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Note

Numerical Modeling of Laser Produced Plasmas: a Second-Order Integration Scheme

I. Introduction

The possibility of using high-power lasers to initiate fusion reactions had led to much activity in the numerical modeling of the dynamics of dense, high-temperature laser produced plasmas. One problem encountered in such models is that for certain combinations of density and temperature, the time scale for the transfer of energy from the electrons to the ions is much shorter than the time scale for the transport of energy by electron thermal conductivity. This would normally preclude the use of explicit integration schemes because of the large amount of computation time required by an appropriately short time step. In this paper we demonstrate an explicit method which avoids this problem.

The hydrodynamic equations for a quasineutral plasma include a continuity equation, a momentum equation and separate energy equations for the ions and electrons which can be transformed into a composite energy equation for the mean plasma temperature and a relaxation-type equation for the temperature difference (electron minus ion temperature) [1]. Since the energy-relaxation scale appears only in the last equation, the exact form of the other three equations is not of interest to us here. The temperature-relaxation equation in normalized form is

$$\frac{\partial \overline{\Delta T}}{\partial \bar{t}} + [\bar{\mathbf{V}} \cdot \bar{\nabla} \overline{\Delta T} + \tfrac{2}{3}\overline{\Delta T}\, \bar{\nabla} \cdot \bar{\mathbf{V}}]\, \bar{t}_a^{-1} - [\bar{\nabla} \cdot (\bar{t}_{HC}^{-1} \bar{\nabla} \bar{T}_e) - \sqrt{\frac{m_e}{m_i}}\, \bar{\nabla} \cdot (\bar{t}_{HC}^{-1} \bar{\nabla} \bar{T}_i)]$$
$$= -\bar{t}_{ei}^{-1}\, \overline{\Delta T} + \overline{W}, \tag{1}$$

where $\overline{\Delta T}$ is the temperature difference normalized to a reference temperature T^*, $\bar{\mathbf{V}}$ the velocity normalized to the acoustic speed at T^*, $\bar{\nabla}$ the gradient operator normalized to a scale L^*, $\overline{W}$ a laser heating term, and $\bar{T}_e$ and $\bar{T}_i$ the normalized species temperatures. Our numerical experiments indicate that an appropriate value for L^* is 1 micron. The time scales $\bar{t}_a$, the time for a disturbance to cross L^*, $\bar{t}_{HC}$, the time for energy equilibration among the electrons in a cell of size L^*, and $\bar{t}_{ei}$ the time for energy relaxation (i.e., the equilibration of temperature) between ions and electrons have all been normalized to the laser rise time t_r.

We are particularly interested in the case

$$\bar{t}_a \gg \bar{t}_{HC} \gg \bar{t}_{ei}\,, \tag{2}$$

where [1, 2]

$$t_{HC} = 3.13 \times 10^{-18} n T_e^{-5/2},$$

$$t_{ei} = 5.31 \times 10^{2} n^{-1} T_e^{3/2},$$

$$T_e = T + \Delta T/2, \qquad T = (T_e + T_i)/2, \qquad \Delta T = T_e - T_i \tag{3}$$

