_1 = \frac{D_1 + G_1}{B_1} \qquad (68)$$

$$E_\ell = \frac{C_\ell}{B_\ell - A_\ell\,E_{\ell-1}}\,, \qquad F_\ell = \frac{D_\ell + G_\ell - A_\ell\,F_{\ell-1}}{B_\ell - A_\ell\,E_{\ell-1}}\,, \quad \ell = 2,N\,. \qquad (69)$$

The temperature can be found from ⟨2.15⟩

$$T_N = F_N \qquad (70)$$

$$T_\ell = F_\ell - E_\ell\,T_{\ell+1} \qquad \ell = N\text{-}1, N\text{-}2, \ldots..2,1\,. \qquad (71)$$

7. SOLUTION OF THE ELECTRON TEMPERATURE EQUATION

If the electrons are assumed to obey perfect gas laws (equation (39)) the solution of equation (51) for the electrons is obtained in the same manner as described in Section 6. The coefficients A,B,C,D and G are those defined by equations (63)-(67), except that $Q_\ell^{n-\frac{1}{2}}$ is omitted from equation (67) and J_ℓ^n, X_ℓ^n and J_ℓ^{n-1}, X_ℓ^{n-1} are included in equations (66) and (67) respectively.

If however the electrons are assumed to behave as a degenerate gas obeying the equations (44) - (46) the coefficients B and D are redefined. Also to solve equation (51) for all ranges of degeneracy we write the analytic form (equation 9) as

$$C_v\,\frac{dT_e}{dt} = -\,(p_e - \frac{1}{V^2}\,B_T)\,\frac{dV}{dt} + S\,. \qquad (71A)$$

We set $\psi = p_e - \frac{1}{V^2}\,B_T$ and from equations (44) and (46) we find ($\gamma_e = 5/3$)

$$\psi = p_F\,(\frac{5\pi^2}{6}\,\xi^2 - \frac{\pi^4}{4}\,\xi^4), \qquad \xi < \xi_{min} \qquad (71B)$$

$$\psi = p_p\,(1 - (6\sqrt{2\pi})^{-1}\,\xi^{-3/2}\,, \qquad \xi_{min} \leq \xi < \xi_{max} \qquad (71C)$$

$$\psi = p_p\,, \qquad \xi_{max} \leq \xi \qquad (71D)$$

where p_F is given by equation (47), and the pressure p_p of a perfect electron gas is

$$p_p = \frac{k}{m_H}\,\frac{Z}{\bar{M}}\,\rho\,T_e\,. \qquad (71E)$$

It is necessary to work with ψ rather than p_e and B_T since for very small $\xi(\sim 10^{-4})$ the difference between p_e and $\frac{1}{V^2}\,B_T$ is below the rounding-off level on many computers (32-bit word length).

We can now write out the expressions used for B,D and G ⟨2.14⟩; A and C are given by equations (63) and (64).

$$B_\ell^n = \tfrac{1}{2}\Big((C_v)_\ell^n + (C_v)_\ell^n\Big) - A_\ell^n - C_\ell^n \qquad (71F)$$

$$D_\ell^n = \tfrac{1}{2}\Big((X_\ell^n + J_\ell^n + Y_\ell^n + 2K_\ell^{n-\frac{1}{2}})\Delta t^{n-\frac{1}{2}} + T_\ell^{n-1}\Big((C_v)_\ell^n + (C_v)_\ell^{n-1}\Big) - (\psi_\ell^n + \psi_\ell^{n-1})(V_\ell^n - V_\ell^{n-1})\Big) \qquad (71G)$$

$$G_\ell^n = \tfrac{1}{2}\Big((X_\ell^{n-1} + J_\ell^{n-1} + Y_\ell^{n-1})\Delta t^{n-\frac{1}{2}} - C_\ell^{n-1}(T_{\ell+1}^{n-1} - T_\ell^{n-1}) + A_\ell^{n-1}(T_\ell^{n-1} - T_{\ell-1}^{n-1})\Big)\,. \qquad (71H)$$

With these definitions of the coefficients A,B,C,D and G we can solve equation (62) as described in Section 6.

