Computer Physics Communications 49 (1988) 475–505
North-Holland, Amsterdam

MULTI – A COMPUTER CODE FOR ONE-DIMENSIONAL MULTIGROUP RADIATION HYDRODYNAMICS

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Received 31 July 1987

The basic physical equations as well as a computer code for the simulation of one-dimensional radiation hydrodynamics are described. The hydrodynamic equations are combined with a multigroup method for the radiation transport. The code, written in standard FORTRAN-77, is characterized by one-dimensional planar geometry with multilayer structure. A time-splitting schema has been adopted with implicit finite-differencing formulation (including the hydrodynamics), and Lagrangian coordinates. Tabulated equations of state and opacities are used.

PROGRAM SUMMARY

Title of program: MULTI

Catalogue number: ABBV

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: CRAY-XMP; *Installation*: RZ Garching

Operating system: COS

Programming language used: FORTRAN 77

High speed storage required: 340000 words

No. of bits in a word: 64

No. of lines in combined program and test deck: 14231

Keywords: inertial confinement fusion, multigroup radiation hydrodynamics, one-dimensional implicit Lagrangian code

Nature of physical problem
In inertial confinement fusion and related experiments with lasers and particle beams energy transport by thermal radiation becomes important. Under these conditions, the radiation field strongly interacts with the hydrodynamic motion through frequency-dependent emission and absorption processes.

Method of solution
The equations of radiation transfer coupled with Lagrangian hydrodynamics are solved using a fully implicit numerical scheme. Frequency and angle dependence is included via a multigroup treatment. A time-splitting algorithm is adopted which feeds in all the groups successively during one hydrodynamic time step. Tabulated equation of state data, Planck and Rosseland opacities, and non-LTE properties of the matter are used which have to be generated externally.

Restrictions on the complexity of the problem
The MULTI code assumes one-dimensional plane symmetry. The target may consist of upto ten layers with up to three different materials. Laser energy deposition is modeled by inverse bremsstrahlung absorption and a dump at the critical density. Electronic heat conduction is flux limited in the usual way. Radiation transport is treated stationary assuming that the matter velocity is much less than the speed of light. Scattering is neglected. There is a single matter temperature and opacities are assumed to depend only on this temperature, the density and frequency.

Typical running time
On the CRAY-XMP the computing time is below 10^{-4} s/(zone timestep group) if the number of groups is not too small.

Unusual features
Call to system routines DNAME0 and ERREXIT. These can be replaced or simply eliminated.

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LONG WRITE-UP

1. Introduction

At the extreme thermodynamic conditions found in inertial confinement fusion (ICF) and related experiments, energy transport by thermal radiation plays an important role [1,2]. The radiation field is strongly coupled to the hydrodynamic motion through emission and absorption phenomena, both essentially frequency dependent. In order to achieve a thorough understanding of the processing going on in such situations a numerical simulation code has been developed. This report describes the physical model and the numerical methods used, and gives also a detailed description of the internal functioning of the code.

The code is called MULTI (MULTIgroup radiation transport in MULTIlayer foils) and solves the one-dimensional planar hydrodynamic equations coupled to the radiation transfer equation.

The equations used in the code are the first terms in the expansion of the radiation hydrodynamic equations in the small parameter v/c (characteristic velocity/light velocity). This means that relativistic effects as well as the time derivatives in the transfer equation are not taken into account. Obviously, this imposes limits on the area of applicability of the code. However, this is not a major shortcoming because in a wide range of situations the matter velocity is really well below the light velocity.

The frequency and angle variables in the equation of transfer are handled by a multigroup method which amounts to a discretization of these variables [3,4]. In this respect, the present treatment goes beyond the usual 'grey' approximation [5,6].

In addition, the code can use the grey description of the radiation, as a particular case in which the number of groups is one. This ability has been intensively used to test the code. The results were compared with that of the grey-approximation code MINIRA [7]. They agree within an error of one percent.

Electronic heat conduction is treated as usual: Spitzer's formula [8] together with a limitation of the flux to a certain fraction of the so-called free-streaming value.

The present version of the code includes laser absorption by inverse bremsstrahlung [9]. Anomalous absorption mechanism are mocked up by a dump at the critical density. Other forms of energy deposition can be easily implemented by changing the appropriate routines.

The properties of the matter are given through tabulated equations of state (usually taken from the SESAME library [10]) and tabulated opacities.

The non-LTE option requires the knowledge of the emission properties of the matter depending only on temperature, density and frequency. These are generated off-line using a stationary model [14] and fed into the code in tabular form.

A time-splitting scheme is used; the physical phenomena are treated successively during the time step. The numerical stability is guaranteed by using a fully implicit method in every substep [11]. Although a time-splitting scheme has only a first order accuracy, several advantages justify its use, namely

i) Since the hydrodynamic equations are solved implicitly, the Courant limit in the time step usually found in the explicit schemes [12], can be exceeded.

ii) The necessary numerical work increases only linearly with the number of photon-groups (in simultaneous resolution schemes this increase occurs quadratically).

iii) A modular design can be easily implemented.

LINPACK library routines [13] have been applied to solve the linear system of equations.

2. Physical model

2.1. Radiation transfer equation

The equation of transfer, also called the transport equation, is the mathematical statement of the conservation of photons. In quite general form

it is given by

$$\left(\frac{1}{c}\partial_t + \boldsymbol{n}\cdot\nabla\right) I(\boldsymbol{r}, \boldsymbol{n}, \nu, t) = \eta(\boldsymbol{r}, \boldsymbol{n}, \nu, t) - \chi(\boldsymbol{r}, \boldsymbol{n}, \nu, t) I(\boldsymbol{r}, \boldsymbol{n}, \nu, t), \tag{2.1}$$

$I(\boldsymbol{r}, \boldsymbol{n}, \nu, t)$ is the specific intensity of radiation of frequency ν at a position $\boldsymbol{r}$ travelling in direction $\boldsymbol{n}$ at time t, η is the total emissivity and χ is the total opacity. The term on the right hand side is the effective rate of energy emission (emission minus absorption) by the matter per unit of volume, frequency and solid angle. The relationship between the photon momentum $\boldsymbol{p}$ and its energy e is given by: $\boldsymbol{p} = (e/c)\boldsymbol{n}$. Consequently the specific rate of momentum emission is $((\eta - \chi I)/c)\boldsymbol{n}$. The total emission rates per unit volume of energy Q and momentum $\boldsymbol{R}$ are obtained by integrating over all frequencies and directions

$$Q = \int_0^\infty \int_{4\pi} (\eta - \chi I)\, \mathrm{d}\boldsymbol{n}\, \mathrm{d}\nu, \tag{2.2}$$

$$\boldsymbol{R} = \int_0^\infty \int_{4\pi} \frac{(\eta - \chi I)}{c} \boldsymbol{n}\, \mathrm{d}\boldsymbol{n}\, \mathrm{d}\nu. \tag{2.3}$$

Under the assumptions that scattering is not important the emissivity may be written as

$$\eta(\boldsymbol{r}, \boldsymbol{n}, \nu, t) = \chi(\boldsymbol{r}, \boldsymbol{n}, \eta, t) I_S(\boldsymbol{r}, \boldsymbol{n}, \nu, t), \tag{2.4}$$

where I_S is the source function [4]. Under conditions of local thermodynamic equilibrium (LTE) Kirchhoff's law is valid and I_S becomes equal to Planck's function (T is the matter temperature)

$$I_P(T, \nu) = \frac{2h\nu^3}{c^2}(\mathrm{e}^{h\nu/kT} - 1)^{-1}. \tag{2.5}$$

Deviations of I_S from I_P may become important in laser plasma problems, in particular in the thin plasma corona. MULTI allows for non-LTE physics, details are described further below.

