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Note

Numerical Treatment of Rapid Equipartition Rates

INTRODUCTION

Many problems in computational plasma hydrodynamics and magnetohydrodynamics are concerned with the spatial transport of mass, momentum, energy, and magnetic flux. The transport of mass and momentum arising from the hydrodynamic motion of the fluid can be dealt with numerically either by an Eulerian or by a Lagrangian description. For either description the transport of energy through the fluid by thermal conduction or the diffusion of a magnetic field can be given one of two alternative numerical formulations: explicit or implicit. Calculations in one space dimension by Hain *et al.* [1] and in two dimensions by Roberts and Potter [2], Lindemuth and Killeen [3], Freeman and Lane [4], and Duchs [5], as well as many others, demonstrate how various spatial transport problems can be handled numerically.

For calculations involving a single fluid the timestep Δt is restricted by numerical stability conditions if an explicit formulation is adopted, e.g. the Courant–Friedrichs–Lewy condition [6]. If an implicit method which guarantees numerical stability is used, then it is often the time rate of variation of fundamental variables such as the temperature T or density ρ that determines the choice of Δt for reasons of accuracy.

When more than one fluid is being studied there may be local exchange of energy between the fluids, e.g. Coulomb interaction between ions and electrons, electron–photon interaction. In most multifluid calculations [1, 2, 4] it is recognized that the rate of energy exchange between the fluids (the equipartition rate) may in some circumstances become so rapid that special measures must be taken to avoid a numerical instability [4]. The simplest cure to this problem is to enforce a restriction on Δt set by the equipartition rate. Such a solution is however usually undesirable. Consider for example as a simple model an N-component system whose composition changes with time due to various types of "radioactive" decay. The fractional density f_k of a component which decays at the rate $\omega_k = 1/\tau_k$ obeys a differential equation of the type

$$\dot{f}_k = -\omega_k f_k + S_k, \qquad k = 1, N, \tag{1}$$

where the source term S_k may be a function of the other component densities.

If a set of coupled differential equations of the type (1) is solved numerically, then it is obviously not desirable to use a timestep restricted by

$$\Delta t \approx \text{Min}(\tau_k, k = 1, N), \tag{2}$$

since the decay times τ_k may vary from, say, 10^{-10}–10^{10} sec.

The plasma calculations referred to above usually aim at studying physical phenomena which occur during a period of order 10^3–10^4 times longer than the timestep Δt determined by the spatial motion. Laser fusion calculations by Nuckolls *et al.* [7], Clarke *et al.* [8], and Christiansen and Ashby [9] aim similarly at studying the phenomena occurring in a compressed and exploding superdense plasma pellet. Here the equipartition rates encountered are several orders of magnitude larger than those usually met in MHD (magnetohydrodynamic) problems. Common to the MHD and laser fusion calculations is a series of physical processes each characterized by a typical timescale τ_k. To enforce a condition on Δt of the type (2) may make these calculations costly, if not impracticable, and in this paper we address ourselves to the question of how to avoid such a restriction.

Section 1 defines the relevant energy equations of a two-component plasma. Section 2 describes a simple method for accurately treating the equipartition of energy between these two components. The method can be applied if the energy equations are transformed into time-centered finite-difference equations which are solved by either an explicit or an implicit treatment of the heat conduction term. The equipartition term itself is isolated from all the other terms and treated explicitly by the use of exponentials. Section 3 summarizes the method while its limitations and applicability are discussed in Section 4.

1. Equations of the Plasma

We consider a plasma consisting of only two fluids representing ions and electrons, moving in one, two, or three space dimensions and described by two temperatures T_i and T_e. The restriction to only two fluids avoids unnecessary complications in the algebra which in the case of three or more fluids (α-particles, radiation, etc.) would swell the bulk of this paper; the method that emerges from the presentation in Section 2 can in principle be applied to multifluid calculations (see Section 4).