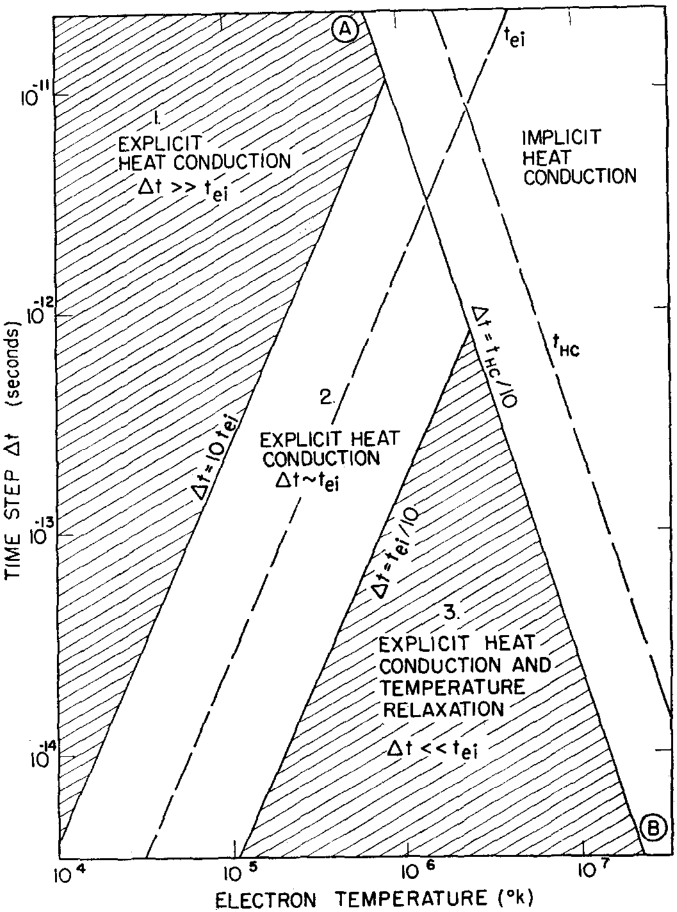

FIG. 1. Time scales as a function of electron temperature. The different types of integration required in each region are indicated.

(all units here are c.g.s.). t_{HC} and t_{ei} are shown in Fig. 1 as functions of the electron temperature (n, the number density of the electrons and ions, has been set equal to the nominal density of the dense plasmas, $4 \times 10^{22}\ \text{cm}^{-3}$). In the region to the left of $A - B$, t_a and t_{HC} are much larger than Δt, and t_{ei} becomes the most important time scale.

Our new method gives second-order accuracy in region 1 where $\Delta t \gg t_{ei}$ (effectively $\overline{\Delta T} \to 0$), in region 2 where $\Delta t \sim t_{ei}$ as well as in region 3 where $\Delta t \ll t_{ei}$ (a standard method such as Euler's would also give second-order accuracy here). The advantages of the method are that the three regions just mentioned need not be specifically identified—the method gives second-order accuracy in all of them—and that the whole region can be treated explicitly with any time step that is short enough for the explicit treatment of the electron-heat conduction. Both of these advantages result in significant savings of computer time.

II. The Second-Order Method

To illustrate the very simple ideas behind this method, we rewrite Eq. (1) as

$$(dy/d\bar{t}) + yf(y) = g, \tag{4}$$

where, for convenience, $\overline{\Delta T}$ has been replaced by y and where the other fluid variables are held constant over the time step $\Delta\bar{t}$. The $\bar{t}_{ei}$ time scale has been incorporated into $f(y)$, but the transport term $\bar{\mathbf{V}} \cdot \bar{\nabla}\, \overline{\Delta T}$ does not appear because our model uses the Fluid-in-Cell techniques of Gentry et al. [3]. Note that $\mathbf{x}$ and t never appear explicitly and that once spatial derivatives are replaced by differences, the differential equation becomes ordinary.

Expanding $f(y)$ and y into Taylor series and retaining only first-order terms, we obtain an explicit integration algorithm for Eq. (1)

$$\begin{aligned} \overline{\Delta T}(\bar{t} + \Delta\bar{t}) &= [g + y_0^2 f_y(y_0)][1 - B]/[f(y_0) + y_0 f_y(y_0)] + By_0\,, \\ B(y_0) &= \exp\{-[f(y_0) + y_0 f_y(y_0)]\,\Delta\bar{t}\}, \end{aligned} \tag{5}$$

where $y_0 = \overline{\Delta T}(\bar{t})$. The error follows directly from the remainder terms

$$E \leqslant \{\tfrac{1}{2} \max_{y_0 < \hat{y} < y} |f_{yy}(\hat{y})|\, y(y - y_0)^2 + |f_y(y_0)|\,(y - y_0)^2\}[1 - B]/[f(y_0) + y_0 f_y(y_0)] \tag{6}$$

(see Ref. [4] for an alternative derivation of the error).