The velocity of the matter is assumed to be small in comparison with the light velocity. Consequently the opacity and the source function can be considered as isotropic (this is equivalent to neglecting the Doppler effect). In addition they are assumed to depend only on the frequency and the thermodynamic properties of the matter: temperature T and density ρ. This is obviously correct for thermodynamic equilibrium and is the simpler choice for more complicated situations:

$$\begin{aligned} \chi(\boldsymbol{r}, \boldsymbol{n}, \nu, t) &= \chi(T, \rho, \nu, N), \\ I_S(\boldsymbol{r}, \boldsymbol{n}, \nu, t) &= I_S(T, \rho, \nu, N), \end{aligned} \tag{2.6}$$

$N(\boldsymbol{r}, t)$ represents the matter composition i.e. a number associated to a specific material. The order of magnitude of the time derivative in (1) is I/ct whereas the convective derivative is of the order I/l, with I, t and l being characteristic values of radiation specific intensity, time and length, respectively. The assumption of small enough matter velocity ($l/t \ll c$) implies then that the time derivative can be dropped in (1). With all those simplifications the equation of transfer, in unidimensional planar geometry reads

$$\begin{aligned} \mu\partial_x I(x, \mu, \nu, t) &= \chi(T, \rho, \nu, N) \\ &\quad \times (I_S(t, \rho, \nu, N) - I(x, \mu, \nu, t)), \end{aligned} \tag{2.7}$$

where μ is the cosine of the angle between the photon direction and the x axis, and T, ρ and N are functions of x and t. Analogously the relations (2) and (3) take the form

$$Q(x, t) = \int_0^\infty \chi(T, \rho, \nu, N)\left[4\pi I_S(T, \rho, \nu, N) - 2\pi\int_{-1}^{1} I(x, \mu, \nu, t)\, \mathrm{d}\mu\right] \mathrm{d}\nu, \tag{2.8}$$

$$R_x(x, t) = \frac{2\pi}{c} \times \int_0^\infty \left[\chi(T, \rho, \nu, N)\int_{-1}^{1} I(x, \mu, \nu, t)\mu\, \mathrm{d}\mu\right] \mathrm{d}\nu, \tag{2.9}$$

$$R_y(x, t) = R_z(x, t) = 0. \tag{2.10}$$

2.2. Hydrodynamic equations

The fluid motion is governed by a set of three equations that state the conservation of mass, momentum and internal energy

$$D_t\rho = -\rho\nabla\cdot\boldsymbol{v}, \tag{2.11}$$

$$\rho D_t \boldsymbol{v} = -\nabla P - \boldsymbol{R}, \tag{2.12}$$

$$\rho D_t e = -P\nabla\cdot\boldsymbol{v} - \nabla\cdot\boldsymbol{q} - Q + S. \tag{2.13}$$

The main variables matter density $\rho(\boldsymbol{r}, t)$, velocity $\boldsymbol{v}(\boldsymbol{r}, t)$, specific internal energy $e(\boldsymbol{r}, t)$ and pressure $P(\boldsymbol{r}, t)$ are considered here to be functions of coordinate and time. D_t is the time derivative in a frame moving with the fluid velocity: ($D_t \equiv \partial_t + \boldsymbol{v}\cdot\nabla$). $\boldsymbol{R}$ and Q are the radiated momentum and energy per unit volume, respectively, $\boldsymbol{q}$ is the thermal flux and S includes other energy sources like laser or ion beam energy deposition. The Eulerian fluid equations for the one-dimensional planar case can be obtained easily from the system (11)–(13), but instead it proves convenient to use the Lagrangian formulation. The Lagrangian coordinate is defined here by

$$m(x, t) = \int_{-\infty}^{x} \rho(x', t)\, \mathrm{d}x', \tag{2.14}$$

m is in fact the total mass per unit area at the left of the considered point. The system (11)–(13) becomes in planar geometry

$$\partial_t \rho = -\rho^2\, \partial_m v, \tag{2.15}$$

$$\partial_t v = -\partial_m (P_{\mathrm{eq}} + P_{\mathrm{vis}}), \tag{2.16}$$

$$\partial_t e = -(P_{\mathrm{eq}} + P_{\mathrm{vis}})\, \partial_m v - \partial_m q - \frac{Q}{\rho} + \frac{S}{\rho}, \tag{2.17}$$

P_{vis} is an artificial viscous pressure that must be included in order to achieve numerical stability and

$$P_{\mathrm{eq}} = P_{\mathrm{eq}}(\rho, e, N) \tag{2.18}$$

is the matter pressure that is assumed to depend only on the thermodynamic variables. Diffusive mixing of different materials is assumed to be not important, consequently the matter composition N depends only on m.

Although the temperature does not enter explicitly in the fluid equation, it is needed in the radiation transfer and thermal flux equations. In analogy to the pressure the temperature is given by

$$T = T_{\mathrm{eq}}(\rho, e, N). \tag{2.19}$$

It must be noticed that the radiation momentum emission has been dropped in (16). This is consistent with the terms which are also dropped in the radiation transfer equation. The equations used in the code are, in fact, the first order equations in a hierarchy of equations obtained by developing in powers of the small factor v_c/c, where v_c is the characteristic velocity ($\equiv l_c/t_c$).

2.3. Heat flux

Most of the energy transported by heat flux is carried away by the electrons. In the quasi-equilibrium limit (small temperature gradients) the heat flux is proportional to the temperature gradient according to Spitzer's formula

$$q = -\bar{K} T^{5/2}\, \partial_x T, \tag{2.20}$$

where $\bar{K}$ is given by

$$\bar{K} = \frac{10.16\epsilon\delta_t k^{7/2}}{\sqrt{m_e}\, e^4 Z_i \log \Lambda} \tag{2.21}$$

with

$$\epsilon\delta_t \approx 0.095 \frac{Z_i + 0.24}{1 + 0.24 Z_i} \tag{2.22}$$

being k Boltzmann's constant, m_e and e the electronic mass and charge, Z_i the effective ion number and $\log \Lambda$ Coulomb's logarithm. The last two quantities are assumed to be constants.

However, for large temperature gradients, Spitzer's formula is no longer valid and overestimates the thermal flux. In this case, the usual procedure is to limit the heat flux artificially by a certain fraction f of the "free-streaming limit"

$$q_{fs} = -n_e kT(kT/m_e)^{1/2}.$$

The interpolation between Spitzer's regime and the flux-limited regime is done by the harmonic mean of the both. Typical values f are determined experimental and range between 0.03 and 0.08.