The equations of state for the ions and electrons are

$$U_i = U_i(\rho, T_i), \qquad p_i = p_i(\rho, T_i), \tag{3}$$

$$U_e = U_e(\rho, T_e), \qquad p_e = p_e(\rho, T_e), \tag{4}$$

where U_i, U_e and p_i, p_e are the internal energies and pressures, respectively. The physical density ρ is in the usual notation

$$\rho = n_i m_i + n_e m_e , \tag{5}$$

n_i, n_e being the number densities. We assume the ions to behave as a perfect gas while the electrons may obey a degenerate gas law. The energy equations (First Law of Thermodynamics) are written separately for ions and electrons as

$$(C_v)_i \, (dT_i/dt) = W_i - K, \tag{6}$$

$$(C_v)_e \, (dT_e/dt) = W_e + K, \tag{7}$$

where the specific heats are obtained from (3) and (4) as

$$(C_v)_i = (\partial U_i/\partial T_i)_\rho ,$$

$$(C_v)_e = (\partial U_e/\partial T_e)_\rho ,$$

and for brevity $(C_v)_i = C_v$, the specific heat of an ideal gas. The quantities W_i and W_e can involve space derivatives and include contributions from thermal conduction, energy release due to thermonuclear reactions, emission and absorption of radiation as well as the terms $-p_i(dv/dt)$ (for ions) and $-p_e(dv/dt)$, $(\partial U_e/\partial \rho)_{T_e} (\partial \rho/\partial t)$ for electrons, v being the specific volume. K is the rate at which energy is transferred from ions to electrons due to Coulomb interactions [10]. The analytic form of K is usually

$$K = C_v(T_i - T_e)(1/\tau), \tag{8}$$

where τ is the equipartition time given by Spitzer [10]:

$$\tau = \omega^{-1} = a T_e^{3/2} n_i^{-1}, \tag{9}$$

and the constant a depends on m_i and the charge number Z. The expressions (8) and (9) are obtained assuming that ions and electrons obey perfect gas laws. If the electrons obey a degenerate gas law the expressions (8) and (9) must be changed according to the degree of degeneracy. In the present context, effects from degeneracy of electrons only appear from the specific heat $(C_v)_e$ not being equal to C_v. Similarly one may use different expressions for K if it represents an energy exchange rate between fluids other than ions and electrons. Our method however assumes K to vary linearly with the temperature difference between the fluids involved, i.e., if applied to multifluid calculations all energy exchange terms between fluids j and l should vary as $K_{jl} \sim (T_j - T_l)$.

The notation may be simplified by introducing:

$$\zeta = T_i - T_e\,,$$
$$\varphi = (W_i/C_v) - (W_e/(C_v)_e),$$
$$\beta = 1 + (C_v/(C_v)_e).$$

Subtracting (7) from (6) we then obtain the linear inhomogeneous equation:

$$d\zeta/dt = \varphi - \omega\beta\zeta. \tag{10}$$

If φ, ω, and β are assumed to be constant over a short time interval, $0 < t < \delta t$, the solution to (10) is

$$\zeta(t) = (\zeta_0 - (\varphi/\omega\beta))\, e^{-\omega\beta t} + (\varphi/\omega\beta), \qquad 0 < t < \delta t, \tag{11}$$

where $\zeta_0 = \zeta(t = 0)$.

2. Method of Solution

In order to solve Eqs. (6) and (7) we transform these into time-centered finite-difference equations, i.e., for Eq. (7)

$$(C_v)_e^{n-1/2}\,(T_e{}^n - T_e^{n-1})/\Delta t^{n-1/2} = W_e^{n-1/2} + K^{n-1/2}, \tag{12}$$

and similarly for Eq. (6); $\Delta t^{n-1/2}$ denotes the time interval between the discrete time levels $n - 1$ and n; superscript $n - \frac{1}{2}$ indicates the time halfway between $n - 1$ and n. If we know T_e^{n-1} and T_i^{n-1}, an algorithm is needed to evaluate $T_e{}^n$ from (12) and similarly for $T_i{}^n$. Since both W_e and K are functions of T_e and T_i we split the terms at time level $n - \frac{1}{2}$ such that Eq. (12) becomes

$$\begin{aligned}(\theta'(C_v)_e^n + (1 - \theta')(C_v)_e^{n-1})(T_e{}^n - T_e^{n-1})/\Delta t^{n-1/2} \\ = \theta'' W_e{}^n + (1 - \theta'')\, W_e^{n-1} + \theta K^n + (1 - \theta)\, K^{n-1}.\end{aligned} \tag{13}$$

The quantities θ, θ', and θ'' measure the degree of implicitness [6] in the approximations to the terms $K^{n-1/2}$, $(C_v)_e^{n-1/2}$ and $W_e^{n-1/2}$, respectively. This splitting principle is often adopted whenever W_e contains a heat conduction term [6]. For calculations in one space dimension the Crank–Nicholson method ($\theta'' = \frac{1}{2}$) is often applied either to the heat conduction term [1] or to all the terms of W_e [9]. In two-dimensional calculations an explicit method ($\theta'' = 0$) as described in [2] can be applied based on the Lax–Wendroff scheme [6]. An implicit method

($\theta'' \neq 0$) in two dimensions necessitates a further splitting of the two spatial components of the heat conduction term [6] and is used in [3].

