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Simultaneous Solution of Temperatures in Plasmas with Rapid Equipartition Rates

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To overcome convergence problems in numerical simulations of plasmas with high exchange rates by the Medusa code (and probably by other similar codes), a new method, which is based on simultaneous solution of all temperatures is developed. This method, which is exact and very stable does not require extra space or time per iteration, thus allowing computing time-saving by the use of larger time steps.

1. INTRODUCTION

The numerical description of a multifluid plasma often runs into difficulties when the time scale for equipartition is much shorter than that of other physical processes in the plasma. As limiting the time step δt by the equipartition time is impractical, other methods, allowing for larger δt have to be used [1, 2]. However, it turns out that some of these methods have convergence problems, that cause unphysical overshooting of the equilibrating temperatures. This happens when the equipartition rate is large, or when a large difference in the specific heat of the substances exists.

Using the Medusa [3] code we found that in some cases we had to reduce the time step considerably, in order not to get overshooting of the temperature to negative values. We believe that this shortcoming is not caused by the degree of implicitness used in the finite difference solution, or by the exact way of averaging the energy exchange during the time interval δt. The source of the problem lies in the fact that the temperatures of the ions and the electrons are solved separately. Thus, in a given iteration, the energy transferred from one fluid to another, is determined by parameters of the former iteration and not by temperatures solved in the present iteration. Being a very sensitive quantity, which depends on the difference of temperatures this term prevents the convergence of the algorithm.

In this paper we describe a different approach which solves the temperatures of the ions and electrons simultaneously. This method which requires the same

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calculation time per iteration as the former one, is stable and converges quickly, even for equipartition times much shorter than the timestep. In the next section we describe the mathematical system, the source of the problem, and a possible solution within the nonsimulataneous scheme. In Section 3 we represent the simultaneous solution of the temperatures. A simple example which demonstrates the type of problems in the original method, and the improvement caused when using the simultaneous solution, is brought in Section 4 together with our concluding remarks.

2. NUMERICAL TREATMENT OF RAPID EQUIPARTITION RATES

We write the energy balance equations of plasma composed of electrons and ions in the form

$$C_{v,i}\frac{dT_i}{dt}+\chi(T_i-T_e)=S_i, \tag{2.1}$$

$$C_{v,e}\frac{dT_e}{dt}+\chi(T_e-T_i)=S_e, \tag{2.2}$$

where $T_i(T_e)$ is the temperature, $C_{v,i}(C_{v,e})$ is the specific heat, $S_i(S_e)$ represents all the source terms except for the energy exchange term of the ions (electrons). The exchange coefficient χ is proportional to the equipartition rate $\omega \sim z^2 ln\lambda \cdot n_i T_e{}^{3/2}$ which can be taken for example from Spitzer [4].

As the source terms S_i, S_e include conductivity processes, Eqs. (2.1) and (2.2) represent (for N calculational mesh cells in one dimension) a set of $2N$ coupled equations. In the Medusa [3] the exchange term is incorporated in a certain way, to be described later, into the source term, and Eqs. (2.1), (2.2) are decoupled into two independent sets of N equations. Each set is transformed into a finite difference scheme of the type

$$A_l^n T_{l-1}^n + B_l^n T_l^n + C_l^n T_{l+1}^n = D_l^n + G_l^{n-1}, \qquad l=1, 2,.., N, \tag{2.3}$$

where upper indices denote time levels and lower indices, mesh cells. The exchange contribution is included here in D_l^n. Equation (2.3) is solved by a Gauss elimination procedure [5] which diagonalizes the three diagonal coefficient matrix.

The origin of the difficulties in treating the exchange term in Eqs. (2.1), (2.2) lies in the fact that unlike the other source terms it is determined by differences of two temperatures. Thus, even when the iterative guess of T_e, T_i has almost converged (giving approximately constant values for S_e, S_i) the difference $(T_e T_i)$ can change by orders of magnitude or even by its sign. If, moreover the coefficient χ is very large convergence problems occurs. Demanding the term $\chi(T_e T_i)$ to change only by a small amount during each time step would lead to extremely small δt, of the order of $\min(C_{v,i}/\chi, C_{v,e}/\chi)$. Thus one should look for a reasonable estimate of the contribution of this term during time intervals typical of the other processes in the system, which may be larger than the equipartition time be several orders of magnitude.