8. CHEMICAL COMPOSITION, VOLUME CHANGES

When thermonuclear reactions take place (equation (30)) the chemical composition, i.e. the material fractions (equation (1)), will change. Here we only describe how the fraction of tritium changes since the fractions of the other components are calculated in an almost identical way. We evaluate ⟨2.28⟩

$$\delta f_T^{n-\frac{1}{2}} = \left(\frac{1}{4}(R_{DD}^n + R_{DD}^{n-1}) - \frac{1}{2}(R_{DT}^n + R_{DT}^{n-1})\right) \frac{\Delta t^{n-\frac{1}{2}}}{n_i^{n-1}} \tag{71I}$$

where the ion number density is obtained from

$$n_i^{n-1} = \rho^{n-1}/(m_H \sum_k f_k^{n-1} M_k) \quad . \tag{71J}$$

The fraction of tritium at level n is calculated as ⟨2.28⟩

$$f_T^n = f_T^{n-1} + \delta f^{n-\frac{1}{2}} \tag{71K}$$

and subsequently modified by a renormalization (equation (2))

$$f_T^n = \frac{f_T^n}{\sum_k f_k^n} \quad . \tag{71L}$$

The volume changes are worked out via the Navier-Stokes equation (34). First we form the hydrodynamic pressure ⟨2.24⟩

$$p_\ell^n = (p_i + p_e)_\ell^n \tag{72}$$

where p_i^n and p_e^n are obtained from the equations of state.

The acceleration of the fluid is obtained from ⟨2.17⟩

$$u_j^{n+\frac{1}{2}} - u_j^{n-\frac{1}{2}} = -(R_j^n)^{g-1} (p_\ell^n - p_{\ell-1}^n + q_\ell^n - q_{\ell-1}^n) \frac{\Delta t^n}{dM_j} \tag{73}$$

where q_ℓ is given by equation (61) and

$$dM_j = \frac{1}{2}(dM_{\ell-1} + dM_\ell) \quad .$$

The cell boundaries can now be moved to new positions ⟨2.19⟩

$$R_j^{n+1} = R_j^n + u_j^{n+\frac{1}{2}} \Delta t^{n+\frac{1}{2}} \quad . \tag{74}$$

Before working out the densities and volumes at level n+1 we evaluate at level n those quantities which have been affected by the burn-up of deuterium and tritium. The mass number, ionic charge number and ion number density have all changed, but also the mass undergoes a change due to the escaping neutrons. Having found the fractions f_k^n (equations (71K) and (71L)) we set

$$M^n = \sum_k f_k^n M_k \ , \quad Z^n = \sum_k f_k^n Z_k \quad . \tag{74A}$$

The change in the ion number density is ⟨2.20⟩

$$\delta n_i^{n-\frac{1}{2}} = -\frac{1}{2}(R_{DT}^n + R_{DT}^{n-1})\Delta t^{n-\frac{1}{2}} - \frac{1}{4}(R_{DD}^n + R_{DD}^{n-1})\Delta t^{n-\frac{1}{2}} \quad . \tag{74B}$$

(Notice that in equations (71I) and (74B) only half the total number of D-D reactions contribute to the changes). The new number density is then

$$n_i^n = n_i^{n-1} + \delta n_i^{n-\frac{1}{2}} \quad , \tag{74C}$$

where n_i^{n-1} is given by equation (71J). For each ion lost a neutron escapes such that the mass becomes ⟨2.20⟩

$$dM_\ell^n = \frac{1}{g}\left((R_{j+1}^n)^g - (R_j^n)^g\right)\left(\rho_\ell^n + (\delta n_i)_\ell^{n-\frac{1}{2}} m_H\right) \quad . \tag{74D}$$

The mass is worked out in this particular way as it is only referred to at one time level. Finally we calculate the specific volumes V_ℓ^{n+1} and densities ρ_ℓ^{n+1} by equation (48) having found the coordinates R_j^{n+1} from equation (74). We notice that the mass dM_ℓ^n used to calculate V_ℓ^{n+1} is only known at level n such that we ignore the slight mass loss which may take place between levels n and n+1.

9. TIMESTEP CONTROL. CONVERGENCE OF ITERATIONS

The implicit method for solving equation (51) guarantees a numerically stable solution [14] and the choice of Δt only serves to determine the accuracy. However the explicit method used to find u (equation (73)) restricts the value of Δt according to the Courant-Friedrichs-Lewy condition [14]

$$\Delta t^{n+\frac{1}{2}} < a_1 \ \mathrm{Min}\left(\frac{R_{j+1}^n - R_j^n}{c_\ell^n}\right) \quad , \tag{75}$$

where c_ℓ^n is the sound speed in cell ℓ and a_1 is a constant less than 1. To monitor the time variation of T_i, T_e and V we enforce ⟨2.16⟩