A commonly adopted procedure for the numerical treatment of the term K retains only the part $(1 - \theta)\, K^{n-1}$ when solving Eq. (12) and the similar equation for T_i. The values T_i^n and T_e^n thus obtained are subsequently modified taking into account the part θK^n which is now a function of the recently obtained values T_i^n and T_e^n. Such a procedure is numerically stable since one can derive from Eq. (12) and the similar equation for T_i that

$$\zeta^n = \frac{1 - (1 - \theta)\,\epsilon\beta}{1 + \theta\epsilon\beta}\,\zeta^{n-1} + \frac{\theta''\varphi^n + (1 - \theta'')\,\varphi^{n-1}}{1 + \theta\epsilon\beta}\,\Delta t^{n-1/2}, \tag{14}$$

where the parameter ϵ is defined as

$$\epsilon = \omega\,\Delta t^{n-1/2}. \tag{15}$$

In the limit $\epsilon \to \infty$ (rapid equipartition rate) the amplification factor $A = \zeta^n/\zeta^{n-1}$,

$$A \xrightarrow[(\epsilon\to\infty)]{} 1 - (1/\theta). \tag{16}$$

For $\theta = \frac{1}{2}$ one gets $A = -1$ which in effect corresponds to "swapping" the two temperatures. The fully implicit case $\theta = 1$ gives $A = 0$, equivalent to setting $T_i^n = T_e^n$, while the explicit case $\theta = 0$ leads to an instability as observed in [1, 2, 4].

The method to be described is used by the laser fusion code MEDUSA [11]. We assume that Eq. (13) is solved by an implicit scheme and that this is done iteratively in order to improve successively on the value $W_e^n = W_e^n(T_e^n, T_i^n)$. The method is simply based on taking an average of the analytic expression (11) over the time interval $\Delta t^{n-1/2}$. For this we require

$$\begin{aligned}\langle e^{-\omega\beta t}\rangle &= \frac{1}{\Delta t^{n-1/2}}\int_0^{\Delta t^{n-1/2}} e^{-\omega\beta t}\,dt \\ &= (\epsilon\beta)^{-1}\,(1 - e^{-\epsilon\beta}).\end{aligned} \tag{17}$$

The temperature difference at time level $n - \frac{1}{2}$ is found from Eqs. (11) and (17) using $\zeta_0 = \zeta^{n-1}$. We get

$$\zeta^{n-1/2} = \left(\zeta^{n-1} - \left(\frac{\varphi\,\Delta t}{\epsilon\beta}\right)^{n-1/2}\right)\left(\frac{1 - e^{-\epsilon\beta}}{\epsilon\beta}\right)^{n-1/2} + \left(\frac{\varphi\,\Delta t}{\epsilon\beta}\right)^{n-1/2}. \tag{18}$$

The energy exchange term to be used when solving Eq. (12) then becomes

$$K^{n-1/2} = C_v\omega^{n-1/2}\zeta^{n-1/2}. \tag{19}$$

That this term is correct for all values of ϵ can be seen by forming the limits $\epsilon \to 0$ and $\epsilon \to \infty$ of the amount of energy exchanged during the time interval $\Delta t^{n-1/2}$. Since

$$K^{n-1/2}\,\Delta t^{n-1/2} = C_v \epsilon^{n-1/2} \zeta^{n-1/2},$$

we get for $\epsilon \to \infty$,

$$K^{n-1/2}\,\Delta t^{n-1/2} \to C_v (1/\beta^{n-1/2})(\zeta^{n-1} + \varphi^{n-1/2}\,\Delta t^{n-1/2}),$$

and for $\epsilon \to 0$,

$$K^{n-1/2}\,\Delta t^{n-1/2} \to 0.$$

Both these limits are equivalent to those obtained by integration of the analytic expression (11).