From Eqs. (1) and (4), we make the identifications

$$f(y) = \bar{t}_{ei}^{-1} + \tfrac{2}{3}\bar{\nabla} \cdot \bar{\nabla}\bar{t}_a^{-1},$$
$$g = \bar{W} + \left[\bar{\nabla} \cdot (\bar{t}_{HC}^{-1}\bar{\nabla}\bar{T}_e) - \sqrt{\frac{m_e}{m_i}}\,\bar{\nabla} \cdot (\bar{t}_{HC}^{-1}\bar{\nabla}\bar{T}_i)\right], \tag{7}$$

where f, f_y and f_{yy} will all be $O(\bar{t}_{ei}^{-1})$. Although $\bar{T}_e$ and $\bar{T}_i$ can be written in terms of $\overline{\Delta T}$, the fact that the time step is small enough for an explicit representation of the heat conduction allows us to treat these two terms as part of g. Equation (7) shows that g is $O(1)$ everywhere that $\bar{t}_{HC}^{-1}$ times the normalized temperature gradient is less than one [$\bar{W} \leqslant O(1)$ already].

To estimate the magnitude of y_0, we multiply (4) by $\bar{t}_{ei}$ and obtain

$$\bar{t}_{ei}\, dy/dt + y\hat{f}(y) = \bar{t}_{ei}\, g, \tag{8}$$

where $\hat{f} = \bar{t}_{ei} f$ is $O(1)$. Since g is $O(1)$, y cannot exceed the current magnitude of $\bar{t}_{ei}$ when it is less than $O(1)$ (by current magnitude, we mean the magnitude of $\bar{t}_{ei}$ for the value of T_e being considered in Fig. 1). When $\bar{t}_{ei}$ is greater than $O(1)$, f in Eq. (4) is small so that in all cases

$$y_0 \leqslant \min[O(\bar{t}_{ei}), O(1)]. \tag{9}$$

Integration over many time steps will not effect this result because $\bar{W} \to 0$ rapidly for $\bar{t} \geqslant 2$ and all mechanisms other than laser heating tend to decrease rather than increase the temperature difference.

Since $y_0 \leqslant O(1)$, the denominator in Eq. (6) and the exponential expression in Eq. (5) can be replaced by $f(y_0)$ and the resulting ratios, f_y/f and f_{yy}/f, by constants of $O(1)$. Using the solution itself to estimate $(y - y_0)$, these changes lead to

$$E \leqslant O\{(g/f(y_0) - y_0)^2(1 - \exp[-\Delta\bar{t}f(y_0)])^3\}. \tag{10}$$

The $\bar{t}_{ei}$ dependence can be exhibited by using Eq. (9) and $f(y) \approx C\bar{t}_{ei}^{-1}$ where C is $O(1)$,

$$E \leqslant O\{\bar{t}_{ei}^2(1 - \exp[-\Delta\bar{t}C/\bar{t}_{ei}])^3\}. \tag{11}$$

To the left of $\bar{t}_{ei}$ in Fig. 1, $\Delta\bar{t} > \bar{t}_{ei}$, and Eq. (11) immediately yields $E \leqslant O(\Delta\bar{t}^2)$. In addition, a simple Taylor expansion shows that $1 - \exp\{-\Delta\bar{t}C/\bar{t}_{ei}\} \leqslant \Delta\bar{t}C/\bar{t}_{ei}$, so Eq. (11) reduces to $O[(\Delta\bar{t}/\bar{t}_{ei})\,\Delta\bar{t}^2]$. This is less than $O(\Delta\bar{t}^2)$ to the right of $\bar{t}_{ei}$ where $\Delta\bar{t} < \bar{t}_{ei}$. The single algorithm (5) is therefore second-order accurate everywhere to the left of $A - B$, and a fully explicit formulation can be used to model the dynamics of laser produced plasmas.

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