2.4. Laser deposition

The laser beam is assumed to come from the right ($x \to \infty$). Electromagnetic waves propagate in a plasma only when the density is below the

critical value. If this density is reached at some point they are reflected. Thus, in general, there are two laser beams, once incident and one reflected whose respective intensities $I_+(x, t)$ and $I_-(x, t)$ are governed by the equations

$$\partial_x I_+ = \kappa I_+, \tag{2.23}$$

$$\partial_x I_- = -\kappa I_-, \tag{2.24}$$

where κ is the attenuation coefficient. If inverse bremsstrahlung is assumed to be the attenuation mechanism, this coefficient is given by

$$\kappa = C\frac{1}{T^{3/2}}\left(\frac{\rho}{\rho_c}\right)^2 \frac{1}{\sqrt{1-\rho/\rho_c}}. \tag{2.25}$$

The critical density ρ_c is determined by $\rho_c = n_c m_i/Z_i$. Here m_i and Z_i are the ion mass and charge number, respectively, and n_c the electron number density given by the condition that the plasma frequency equals the laser frequency ν_L

$$n_c = \pi\nu_L^2 m_e/e^2. \tag{2.26}$$

On the other hand, the constant C is given by

$$C = \frac{16\pi Z_i n_c^2 e^6 \log \Lambda}{3c^2\nu_L^2(2\pi m_e k)^{3/2}}. \tag{2.27}$$

It must be noticed that the eqs. (23), (24) become singular when $\rho = \rho_c$.

The incident laser intensity $I_+(\infty, t)$ is assumed to be known and consequently eq. (23) can be integrated from $x = \infty$ to the point x_c where $\rho = \rho_c$. In this way the value $I_+(x_c, t)$ can be achieved. A given fraction αI_+ is absorbed there and the rest is reflected ($I_-(x_c, t) = (1 - \alpha)I_+(x_c, t)$). Starting from this value eq. (24) can be integrated from x_c to ∞.

In the case that the density is everywhere below the critical value, (23) can be integrated from ∞ to $-\infty$ and (24) implies $I_-(x, t) = 0$ because $I_-(\infty, t) = 0$ (there is no laser incident on the left hand side).

Once I_+ and I_- are known the deposition term is given by

$$S = \partial_x I_+ - \partial_x I_-. \tag{2.28}$$

The code includes also the possibility that the laser incidents from the left hand side; the discussion is analogous.

2.5. Other energy sources

There is the possibility to modify the code to include other forms of energy deposition. Only the routines QUELLE and QUELIN must be changed.

2.6. Boundary conditions

The preceding equations must be complemented by appropriate boundary conditions. In planar geometry the problem is confined between two limiting planes, at the left and at the right sides, whose position change with time. However, their Lagrangian mass coordinates, denoted by m_L and m_R, respectively, are constant. ($m_L = 0$ because there is no mass to the left of the left boundary, and m_R, the total mass per unit area, is constant if the mass is conserved).

First the specific radiation intensity $I(m, \mu, \nu, t)$ will be considered. For positive μ this function represents the intensity of radiation travelling from left to right. Consequently the natural boundary conditions must be, in this case, imposed on the left boundary m_L. Once these are known, (7) can be integrated and the values at the right boundary determined. Conversely, the boundary conditions for I with negative μ must be imposed at m_R. Some of the possible combinations at the left hand side are (for $\mu > 0$)

No incident radiation

$$I(m_L, \mu, \nu, t) = 0; \tag{2.29}$$

Incident Planckian radiation at temperature T_L

$$I(m_L, \mu, \nu, t) = I_p(T_L, \nu); \tag{2.30}$$

Specular reflection

$$I(m_L, \mu, \nu, t) = I(m_L, -\mu, \nu, t); \tag{2.31}$$

Partial specular reflection

$$I(m_L, \mu, \nu, t) = \alpha_L I(m_L, -\mu, \nu, t) \quad (0 < \alpha_L < 1). \tag{2.32}$$

The third condition can be used in the case of a

symmetric 'Hohlraum', that is two symmetric layers, each of them receiving the radiation emitted by the other. The program actually carries out only one layer computations, the plane of symmetry is modeled as a mirror. The fourth condition takes into account some possible losses in the 'Hohlraum', i.e. non-planar effects, holes in the layer, and so on. It must be noted that the second and third condition are particular case of the fourth one for $\alpha_L = 0$ and $\alpha_L = 1$, respectively. That is actually the condition implemented in the code. The boundary conditions on the right hand side are completely analogous. The corresponding 'reflection factor' is denoted by α_R.

The boundary conditions for the hydrodynamics take the usual form. At a free surface the pressure must be zero, while the density, specific internal energy and velocity can take in principle arbitrary values (in the case of a gas this condition implies also zero density). At a rigid wall the velocity must be zero whereas all the other variables can take arbitrary values. The input variable IFLAG2 controls these conditions. It must be set to 1 to have free left and right surfaces and 0 for rigid walls.

In addition a condition for the thermal flux is needed. It is assumed always to have isolated boundaries $q(m_L, t) = q(m_R, t) = 0$.

Although the program manages composed layers there are no explicit boundary conditions at the interfaces. Instead a matter composition function $N(m)$ (usually taking integer values) is given, which enters as a parameter in the opacity and equation of state.

3. Multigroup radiation model

3.1. Introduction

The radiation transfer equation can be rewritten as

$$\mu\, \partial_m I(m, \mu, \nu, t) = \kappa(T, \rho, \nu, N) \times (I_S(T, \rho, \nu, N) - I(m, \nu, \nu, t)). \quad (3.1)$$

Now the radiation intensity is considered to depend on the Lagrangian coordinate. The quantity κ ($\equiv \chi/\rho$) is the opacity expressed in units of surface per mass. The above equation is obviously very complicated; the specific intensity depends on four variables. Careless discretization can easily lead to an enormous amount of computational work or a substantial loss of accuracy. The approach adopted here carries out the discretization in two steps. First eq. (1) is replaced by its integrals over the variables ν and μ in a finite number of domains called 'groups'. This procedure leads to a finite number of differential equations involving a finite number of variables depending only on m and t. In the second step, discussed in the next sections, this set of equations together with the fluid, thermal flux and laser equations is discretized in a computational mesh in the m, t space, generating finite difference equations.

3.2. Group definition

Let us consider the set of possible pairs of values (ν, μ) of frequency and cosine $(0 < \nu < \infty, -1 < \mu < 1)$. This set can be partitioned in a finite number NG of subsets that will be called here 'groups' (although properly speaking a 'group' is formed by the photons whose frequency and cosine belong to such a subset). The groups considered here are defined by two boundary frequencies $(\nu_a^k < \nu_b^k)$ and two boundary cosines $(0 < \mu_a^k < \mu_b^k)$, where the superindex k stands for the number of the group. The group k is thus the set of photons whose frequency verifies $\nu_a^k < \nu < \nu_b^k$ and whose cosine verifies $\mu_a^k < \mu < \mu_b^k$ (photons travelling to the right) or $-\mu_b^k \lambda \mu < -\mu_a^k$ (travelling to the left). It is assumed, of course, that the groups do not overlap and that they cover the whole ν, μ space.