In order to use the expression (19) in solving Eq. (12) it is necessary to work out three quantities at time level $n - \frac{1}{2}$. We set

$$\epsilon^{n-1/2} = \omega^{n-1/2}\,\Delta t^{n-1/2} = (\theta\omega^n + (1-\theta)\,\omega^{n-1})\,\Delta t^{n-1/2}, \tag{20}$$

$$\beta^{n-1/2} = \theta'\beta^n + (1-\theta')\,\beta^{n-1}, \tag{21}$$

since ω and β are functions of T_e and ρ. To find the value of $\varphi^{n-1/2}$ we avoid a cumbersome summing up of all the contributions to the source terms W_e and W_i by transforming Eq. (10) into finite-difference form, i.e.,

$$\varphi^{n-1/2} = [(\zeta^n - \zeta^{n-1})/\Delta t^{n-1/2}] + (\beta^{n-1/2}/C_v)\,K^{n-1/2}. \tag{22}$$

3. Summary

To summarize the procedure for the present treatment of the energy exchange term we assume as mentioned above that Eq. (13) and the similar equation for T_i are solved by iteration. The following five stages illustrate how a single step from level $n-1$ to level n in a calculation can be performed.

(1) At the first iteration assume that the new quantities T_i^n and T_e^n take the same values as T_i^{n-1} and T_e^{n-1}.

(2) Evaluate $\epsilon^{n-1/2}$ and $\beta^{n-1/2}$ from Eqs. (20) and (21) and $\varphi^{n-1/2}$ from Eq. (22). At the mth iteration the values of ζ^n, β^n, ω^n, and $K^{n-1/2}$ from the $m-1$ iteration are used. (If $m = 0$ then of course $\zeta^n = \zeta^{n-1}$, $\beta^n = \beta^{n-1}$, $\omega^n = \omega^{n-1}$, and $K^{n-1/2} = K^{n-3/2}$).

(3) Find $K^{n-1/2}$ from Eqs. (18) and (19).

(4) Calculate all other contributions to the source terms W_e and W_i, i.e., thermal conductivities, thermonuclear reaction rates, etc.

(5) Solve Eq. (13) to give a new value of T_e^n (similarly for T_i^n). The next iteration starts at (2).

4. Applications and Limitations

The procedure described in Sections 2 and 3 is employed by the two-fluid code MEDUSA [11] which has been used for laser fusion calculations in one space dimension [9]. Section 2 applied the method to the equipartition of energy between two fluids, but in principle it can be used for calculations on a multifluid system. One then gets a set of equations of the type (11) and the solutions for the temperature differences $\zeta_{jl} = T_j - T_l$ will contain several terms of the form $f(t)\, e^{-\omega_{jl}t}$, where $f(t)$ may be 1, t or $\cos \omega_{jl}t$. These solutions must be examined in order to decide if the averaging (Eq. (18)) is suitable.

The application of the method is, however, confined to those cases in which Eq. (13) is solved implicitly and by iterations. For $\theta = \frac{1}{2}$, a second-order treatment is formally obtained. If no iterations are made the method degenerates to a first-order treatment as can be seen from Section 3, and similarly if Eq. (13) is solved explicitly ($\theta'' = 0$). In such cases Δt is restricted by the equipartition rate as reported in [12] and [13].

Furthermore it should be noticed that the method for solving Eq. (13) by iterations does not in general ensure convergence of the solutions. In some situations a lack of ability to center ϵ, β, and φ (Eqs. (20)–(22)) can arise, causing a small rate of convergence. This difficulty, which is inherent in all splitting techniques, may be overcome either by further restrictions of the permissible time variations of T_e and T_i via Δt or simply by ignoring the lack of convergence of T_e or T_i if the resulting physics is justified. These two principles have been adopted in the laser fusion calculations [9] in which a spatial variation of ϵ ranging from 10^5 (compressed, cold plasma) to 10^{-7} (tenuous plasma with hot electrons) has been encountered at a given instant.

The method described in this paper has been developed to confine the number of timesteps required to carry out plasma calculations in one space dimension without a significant increase in computing time. Although the method does make use of an exponential library function, this does not in practice inhibit its application to two- or three-dimensional calculations. The small increase in computing time arising from the evaluation of Eqs. (18)–(22) rather than the simpler explicit formulas (8) and (9) is marginal for complex calculations which treat thermal conduction, radiation, or thermonuclear burn-up of a plasma. The distinct advantage of using the expression (18) is its validity for all values of ϵ.

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