$$\Delta t^{n+\frac{1}{2}} \leqslant a_2 \ \mathrm{Min}\left(\frac{V^{n+1} - V^n}{V^{n+1} + V^n}\right)_\ell \tag{76}$$

$$\Delta t^{n+\frac{1}{2}} \leqslant a_3 \ \mathrm{Min}\left(\frac{T_i^{n+1} - T_i^n}{T_i^{n+1} + T_i^n}\right)_\ell \tag{76A}$$

$$\Delta t^{n+\frac{1}{2}} \leqslant a_4 \ \mathrm{Min}\left(\frac{T_e^{n+1} - T_e^n}{T_e^{n+1} + T_e^n}\right)_\ell \quad . \tag{76B}$$

If the electrons are strongly degenerate, i.e. $\xi < \xi_{min}$, p_e replaces T_e in equation (76B). The variation of Δt is itself restricted by either

$$\frac{1}{a_o} \Delta t^{n-\frac{1}{2}} \leqslant \Delta t^{n+\frac{1}{2}} \quad \text{or} \quad \Delta t^{n+\frac{1}{2}} \leqslant a_o \Delta t^{n-\frac{1}{2}} \quad . \tag{77}$$

This restriction is enforced ⟨2.16⟩ to keep equation (73) reasonably well time-centred. Finally Δt is

restricted by the time variation of the applied external "force", i.e. laser, boundary temperature, pressure or velocity.

Having chosen the smallest Δt satisfying these conditions we check whether the iterations on T_i , T_e and u converge by evaluating ⟨2.21⟩

$$\delta u = \mathrm{Max}\left(\frac{|{}^{m}u - {}^{m-1}u|}{|{}^{m}u + {}^{m-1}u|}\right)_j^{n+\frac{1}{2}} \qquad (78)$$

$$\delta T_i = \mathrm{Max}\left(\left|\frac{{}^{m}T_i - {}^{m-1}T_i}{{}^{m}T_i + {}^{m-1}T_i}\right|\right)_\ell^{n} \qquad (78A)$$

$$\delta T_e = \mathrm{Max}\left(\left|\frac{{}^{m}T_e - {}^{m-1}T_e}{{}^{m}T_e + {}^{m-1}T_e}\right|\right)_\ell^{n} \quad . \qquad (78B)$$

In these equations m and m-1 indicate the values obtained after m and m-1 iterations respectively. If the electrons are strongly degenerate, i.e. $\xi < \xi_{min}$, then $(\delta T_e)_\ell^n = 0$. Similarly if

$$|{}^{m}u|_j^{n+\frac{1}{2}} < u_{min}$$

or if

$$|{}^{m}u - {}^{m-1}u|_j^{n+\frac{1}{2}} \Delta t^n < \delta R_{min}$$

we set $(\delta u)_j^{n+\frac{1}{2}} = 0$. If the maximum deviations found by equations (78), (78A) and (78B) are below specified values convergence is established. Otherwise a new iteration is performed with ${}^{m}u$, ${}^{m}T_i$ and ${}^{m}T_e$ replacing the values obtained after the m-1 iteration. At the first iteration of each timestep we assume $T_i^n = T_i^{n-1}$ and $T_e^n = T_e^{n-1}$.

10. ENERGY CALCULATION

When a timestep is completed we calculate all relevant energies at level n ⟨2.22⟩. The thermal energy is

$$E_{th}^n = \frac{1}{\gamma-1} \sum_\ell p_\ell^n v_\ell^n \, dM_\ell \quad . \qquad (79)$$

The kinetic energy is averaged over levels $n-\frac{1}{2}$ and $n+\frac{1}{2}$

$$E_k^n = \frac{1}{8} \sum_{j \text{ or } \ell} (dM_\ell + dM_{\ell-1})\left[(u_j^{n+\frac{1}{2}})^2 + (u_j^{n-\frac{1}{2}})^2\right] \quad . \qquad (80)$$

The energy input depends on which boundary condition (equation (38)) has been chosen :

Case 1 : $$\frac{d}{dt} E_{in}^n = \sum_\ell X_\ell^n \, dM_\ell \qquad (81)$$

Case 2 : $$\frac{d}{dt} E_{in}^n = \frac{(R_{N+1}^n)^{g-1}}{R_{N+1}^n - R_N^n} \left\{\left[\kappa (T_{N+1} - T_N)\right]_i^n + \left[\kappa (T_{N+1} - T_N)\right]_e^n\right\} \qquad (82)$$