3.3. Group equations

It proves convenient to introduce first a few definitions. If f is an arbitrary function of the variables m, ν, μ and t, it can be transformed into a function of m and t only through the use of the integral operators L_+^k, L_-^k and L^k defined by

$$L_+^k(f) = 2\pi \int_{\mu_a^k}^{\mu_b^k} \int_{\nu_a^k}^{\nu_b^k} f(m, \nu, \mu, t)\, d\nu\, d\mu, \quad (3.2)$$

$$L_-^k(f) = 2\pi \int_{-\mu_b^k}^{-\mu_a^k} \int_{\nu_a^k}^{\nu_b^k} f(m, \nu, \mu, t)\, d\nu\, d\mu, \quad (3.3)$$

$$L^k(f) = L_+^k(f) + L_-^k(f). \quad (3.4)$$

The last of these operators is the integration over all the frequencies and angles in the group k. The density of the energy U_k and the energy flux S_k of the photons belonging to the group k can be expressed as

$$U_k = \frac{1}{c} L^k(I), \quad (3.5)$$

$$S_k = L^k(\mu I). \quad (3.6)$$

Analogously the rate of energy emission per volume by the photons of this group is given by

$$Q_k = L^k(\chi(I_S - I)) \quad (3.7)$$

and consequently the total rate is computed adding all the groups

$$Q = \sum_{1 \le k \le NG} Q_k. \quad (3.8)$$

This expression coincides with eq. (2.8). The following properties of these operators will be needed below: if g is some function of m, ν and t but not dependent on μ, it is verified that

$$L_+^k(g) = L_-^k(g) = \tfrac{1}{2} L^k(g), \quad (3.9)$$

$$L_+^k(\mu g) = -L_-^k(\mu g) = \tfrac{1}{4}\left(\mu_a^k + \mu_b^k\right) L^k(g), \quad (3.10)$$

$$L_+^k(\mu^2 g) = L_-^k(\mu^2 g) = \tfrac{1}{6}\left(\mu_a^{k^2} + \mu_a^k \mu_b^k + \mu_b^{k^2}\right) L^k(g). \quad (3.11)$$

In order to obtain the group-k equations, eq. (1) is integrated separately over the photons travelling to the right and over the photons travelling to the left. This is done by applying the operators L_+^k and L_-^k, respectively,

$$\partial_m L_+^k(\mu I) = L_+^k(\kappa I_S) - L_+^k(\kappa I), \quad (3.12)$$

$$\partial_m L_-^k(\mu I) = L_-^k(\kappa I_S) - L_-^k(\kappa I). \quad (3.13)$$

In order to make these equations useful, it is necessary to make some reasonable assumptions about the form of the function I. Between the wide range of possible choices, I is selected such that one is able, with a reduced number of groups, to manage situations near the thermodynamical equilibrium with a reasonable accuracy. In these situations $I \approx I_p$ and applying perturbation methods to (1) results in

$$I = I_p - \mu \frac{I_p'}{\kappa} \partial_m T + \cdots, \quad (3.14)$$

where I_p and I_p' ($\equiv \partial I_p / \partial T$) are functions of ν and T only. This equation suggests to assume for the group k the following form of I

$$I(m, \mu, \nu, t) = \alpha_k(m, t) I_p(T, \nu) + \mu \beta_k(m, t) \frac{I_p'(T, \nu)}{\kappa(T, \rho, \nu, N)}, \quad (3.15)$$

α_k and β_k being the functions that describe completely the group. If there is local quasi-equilibrium they take the values 1 and $-\partial_m T$, respectively; this makes it possible to manage correctly situations with one group only. On the other hand, when the system is far away from the equilibrium, the present assumption is not worse as any other; in this case the accuracy can be reached only by taking a large number of groups. Using the properties (9)–(11) the energy density and flux expressions take now the form

$$U_k = \frac{1}{c} \alpha_k L^k(I_p), \quad (3.16)$$

$$S_k = \frac{\beta_k}{3}\left(\mu_a^{k^2} + \mu_a^k \mu_b^k + \mu_b^{k^2}\right) L^k(I_p'/\kappa), \quad (3.17)$$

Whereas the eqs. (12), (13) can be rewritten as

$$\partial_m \left(\pm \frac{\mu_a^k + \mu_b^k}{4} \alpha_k L^k(I_p) + \frac{\mu_a^{k^2} + \mu_a^k \mu_b^k + \mu_b^{k^2}}{6} \beta_k L^k(I_p'/\kappa) \right) = \tfrac{1}{2} L^k(\kappa I_S) - \frac{\alpha_k}{2} L^k(\kappa I_p) \mp \frac{\mu_a^k + \mu_b^k}{4} \beta_k L^k(I_p'). \quad (3.18)$$

Now these equations are linearly combined adding and substracting each other; after some straight-

forward algebra this results in

$$\partial_m S_k(m, t) = c\kappa_P^k(\rho, T, N)(U_{Sk}(\rho, T, N) - U_k(m, t)), \tag{3.19}$$

$$g_k^2 c\partial_m U_k(m, t) = -\kappa_R^k(\rho, T, N) S_k(m, t). \tag{3.20}$$

The source energy density U_{Sk} is written in the form

$$U_{Sk}(\rho, T, N) = \epsilon_k(\rho, T, N) U_{Pk}(T)$$

with the Planckian energy density

$$U_{Pk}(T) = \frac{4\pi(\mu_b^k - \mu_a^k)}{c} \int_{\nu_a^k}^{\nu_b^k} I_P(T, \nu)\, d\nu. \tag{3.21}$$

The material coefficients κ_P^k and κ_R^k are usually named Planck and Rosseland mean opacities and are defined by

$$\kappa_P^k = \int_{\nu_a^k}^{\nu_b^k} \kappa I_P\, d\nu \Big/ \int_{\nu_a^k}^{\nu_b^k} I_P\, d\nu, \tag{3.22}$$

$$\kappa_R^k = \int_{\nu_a^k}^{\nu_b^k} I_P'\, d\nu \Big/ \int_{\nu_a^k}^{\nu_b^k} \frac{I_P'}{\kappa}\, d\nu. \tag{3.23}$$

Deviations from LTE conditions in the source function are taken into account by the coefficients

$$\epsilon_k = \int_{\nu_a^k}^{\nu_b^k} \kappa I_S\, d\nu \Big/ \int_{\nu_a^k}^{\nu_b^k} \kappa I_P\, d\nu.$$

This is done in the approximation that $\epsilon_k(\rho, T, N)$ can be expressed as a function of the local density, temperature and material species alone. In practice, one may use some interpolation between SAHA (LTE) and corona equilibrium [14]. In LTE, all ϵ_k are equal to unity.