We thus transform to a new set of equations, where the problematic quantity $T_i - T_e$ is treated explicitly. Adding and subtracting Eqs. (2.1) and (2.2) from each other, we obtain after integrating over the time interval δt

$$C_{v,i}(T_i - T_{i,0}) + C_{v,e}(T_e - T_{e,0}) = (S_i + S_e)\,\delta t, \tag{2.4}$$

$$\frac{d}{dt}(T_i - T_e) + f(T_i - T_e) = g, \tag{2.5}$$

$$T_i - T_e = (T_{i,0} - T_{e,0})\,e^{-f\delta t} + \frac{g}{f}(1 - e^{-f\delta t}), \tag{2.6}$$

where the subscript 0 denote the beginning of the time step, and in performing the integration we assumed that S_i, S_e do not change much during the interval δt. The transformed source and exchanged terms in Eqs. (2.5), (2.6) are defined by

$$g = \frac{S_i}{C_{v,i}} - \frac{S_e}{C_{v,e}}, \tag{2.7}$$

$$f = \left(\frac{1}{C_{v,i}} + \frac{1}{C_{v,e}}\right)\chi. \tag{2.8}$$

In the Medusa one uses the method proposed by Christiansen and Roberts [1] and averages the exchange contribution over the interval δt, i.e.,

$$\begin{aligned}\chi(T_i - T_e) \rightarrow \chi\langle T_i - T_e\rangle &= \chi\cdot\frac{1}{\delta t}\int_0^{\delta t}(T_i(t) - T_e(t))\,dt \\ &= \frac{C_{v,i}}{1 + C_{v,i}/C_{v,e}}\left[\frac{1}{\delta t}\left(T_{i,0} - T_{e,0} - \frac{g}{f}\right)(1 - e^{-f\delta t}) + g\right],\end{aligned} \tag{2.9}$$

where g is estimated iteratively from the difference equation derived from (2.5)

$$g = [T_i - T_e - (T_{i,0} - T_{e,0})]/\delta t + f(T_i + T_{i,0} - T_e - T_{e,0})/2. \tag{2.10}$$

As was mentioned earlier, this scheme is not stable when exchange rates are high, giving rise to overshooting of the exchanged energy, as will be demonstrated in Section 4. In some cases, the simulation is terminated as negative temperatures appear during iterations.

We now present a possible way of preventing the overshooting, in a method similar to that of Ref. [2]. In this method Eqs. (2.1) and (2.2) are solved in two stages. First, we insert $\chi = 0$ and obtain a zeroth-order solution which we denote by $T_{i,B}$, $T_{e,B}$. This solution satisfies Eqs. (2.4), (2.6) in the special case were $f \to 0$, i.e.,

$$C_{v,i}(T_{i,B} - T_{i,0}) + C_{v,e}(T_{e,B} - T_{e,0}) = (S_i + S_e)\,\delta t, \tag{2.11}$$

$$T_{i,B} - T_{e,B} = T_{i,0} - T_{e,0} + g\,\delta t. \tag{2.12}$$

In practice this solution can be obtained by the usual procedure of the Medusa, applied with zero exchange. We note that when $\chi = 0$ this solution, obtained by decoupling Eq. (2.1) from (2.2) is exact. After solving this primary problem we are left with the residual problem obtained by the subtraction of (2.11) from (2.4) and (2.12) from (2.6),

$$C_{v,i}(T_i - T_{i,B}) + C_{v,e}(T_e - T_{e,B}) = 0, \tag{2.13}$$

$$T_i - T_e = T_{i,B} - T_{e,B} + (T_{i,0} - T_{e,0})(e^{-f\delta t} - 1) + \frac{g\,\delta t}{f\,\delta t}(1 - e^{-f\delta t} - f\,\delta t). \tag{2.14}$$

Denoting the right-hand side of (2.14) by P we obtain

$$T_i = (Q + C_{v,e}P)/(C_{v,i} + C_{v,e}), \tag{2.15}$$

$$T_e = (Q - C_{v,i}P)/(C_{v,i} + C_{v,e}), \tag{2.16}$$

with

$$Q = C_{v,i}T_{i,B} + C_{v,e}T_{e,B}. \tag{2.17}$$

The source term g which enters the solution through P is determined self consistently with the known solution of (2.12), which means that in calculating P we substitute.

$$g\,\delta t = T_{iB} - T_{eB} - (T_{i0} - T_{e0}). \tag{2.18}$$

For any value of f and δt this solution behaves as expected from physical intuition. When the exchange rate is very small $f\,\delta t \to 0$, $P \to T_{i,B} - T_{e,B}$ so that $T_i \to T_{i,B}$, $T_e \to T_{e,B}$ giving the exact solution of the problem, where there is no exchange. In the opposite limit of high exchange rates $f\,\delta t \to \infty$, $P \to T_{i,B} - T_{e,B} - (T_{i,0} - T_{e,0}) - g\,\delta t = 0$, and we get

$$T_i = T_e = (C_{v,i}T_{i,B} + C_{v,e}T_{e,B})/(C_{v,i} + C_{v,e}) \tag{2.19}$$

which describes a thermal equilibrium with a final temperature that conserves the total energy. Thus, even for an infinite exchange rate, or very long time steps, overshooting cannot occur, and we get just the expected equalization of the ions and electrons temperature.