Case 3 : $$\frac{d}{dt} E_{in}^n = \frac{1}{4} (p_{N+1}^n + p_{N+1}^{n-1}) u_{N+1}^{n-\frac{1}{2}} \left[(R_{N+1}^n)^{g-1} + (R_{N+1}^{n-1})^{g-1}\right] \qquad (83)$$

Case 4 : As case 3 but with p_{N+1}^n replaced by

$$p_{N+1}^n = p_N^n + \tfrac{1}{2}(q_N^{n+\frac{1}{2}} + q_N^{n-\frac{1}{2}}) - \tfrac{1}{2} dM_N \frac{u_{N+1}^{n+\frac{1}{2}} - u_{N+1}^{n-\frac{1}{2}}}{\Delta t^n (R_{N+1}^n)^{g-1}} \quad . \qquad (84)$$

The total energy input at level n becomes

$$E_{in}^n = E_{in}^{n-1} + \tfrac{1}{2}\left(\frac{d}{dt} E_{in}^n + \frac{d}{dt} E_{in}^{n-1}\right) \Delta t^{n-\frac{1}{2}} \quad , \qquad (85)$$

where $E_{in}^o = E_k^o + E_{th}^o$.

The energy released by the thermonuclear reactions is

$$E_f^n = E_f^{n-1} + \tfrac{1}{2} \Delta t^{n-\frac{1}{2}} \sum_\ell \left[(Y_i + Y_e)_\ell^n + (Y_i + Y_e)_\ell^{n-1}\right] dM_\ell \quad . \qquad (86)$$

The energy carried away by the neutrons is found from

$$E_{neu}^n = E_{neu}^{n-1} + \tfrac{1}{2} (\dot{E}^n + \dot{E}^{n-1}) \Delta t^{n-\frac{1}{2}} \quad , \qquad (86A)$$

where $\dot{E}^n$ is given by equation (59U). The total number of neutrons released so far is

$$N_{neu}^n = N_{neu}^{n-1} + \tfrac{1}{2} (R_{neu}^n + R_{neu}^n) \Delta t^{n-\frac{1}{2}} \quad , \qquad (86B)$$

where R_{neu}^n is expressed by equation (59T). The bremsstrahlung radiation loss is

$$E_b^n = E_b^{n-} + \tfrac{1}{2} \Delta t^{n-\frac{1}{2}} \sum_\ell (J_\ell^n + J_\ell^{n-1}) dM_\ell \quad . \qquad (87)$$

The error in the energy calculations is represented by

$$\Delta E^n = E_k^n + E_{th}^n - E_{in}^n - E_f^n - E_b^n \quad . \qquad (88)$$

ΔE is a measure of the truncation errors arising from the use of a finite difference scheme. Finally as a check of the "Lawson criterion" we evaluate

$$\overline{\rho r} = \frac{\int_0^{R_o} \rho r \, \rho r^{g-1} \, dr}{\int_0^{R_o} \rho r^{g-1} \, dr}$$

The quantity $\overline{\rho r}$ is proportional to $\overline{n_i \tau}$ [2], where τ is the confinement time of a plasma. We calculate $\overline{\rho r}$ as

$$(\rho R)^n = \frac{\sum_{\ell=1}^{N} \rho_\ell^n \, R_\ell^n \, \delta M_\ell}{\sum_{\ell=1}^{N} \delta M_\ell} \qquad (89)$$

where R_ℓ^n is given by equation (50).

11. STRUCTURE OF THE COMPUTER CODE

The MEDUSA 1 code comprises a main program and 144 subprograms of which 40 are part of the ICL 4-70 Multijob Operating System. 36 subprograms form the graphical output package and these are not included in the version presented here. The main program and 22 subprograms are part of the OLYMPUS package [6,7] and the remaining 46 subprograms are divided into 5 classes as described in [6,7]. To run the MEDUSA 1 code on a particular computer one thus requires the OLYMPUS package and the 46 subprograms as well as 11 dummy subroutines which eliminate the use of the graphical output package.

Each of the 46 subprograms of MEDUSA 1 is decimally numbered according to the conventions of [6,7]. The references in this report of the type ⟨2.9⟩ can be correlated with the subprogram index shown in the Appendix of [8]. This index also appears in the source deck. On the ICL 4-70 the corresponding file name is denoted by C2S9 (Class 2, subprogram 9) followed by a type code defining the type of file (e.g. Fortran source code F, object module Y).