The coefficients κ_P^k, κ_R^k and ϵ_k have to be provided in tabular form. The constant g_k^2 plays the role of the Eddington factor for the group and is given

$$g_k = \sqrt{\frac{\mu_a^{k^2} + \mu_a^k \mu_b^k + \mu_b^{k^2}}{3}}. \tag{3.24}$$

Finally, eq. (7) can be rewritten as

$$Q_k(m, t) = c\rho(m, t)\kappa_P^k(\rho, T, N) \times (U_{Sk}(\rho, T, N) - U_k(m, t)). \tag{3.25}$$

3.4. Boundary conditions

As had been pointed out, every group is composed of photons traveling in two directions. Let us consider the partial energy densities U_k^+ and U_k^- of the photons traveling to the right and to the left, respectively, and also the corresponding energy fluxes S_k^+ and S_k^-. They are given by

$$U_k^\pm = \frac{1}{c} L_\pm^k(I) = \tfrac{1}{2} U_k \pm \frac{\mu_a^k + \mu_b^k}{4cg_k^2} S_k, \tag{3.26}$$

$$S_k^\pm = L_\pm^k(I) = \tfrac{1}{2} S_k \pm \frac{\mu_a^k + \mu_b^k}{4} cU_k. \tag{3.27}$$

The boundary conditions (2.32) can be written in terms of energy fluxes instead of specific intensities. Multiplying by μ and carrying out the integration over frequencies between ν_a^k and ν_b^k and cosines between μ_a^k and μ_b^k results in

$$S_k^+(m_L, t) = -\alpha_L S_k^-(m_L, t). \tag{3.28}$$

Taking into account the previous expressions it becomes

$$S_k(m_L, t) = -\frac{\mu_a^k + \mu_b^k}{2}\left(\frac{1 - \alpha_L}{1 + \alpha_L}\right) cU_k(m_R, t). \tag{3.29}$$

Analogously, the corresponding condition at the right boundary is

$$S_k(m_R, t) = \frac{\mu_a^k + \mu_b^k}{2}\left(\frac{1 - \alpha_R}{1 + \alpha_R}\right) cU_k(m_L, t). \tag{3.30}$$

3.5. Alternative model

Besides the above outlined model, it is interesting to consider other possible assumptions for the specific intensity. One simple choice is, for the

group k, given by

$$I_k(m, \mu, \nu, t) = \alpha_k^+(m, t) I_p(T, \nu), \quad (\mu > 0), \tag{3.31}$$

$$I_k(m, \mu, \nu, t) = \alpha_k^-(m, t) I_p(T, \nu), \quad (\mu < 0). \tag{3.32}$$

Proceeding analogously as in the previous sections the equations for the groups become

$$\partial_m S_k(m, t) = c\kappa_P^k(\rho, T, N)(U_{Sk}(\rho, T, N) - U_k(m, t)), \tag{3.33}$$

$$g_k'^2 c\, \partial_m U_k(m, t) = -\kappa_P^k(\rho, T, N) S_k(m, t), \tag{3.34}$$

where the Eddington factor $g_k'^2$ is given now by

$$g_k' = (\mu_a^k + \mu_b^k)/2. \tag{3.35}$$

On the other hand, the boundary conditions are the same, provided that g_k' is used instead of g_k. These equations can be compared with the system (19), (20). There are two differences, namely: the appearance of the Planck opacity instead of the Rosseland opacity and the different expression for the factor g_k' in (34). Nevertheless, both descriptions are equivalent. In fact, they coincide when the size of the groups is made arbitrarily small. That is: $\kappa_R^k \to \kappa_P^k$ and $g_k' \to g_k$ when $\nu_a^k \to \nu_b^k$ and $\mu_a^k \to \mu_b^k$. The advantage of the previous model had been already pointed out. On the other hand, the alternative model has an interesting property: eqs. (33), (34) can be linearly combined giving

$$\partial_m(S_k + g_k' c U_k) = c\kappa_P^k U_{Sk} - \frac{\kappa_P^k}{g_k'}(S_k + g_k' c U_k) \tag{3.36}$$

while the boundary condition in m_L implies $S_k + g_k' c U_k > 0$ there, because α_L must be less than unity. The above equation implies that $S_k + g_k' c U_k > 0$ everywhere (otherwise, starting from positive values of $S_k + g_k' c U_k$ at the left hand side implies that as soon as this quantity changes sign the slope needs to be negative, in contradiction to the above equation). Consequently $S_k < g_k' c U_k$. Analogously the condition $S_k > -g_k' c U_k$ is obtained. Thus the alternative model supplies a natural 'flux-limit' without the need of ad-hoc assumptions. The program is written in such a way that both models can be easily used.

3.6. Specific intensity

Although the equations actually solved by the code have been already given in the previous sections, it is interesting to write down expressions for the specific intensity of the radiation that could be used to display the results. This is done assuming two constant intensities $\langle I_k^+ \rangle$ and $\langle I_k^- \rangle$ for the photons traveling in two directions in every group. They are defined by the condition that by integrating over their respective half-groups the energy densities U_k^+ and U_k^- are obtained. This gives

$$\langle I_k^\pm \rangle = \frac{c U_k^\pm}{2\pi(\mu_b^k - \mu_a^k)(\nu_b^k - \nu_a^k)}. \tag{3.37}$$

Obviously, these expressions make only sense when the number of groups is large enough.

4. Spatial discretization

4.1. Introduction

Once the radiation transfer equation has been replaced by a finite set of group equations, the only independent variables are the mass coordinate m and the time t. The discretization of the system is carried out in two steps. First the spatial operators are replaced by finite-difference operators; the equations thus become a system of ordinary differential equations with the time as independent variable. In the second step this system is again discretized in time; a set of algebraic equations are obtained. This section is devoted to the first step.

In terms of the Lagrangian variable m, the matter (and thus the problem) is confined between the boundaries m_L and m_R. Let us divide this interval in N subintervals, called 'cells', not necessarily equal. Each of them will be referenced by the index i, that increases from left to right; $i = 1$

corresponds to the leftmost cell and $i = N$ is the rightmost. The thickness of the subinterval itself is denoted by Δm_i. The cut points will be called 'interfaces'. Obviously there are $N+1$ interfaces; their index i varies from 1 (left boundary) to $N+1$ (right boundary). With this notation the cell i lies between the interface i and $i+1$ while the interface i $(2 \le i \le N)$ lies between the cells $i-1$ and i. The advantage of this notation is that it corresponds directly to the index on the storage arrays used by the program.

Here, as customary, the quantities that imply a flux (velocity, laser intensity, heat flux and radiation flux) are assumed to be known on the interfaces whereas all the others are assumed to be known in the cells. They are usually named interface-centered and cell-centered quantities, respectively. The finite diference equations are obtained in a rather straightforward way; only special refinements are needed for the laser deposition.

Although the equations are coupled, they are presented separately.

4.2. Fluid equations

The equations for mass, momentum and internal energy conservation take the form

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i^2 \frac{v_{i+1} - v_i}{\Delta m_i}, \quad (i = 1, \ldots, N), \tag{4.1}$$

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = -\frac{P_i - P_{i-1}}{\frac{1}{2}(\Delta m_i + \Delta m_{i-1})}, \quad (i = 2, \ldots, N), \tag{4.2}$$

$$\frac{\mathrm{d}e_i}{\mathrm{d}t} = -P_i \frac{v_{i+1} - v_i}{\Delta m_i} - \frac{q_{i+1} - q_i}{\Delta m_i} - \left(\frac{Q}{\rho}\right)_i + \left(\frac{S}{\rho}\right)_i,$$

The pressure is given by the static term plus the artificial viscosity term

$$P_i = P_{\mathrm{eq},i} + a_{\mathrm{v}}^2 \rho_i \min(0, v_{i+1} - v_i)^2, \quad (i = 1, \ldots, N), \tag{4.6}$$

Where a_{v} is a dimensionless parameter that represents the number of cells needed to describe numerically the shock waves; typically $a_{\mathrm{v}} = 2$. Thermal flux q_i, specific radiated power $(Q/\rho)_i$ and specific laser power deposition $(S/\rho)_i$ are given in the following sections.

4.3. Thermal flux

The classical flux, in the form given by Spitzer, would take the form

$$q_{\mathrm{c}i} = -\tfrac{2}{7}\overline{K}(\rho_i + \rho_{i-1})\left(\frac{T_i^{7/2} - T_{i-1}^{7/2}}{\Delta m_i + \Delta m_{i-1}}\right), \quad (i = 2, \ldots, N), \tag{4.7}$$

whereas the maximum allowable flux is given by

$$q_{\mathrm{s}i} = \left(\frac{fk^{3/2} Z_i}{m_{\mathrm{e}}^{1/2} m_i}\right) \frac{(T_i^{3/2} + T_{i-1}^{3/2})}{2} \frac{(\rho_i + \rho_{i-1})}{2}, \quad (i = 2, \ldots, N), \tag{4.8}$$

the program uses the harmonic mean

$$q_i = \frac{q_{\mathrm{c}i}}{1 + |q_{\mathrm{c}i}|/q_{\mathrm{s}i}}, \quad (i = 2, \ldots, N),$$

the boundary conditions reads $q_1 = q_{N+1} = 0$.

4.4. Group equations

The specific energy radiated by the matter is

eqs. (3.19), (3.20) for the group k take the form

$$\frac{S_{k,i+1}-S_{k,i}}{\Delta m_i}=c\kappa^k_{\mathrm{P},i}(U_{\mathrm{S}k,i}-U_{k,i}),\quad (i=1,\ldots,N), \tag{4.11}$$

$$cg_k^2\frac{U_{k,i}-U_{k,i-1}}{\frac{1}{2}(\Delta m_i+\Delta m_{i-1})}=-\left(\frac{2}{1/\kappa^k_{\mathrm{R},i}+1/\kappa^k_{\mathrm{R},i-1}}\right)S_{k,i},\quad (i=2,\ldots,N) \tag{4.12}$$

and the boundary conditions (3.29), (3.30) can be written as

$$S_{k,1}=-\frac{\mu^k_{\mathrm{a}}+\mu^k_{\mathrm{b}}}{2}\left(\frac{1-\alpha_{\mathrm{L}}}{1+\alpha_{\mathrm{L}}}\right)cU_{k\mathrm{L}}, \tag{4.13}$$

$$S_{k,N+1}=\frac{\mu^k_{\mathrm{a}}+\mu^k_{\mathrm{b}}}{2}\left(\frac{1-\alpha_{\mathrm{R}}}{1+\alpha_{\mathrm{R}}}\right)cU_{k\mathrm{R}}. \tag{4.14}$$

The values of $U_{k\mathrm{L}}$ and $U_{k\mathrm{R}}$ at the boundaries are computed by extrapolating the values in the adjoint cells (U_k is a cell centered quantity)

$$U_{k\mathrm{L}}=\left(1+\frac{\Delta m_1}{\Delta m_1+\Delta m_2}\right)U_{k,1}+\left(-\frac{\Delta m_1}{\Delta m_1+\Delta m_2}\right)U_{k,2}, \tag{4.15}$$

$$U_{k\mathrm{R}}=\left(1+\frac{\Delta m_N}{\Delta m_N+\Delta m_{N-1}}\right)U_{k,N}+\left(-\frac{\Delta m_N}{\Delta m_N+\Delta m_{N-1}}\right)U_{k,N-1}. \tag{4.16}$$

It must be noted that in (12) the Rosseland opacity in the interfaces is obtained as the inverse of the average of the inverses in the adjoint cells. This procedure gives smaller values than the direct average, especially with large gradients. Thus allowing for large fluxes makes it possible to smooth such gradients.

4.5. Laser equation

Some case is needed in computing specific laser energy deposition in the cell i, as the laser equations are strongly non-linear. The procedure adopted here computes the energy deposited in one cell integrating eq. (2.28) between cell boundaries; the specific deposition is given by this quantity divided by the thickness of the cell

$$\left(\frac{S}{\rho}\right)_i=\frac{1}{\rho_i\,\Delta x_i}\int_{x_i}^{x_{i+1}}S\,\mathrm{d}x=\frac{I_{+,i+1}-I_{+,i}-I_{-,i+1}+I_{-,i}}{\Delta m_i}. \tag{4.17}$$

The laser intensities $I_{+,i}$ and $I_{-,i}$ are computed in the interfaces between cells as follows. $I_{+,N+1}$ is the known incident laser intensity while the other values $I_{+,i}$ are computed applying successively the formula

$$I_{+,i}=I_{+,i+1}\exp\left(-\frac{C}{T_i^{3/2}}\int_{x_i}^{x_{i+1}}\frac{(\rho/\rho_{\mathrm{c}})^2\,\mathrm{d}x}{\sqrt{1-\rho/\rho_{\mathrm{c}}}}\right), \tag{4.18}$$

where the temperature T_i is assumed constant through the cell. If ρ is assumed to vary linearly between the values at the interfaces, the integral can be carried out analytically. The needed interface-centered values of ρ are assumed to be the mean between cell centered-values, except the first and the last ones that are taken equal to zero. This method can be applied only if the density at x_i is higher than critical. Otherwise, the incident intensity at the critical point can be determined by the similar expression

$$I_+^{\mathrm{cr}}=I_{+,i_{\mathrm{cr}}+1}\exp\left(-\frac{C}{T_i^{3/2}}\int_{x_{\mathrm{cr}}}^{x_{i_{\mathrm{cr}}+1}}\frac{(\rho/\rho_{\mathrm{c}})^2\,\mathrm{d}x}{\sqrt{1-\rho/\rho_{\mathrm{c}}}}\right), \tag{4.19}$$

where i_{cr} is the cell where the critical density is located. Once I_+^{cr} is known the reflected intensity is given by $I_-^{\mathrm{cr}}=(1-\alpha)I_+^{\mathrm{cr}}$. Then, observing that (2.23), (2.24) implies $I_+I_-=$ constant, the values of the reflected intensity are easily computed by

$$I_{-,i}=I_+^{\mathrm{cr}2}(1-\alpha)/I_{+,i}. \tag{4.20}$$

Finally, the energy deposition corresponding to i_{cr} is divided between this cell and its neighbours. This smoothing is needed in order to prevent

strong numerical noise when the critical point jumps from one cell to another.

4.6. Matter equations

The above equations must be completed by the equation of state, opacities and other matter properties

$$P_{\mathrm{eq},i} = P_{\mathrm{eq}}(\rho_i, e_i, N_i), \quad (i=1,\ldots,N), \tag{4.21}$$

$$T_i = T(\rho_i, e_i, N_i), \quad (i=1,\ldots,N), \tag{4.22}$$

$$\kappa^k_{\mathrm{P},i} = \kappa^k_{\mathrm{P}}(\rho_i, T_i, N_i), \quad (i=1,\ldots,N,\ k=1,\ldots,\mathrm{NG}), \tag{4.23}$$

$$\kappa^k_{\mathrm{R},i} = \kappa^k_{\mathrm{R}}(\rho_i, T_i, N_i), \quad (i=1,\ldots,N,\ k=1,\ldots,\mathrm{NG}), \tag{4.24}$$

$$\epsilon_{k,i} = \epsilon_k(\rho_i, T_i, N_i), \quad (i=1,\ldots,N,\ k=1,\ldots,\mathrm{NG}). \tag{4.25}$$

The composition N_i is constant in time. These relations are implemented in the standard version of the code interpolating between tabulated values. Nevertheless it is possible, by changing the appropriate routines, to use analytic expressions.