The overall structure of MEDUSA is based on the underlying structure provided by OLYMPUS [6,7]. In Figure 3 we show the flow diagram for the subprograms of the calculation Class 2. The classes 1, 3, 4 and 5 are almost identical to those of [6,7].

The common blocks used by MEDUSA 1 also follow the conventions of [6,7]. There are 13 common blocks labelled as follows:

[C1.1]	COMBAS	Basic system parameters
[C1.9]	COMDDP	Development and diagnostic parameters
[C2.1]	COMHYD	Hydrodynamics
[C2.2]	COMTH	Thermodynamics
[C2.3]	COMIE	Ions and electrons
[C2.4]	COMLAS	Laser data
[C2.5]	COMFUS	Fusion
[C2.6]	COMEN	Energy
[C2.7]	COMCON	Physics control
[C3.1]	COMNC	Numerical control parameters
[C3.2]	COMNUM	Mesh and numerical methods

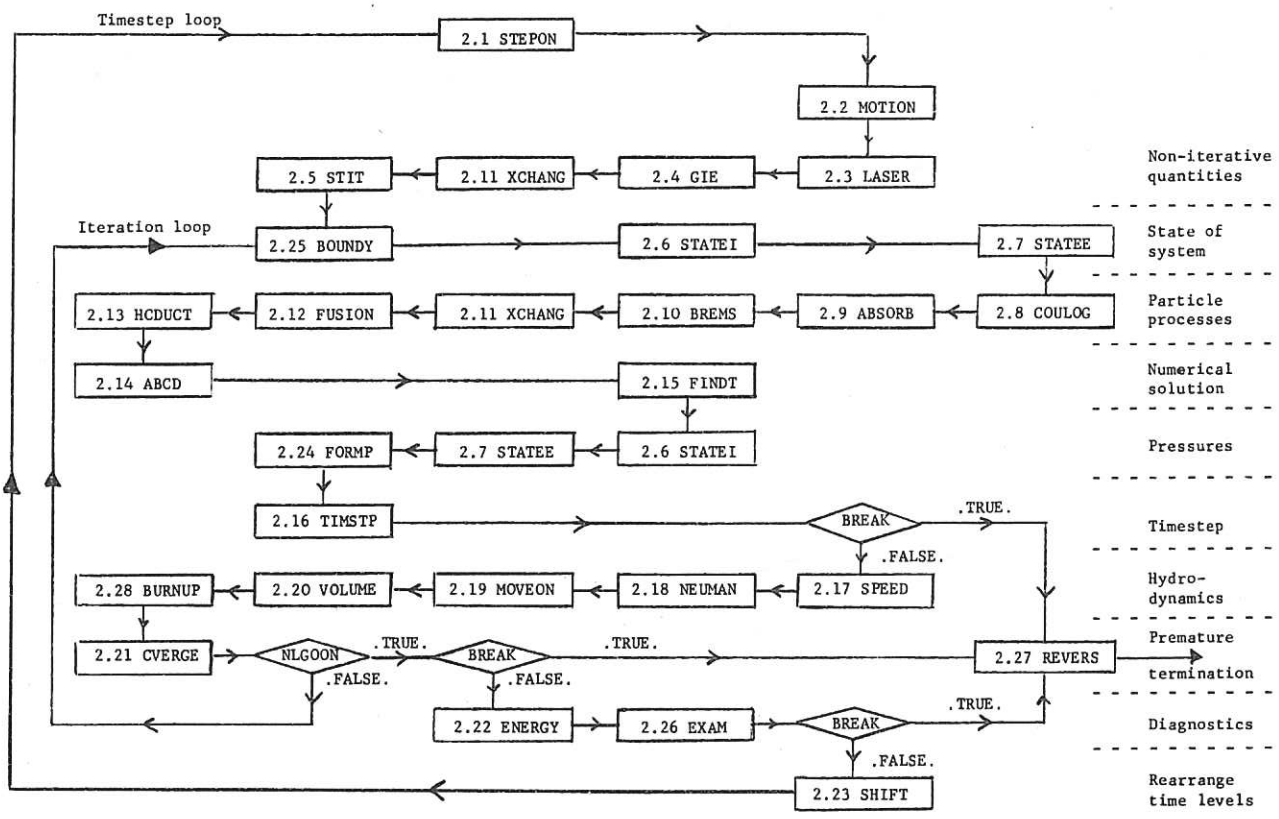

Figure 3. Flow diagram for the calculation in MEDUSA 1.