5. Temporal discretization

5.1. Time splitting

Once the equations have been discretized in space, the physical system is represented by a finite set of variables which are continuous in time but defined only on a finite number of points (computational mesh). From the mathematical point of view, the equations consist of the rate equations for the variables ρ_i, v_i and e_i joined to a set of algebraic equations for q_i (thermal flux equation), $(Q_k/\rho)_i$, $S_{k,i}$ and $U_{k,i}$ (group equations), $(S/\rho)_i$, $I_{+,i}$ and $I_{-,i}$ (laser equations) and $P_{\mathrm{eq},i}$, T_i, $\kappa^k_{\mathrm{P},i}$, $\kappa^k_{\mathrm{R},i}$ and $\epsilon_{k,i}$ (matter properties). The system can be thought of as a set of ordinary differential equations depending on the main variables ρ_i, v_i and e_i whose right hand side depend only on these variables, since all the other variables can be written in terms of the main variables solving the algebraic equations. Thus, denoting by X the vector whose $3N+1$ components are the functions ρ_i, v_i and e_i, the system can be represented schematically by

$$\mathrm{d}X/\mathrm{d}t = f(X). \tag{5.1}$$

This system can be solved, in principle, by standard methods. For example, denoting by X^n the representation of X at time t^n ($\equiv n\,\Delta t$), it is clear that the recurrence relation

$$\frac{X^{n+1}-X^n}{\Delta t} = f(X^n) \tag{5.2}$$

supplies the required solution, provided that Δt is small enough. In general, this explicit scheme needs a prohibitively small value for the time step Δt in order to be numerically stable. This makes it useless in practice. The numerically stable implicit scheme

$$\frac{X^{n+1}-X^n}{\Delta t} = (1-\theta)f(X^n) + \theta f(X^{n+1}), \quad (\tfrac{1}{2} < \theta \le 1) \tag{5.3}$$

is unfortunately very complicated, it involves the simultaneous solution of a set of $3N+1$ non-linear equations.

Thus, it becomes necessary to use a different approach which is able to achieve the necessary stability which a reasonable amount of computational work. The procedure adopted here is the so-called 'time-splitting'. Before continuing, it proves convenient to explain briefly the basis of this method. Let us consider the equation

$$\frac{\mathrm{d}X}{\mathrm{d}t} = f_1(X) + f_2(X) \tag{5.4}$$

and the two substeps integration method given by

$$\frac{X^*-X^n}{\Delta t} = f_1(X^*), \tag{5.5}$$

$$\frac{X^{n+1}-X^*}{\Delta t} = f_2(X^{n+1}), \tag{5.6}$$

Where X^* is some intermediate value. If the functions f_1 and f_2 have some reasonable mathematical properties (continuous derivatives), it is straightforward (but rather cumbersome),

applying Taylor's series, to show that

$$\frac{X^{n+1}-X^n}{\Delta t}=f_1(X^n)+f_2(X^n)+\mathcal{O}(\Delta t). \quad (5.7)$$

The notation $\mathcal{O}(\Delta t)$ stands for terms that verify $|\mathcal{O}(\Delta t)|<\text{constant}\times\Delta t$ for $\Delta t<\Delta t_0$. This expression implies the so-called 'consistency' of the method. If, in addition, the method is stable, this leads to the appropriate solutions. If both (5), (6) are stable it is reasonable to think that the two substeps method is also stable; this occurs in practice. The global method has only a first order accuracy (the error is of order $\mathcal{O}(\Delta t)$), but this is scarcely a trouble; the main (and unavoidable) sources of error had been made in modelling the physics. The extension to more than two terms on the right of (4) is straightforward.

Now coming back to the physical equations, it is clear that the different terms can be grouped in the following way

f_H (Hydrodynamics)	f_T (Thermal flux)	f_R^1 (Group-1)	$\cdots$	f_R^{NG} (group-NG)	f_L (Laser)
$\partial_t\rho=-\rho^2\,\partial_m v$	$+0$	$+0$	$+\cdots+$	$+0$	$+0$
$\partial_t v=-\partial_m(P_{eq}+P_{vis})$	$+0$	$+0$	$+\cdots+$	$+0$	$+0$
$\partial_t e=-(P_{eq}+P_{vis})\,\partial_m v$	$-\partial_m q$	$-Q_1/\rho$	$-\cdots-$	$-Q_{NG}/\rho$	$+S/\rho$

And thus eq. (1) can be written as

$$\frac{dX}{dt}=f_H+f_T+f_R^1+f_R^2+\cdots+f_R^{NG}+f_L. \quad (5.8)$$

Before applying the time-splitting method to this equation, two points must be taken into account:

i) The laser energy deposition has usually a very sharp profile. This fact would produce strong oscillations in the temperature through the time step; first the deposition of energy produces a very hot spot that is cooled immediately by the heat and radiation transport terms. This phenomena can be the source of important errors. It can be avoided by splitting the energy deposition in NG + 1 pieces, each of them will be solved together with one of the transport terms. This is made using weight factors η_k ($k=1,2,\ldots,\text{NG}$) for the radiation transport, and η_0 for the heat flux transport. The appropriate values for these factors will be discussed at the end of this section.

ii) Often the structures related to the hydrodynamics (i.e. shock waves) move faster than the structures related to the heat or radiation transport (i.e. thermal waves). Consequently, the maximum bound for the time step would be related to the fluid motion, usually leading to quite strong restrictions. This can be overcome using 'subcycling' for the hydrodynamics; i.e. the fluid equations are advanced NS times during one time step. This is implemented in the code by dividing the term f_H into NS pieces and placing them between the radiation transport terms. Although not strictly necessary, the same is done with the thermal heating.

Eq. (8) now takes the form

$$\begin{aligned}\frac{dX}{dt}=&\,g_H+g_R^1+g_R^{NS+1}+g_R^{2NS+1}+\cdots\\&+g_R^{NG-NS+1}+g_T+g_H+g_R^2+g_R^{NS+2}\\&+g_R^{2NS+2}+\cdots+g_R^{NG-NS+2}+g_T\\&\cdots\\&+g_H+g_R^{NS}+g_R^{2NS}+g_R^{3NS}+\cdots\\&+g_R^{NG}+g_T,\end{aligned} \quad (5.9)$$

where

$$g_H=f_H/\text{NS}, \quad (5.10)$$

$$g_R^k=f_R^k+\eta_k f_L, \quad (5.11)$$

$$g_T=(f_T+\eta_0 f_L)/\text{NS}. \quad (5.12)$$

Now the time-splitting method can be directly applied to this equation; the NG + 2NS terms are added in successive substeps, in the order given above. However, it proves convenient to introduce still some minor approximations that, without spoiling the accuracy, reduce the computational work:

i) The laser deposition profile is rather insensitive to the exact temperature and density profiles; thus the f_L term will be computed only after every hydrodynamic substep and used without changes until the next hydrodynamic substep (it will be computed only NS times instead of NG + NS).

ii) The equations of state will be evaluated only before every hydrodynamic substep and approximated by the linearized formulae

$$P_{eq}(\rho, e) = P_{eq}(\rho_0, e_0) + \partial_\rho P_{eq0}(\rho_0, e_0)(\rho - \rho_0) + \partial_e P_{eq0}(\rho_0, e_0)(e - e_0), \tag{5.13}$$

$$T(\rho, e) = T(\rho_0, e_0) + \partial_\rho T_0(\rho_0, e_0)(\rho - \rho_0) + \partial_e T_0(\rho_0, e_0)(e - e_0), \tag{5.14}$$

until the next hydrodynamic substep.

iii) Although the substeps involved by the time-splitting are given fully implicitly (the operators at the right hand sides of (5), (6) are evaluated at the new values of the solution), in order to guarantee numerical stability, the values of the transport coefficients κ_P^k, κ_R^k and ϵ_k are computed with the old values of the thermodynamical variables. This does not affect stability.

Details on every of the substeps are given in the following sections.

5.2. Hydrodynamical substep

As had been pointed out, the fluid state is advanced NS times every time step. The fluid variables before and after the advancing will be denoted by the superindexes O and N, respectively. The substep is then given by

$$\frac{X^N - X^O}{\Delta t} = g^H(X^N) \equiv \frac{f_H(X^N)}{NS}. \tag{5.15}$$

This equation is non-linear and in principle it would be necessary to use some iteration procedure. However, this is not actually carried out; instead the equation is linearized expanding the right hand side into Taylor's series

$$\frac{X^N - X^O}{\Delta t'} = f_H(X^O) + \frac{\partial f_H}{\partial X}(X^O)(X^N - X^O), \tag{5.16}$$

where $\Delta t' = \Delta t/NS$. This equation is now linear in the unknown value X^N, $\partial f_H/\partial X$ being a 7-diagonal matrix. Standard library routines are employed to solve this system. The dropped terms in the Taylor series are of the order $\mathcal{O}(\Delta t^2)$ and thus do not spoil the overall accuracy of the method (of order $\mathcal{O}(\Delta t)$).

5.3. Heat flux substep

All that is said for the hydrodynamics can be directly applied to the heat flux. However, in this case, the density and velocity are not advanced (its derivatives in f_T are zero), consequently the resulting system is only tridiagonal.

5.4. Group substep

The equation for a group can be written as

$$\frac{X^N - X^O}{\Delta t} = g_R^k(X^N). \tag{5.17}$$

On the right hand side there is only one non-linear term, namely $U_{Pk}(T_i^N)$. This term will be linearized in the following way

$$U_{Pk}(T_i^N) \approx U_{Pk}(T_i^*) + \frac{\partial U_{Pk}}{\partial T}(T_i^*)(T_i^N - T_i^*), \tag{5.18}$$

where T_i^* is a reference value. The resulting equation is a tridiagonal system that can be easily solved once T_i^* is given. The code uses an iterative procedure; for the first iteration it takes $T_i^* = T_i^O$ and a provisional T_i^N result, for the second iteration it takes $T_i^* = T_i^N$ and so on. The number of iterations is given by the input variable NITER. Usually, the results are reasonable good with one iteration only.

5.5. Laser deposition partition

In this section the algorithm used by the program to avoid strong oscillations in the temperature during one time step will be explained. This problem can be especially serious in the cell i_{max} where the laser deposition is at its maximum.

Let us consider first the thermal flux substep. It

is given by

$$\left(\frac{\partial e}{\partial T}\right)_i \frac{T_i^{\mathrm{N}} - T_i^{\mathrm{O}}}{\Delta t} = \eta_0 \left(\frac{S}{\rho}\right)_i + \text{transport terms.} \tag{5.19}$$

If the time step is small enough, the transport terms are not affected by the deposition. Thus, the temperature increment in $i_{\max}$ can be rewritten as

$$\Delta T_0 = \eta_0 a + b_0, \tag{5.20}$$

where $a = (S/\rho)_{i_{\max}} (\partial T/\partial e)_{i_{\max}} \Delta t$, while b_0 does not depend on η_0. Analogous relations can be obtained for the group substeps

$$\Delta T_k = \eta_k a + b_k, \quad (k = 1, 2, \ldots, \mathrm{NG}), \tag{5.21}$$

the value a being common to all the transport processes. The global increment of the temperature at $i_{\max}$ is obviously

$$\Delta_T T = \sum_{0 \le k \le \mathrm{NG}} \Delta T_k. \tag{5.22}$$

The factors η_k can be freely chosen. If the values

$$\eta_k = \frac{1}{a}\left(\frac{\Delta_T T}{\mathrm{NG}+1} - b_k\right) \tag{5.23}$$

are selected, the temperature increments in all the transport processes are the same, supplying the desired smoothing through the step.

The program initializes first the values of the factors to

$$\eta_k = 0, \quad (k = 0), \tag{5.24}$$

$$\eta_k = 1/\mathrm{NG}, \quad (k = 1, 2, \ldots, \mathrm{NG}). \tag{5.25}$$

These values are applied in the first time step. During this step the values of ΔT_k are stored and the values of b_k computed by (21). Finally, the formula (23) provides the most appropriate values that will be used in the next time step. This process is carried out in successive time steps. If the input parameter IWCTRL (normally set to 1) is set to 0, the initial values of η_k are always used.

6. Program description

6.1. General

The program is written (as much as possible) in a modular way; only four routines have more than 56 source lines. Some parts of the program (modules) are completely interchangeable. For example, the routines QUELIN, QUELLE and LASER3, that compute the laser power deposition, can be substituted by other routines with the same name and arguments, but with completely different physics, without the need of additional changes in other program units. The modules are the following:

QUELIN-QUELLE-LASER3
HYDRO-LEICHT-ABLTNG
EOSM-EOSIN1-EOSIN2-EOSBIN-EOSLIN
WFIN-WFLUSS-LEICHT-WFDER
OPA-OPAIN-OPABIN

The program input is done through FORTRAN units 12 to 19. Every unit has assigned a conceptually different sort of data (i.e. on 16 are given the laser characteristics). In some units the read process is carried out until the 'end-of-file' is reached.

Matrices are used at different places of the program. In general they have a banded structure and thus can be stored in condensed format. Every diagonal of the 'mathematical' matrix is stored in one row of the 'FORTRAN' matrix. This format is required by the library routines that perform operations over these matrices.

The program uses the c.g.s. system of units, with the exception of the temperature which is given in electron volts. However, for compatibility with other programs, the equation of state tables must be supplied in SESAME [10] units.

6.2. Main body

In this section the main program (MULTI) and some auxiliary routines for input and initialization (INITVR, GDTGEN, WCTRL, ZONING) will be described. The different tasks carried out are the following

i) The program reads from the FORTRAN unit 12 a series of parameters that control the subsequent operations. These parameters must be given in a NAMELIST block with the name INPUT as in table 1.