[C4.1] COMADM Housekeeping data

[C5.1] COMOUT Input-output control variables .

The variables and arrays of these common blocks appear in an index following the source code. Those variables which can be specified by the user are listed in the Appendix of [8]. A common block such as COMOUT is referred to in the text as [C5.1].

12. INSTRUCTIONS FOR THE USER

An understanding of the code listing is facilitated by the inclusion of references to the numbered equations in this report as well as the corresponding paper [8]. The notation has also been chosen, whenever possible, to indicate the time level at which a quantity is known. The 5 time levels n-1, n-½, n , n+½ and n+1 are denoted by 1,2,3,4 and 5 respectively, so that for example R1, R3 and R5 are three arrays containing the mesh coordinates at levels n-1, n, n+1, while U2 and U4 contain the velocities of levels n-½ and n+½, and so on.

Although all physical quantities are currently expressed in SI units it is possible to scale these to any arbitrary set of units (say CGS) by means of the scaling factors in the common block COMOUT [C5.1]. This will however only affect input-output, the internal variables of MEDUSA 1 always being expressed in SI units.

The physical coefficients appearing in the laws for conductivity, absorption, bremsstrahlung etc. can be altered by setting elements of the array PIQ of [C5.1] to values different from zero. PIQ acts as a general-purpose array which enables modifications of the code to be communicated from subprogram DATA ⟨1.4⟩ to any other subprogram (see file INTRO).

To run the MEDUSA 1 code under conditions different from those of the tests described in Section 9 a user can control the calculation in 4 principal ways:

1. The boundary conditions ⟨2.25⟩ explained in equation (38) can be arbitrarily specified. This means replacing the existing expressions for p(t), u(t), $T_e(t)$ and $T_i(t)$ in ⟨2.25⟩ and recompiling the subprogram.

2. The laser power $P_L(t)$ programmed into ⟨2.3⟩ can similarly be changed if necessary.

3. A user can overwrite any of the physical laws coded in MEDUSA 1, as well as modifying other sections of the program. For this purpose a subprogram EXPERT ⟨0.4⟩ is called at many places in the program, with 3 parameters defining the class, subprogram and point at which the call is made. The version of EXPERT provided is a dummy, the idea being that the user should "slot" into EXPERT the ad hoc coding which may be required to replace or extend the existing action of any sections that are to be modified, without disturbing the program itself.

4. The last and simplest method of control concerns the input of parameters to the calculation. This is done in subprogram DATA ⟨1.4⟩ using the NAMELIST facility which is available on most computer systems including the Culham ICL 4/70. The variables and arrays contained in namelist NEWRUN are listed in the Appendix of [8]. (No specific provision for a restart [6,7] is made in this version). If the namelist facility is not available it is necessary to replace the statement

READ (NREAD, NEWRUN) (90)

in DATA ⟨1.4⟩ by a normal FORTRAN READ statement which includes all the variables of the namelist.

If desired, any part of the physics calculation can be excluded by setting the logical variables of block COMCON [C2.7] to .FALSE. , e.g. NLBRMS = .FALSE. will switch off the bremsstrahlung calculation. If NLBRMS = .TRUE. the bremsstrahlung calculation will be switched on only if the variable MLBRMS = .TRUE. as set by the code itself. The criteria for setting the variables ML.... to .TRUE. depend on the current state of the plasma ⟨2.26⟩, but also on the finite word length (32 bits), so that the code neglects terms whose contributions cannot be accommodated within the accuracy of the floating-point calculations. This arrangement saves CPU time and makes the testing much easier.

Premature termination of a calculation may arise from a variety of checks made by the code. The initial conditions are checked ⟨1.10⟩ and at the end of each timestep the fundamental variables t, R, ρ, T_i and T_e are examined ⟨2.26⟩. If certain maximum or minimum values are exceeded termination occurs. This also happens if the iterations on u, T_i and T_e fail to satisfy the convergence criteria ⟨2.21⟩.

13. TESTING THE PROGRAM

There are no analytic solutions to equations (9) and (34) when the right-hand side of equation (9) is given by equations (11) and (12). This means that the overall testing of the MEDUSA 1 code relies on a series of independent tests which deal with each individual physical process included in the code. The results from such tests can be compared with analytic solutions.

By setting the logical switches of Table 2 of

[8] as appropriate, a comprehensive series of tests can be made. Three such tests are shown in [8] along with the corresponding output generated by the MEDUSA 1 code.

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