This model would have been exact if we were dealing with a single cell, or if there was no conductivity. However, when we have a strong exchange, the solution to the conductivity problem, obtained by the implicit sweep over cells in (2.11), (2.12), deviates from the exact solution. The temperature T_B in cell l should be determined recursively from the exact temperature T in cell $l+1$ and not from the intermediate temperature T_B in this cell. Again, the method described in (2.11), (2.12) is not solving the set of $2N$ coupled equations, that is our real problem.

However, there is no need for approximations in solving (2.1), (2.2) as the set of $2N$ equations can be solved simultaneously and exactly. This solution is presented in the following section.

3. Simultaneous Solution of the Ions and Electrons Temperature

As a difference equations with the time centering system adopted in the Medusa (source terms defined as averages of their values at times t^{n-1}, t^n) we write Eqs. (2.1) and (2.2) in the form (omitting cell indices for brevity):

$$\begin{aligned} &T_i^n(C_{v,i}^{n-(1/2)} + \tfrac{1}{2}\chi^n\,\delta t)/\delta t - \tfrac{1}{2}\chi^n T_e^{n-(1/2)} S_i^n \\ &\quad = \tfrac{1}{2}S_i^{n-1} + C_{v,i}^{n-(1/2)} T_i^{n-1}/\delta t + \tfrac{1}{2}\chi^{n-1}(T_e^{n-1} - T_i^{n-1}), \qquad (3.1) \\ &T_e^n(C_{v,e}^{n-(1/2)} + \tfrac{1}{2}\chi^n\,\delta t)/\delta t - \tfrac{1}{2}\chi^n T_i^n - \tfrac{1}{2}S_e^n \\ &\quad = \tfrac{1}{2}S_e^{n-1} + C_{v,e}^{n-(1/2)} T_e^{n-1}/\delta t + \tfrac{1}{2}\chi^{n-1}(T_i^{n-1} - T_e^{n-1}), \qquad (3.2) \end{aligned}$$

where the upper indices denote time steps t^n, t^{n-1} and $t^{n-(1/2)} = \frac{1}{2}(t^{n-1} + t^n)$. The heat conduction terms in S_i, S_e couples each cell to its neighbours so that Eqs. (3.1), (3.2) can be arranged in the form

$$A_{i,l}^n T_{i,l-1}^n + B_{i,l}^n T_{i,l}^n + C_{i,l}^n T_{i,l+1}^n + EX_l T_{e,l}^n = D_{i,l}^n + G_{i,l}^{n-1}, \qquad (3.3)$$

$$A_{e,l}^n T_{e,l-1}^n + B_{e,l}^n T_{e,l}^n + C_{e,l}^n T_{e,l+1}^n + EX_l T_{i,l}^n = D_{e,l}^n + G_{e,l}^{n-1}, \qquad (3.4)$$

where the lower indices, $l-1$, l, $l+1$ indicate different mesh cells and $EX_l = -\frac{1}{2}\chi_l$. The correlation with the original notation of the Medusa represented by Eq. (2.3) is obtained by setting the exchange contribution in D_e, D_i to zero and transforming

$$\begin{aligned} B_{i,l}^n &\to B_{i,l}^n + \tfrac{1}{2}\chi_l^n\,\delta t, \\ B_{e,l}^n &\to B_{e,l}^n + \tfrac{1}{2}\chi_l^n\,\delta t, \\ G_{i,l}^{n-1} &\to G_{i,l}^{n-1} + \tfrac{1}{2}\chi_l^{n-1}\,\delta t(T_{e,l}^{n-1} - T_{i,l}^{n-1}), \\ G_{e,l}^{n-1} &\to G_{e,l}^{n-1} + \tfrac{1}{2}\chi_l^{n-1}\,\delta t(T_{i,l}^{n-1} - T_{e,l}^{n-1}). \end{aligned} \qquad (3.5)$$

From test runs that were performed we came to the conclusion that the scheme is more stable when the exchange term is treated fully implicitly as $\chi^n(T_i^n - T_e^n)$ and not as an average of contributions at times t^n and t^{n-1}. In this approach the exchange terms at the right hand side of Eqs. (3.1), (3.2) (with χ^{n-1}) appear in the left side. All the former and later to come algebra remains the same if we define in (3.3), (3.4) $EX_l = -\chi_l$ and change the transformation (3.5) to

$$\begin{aligned} B^n_{i,l} &\to B^n_{i,l} + \chi^n_l\,\delta t, \\ B^n_{e,l} &\to B^n_{e,l} + \chi^n_l\,\delta t, \end{aligned} \tag{3.5'}$$

with no changes in $G^{n-1}_{i,l}$, $G^{n-1}_{e,l}$.

The stability of this implicit scheme is independent on the specific way in which χ_l is averaged over the interval δt. Unlike the general approach adopted in the Medusa which averages values of χ at the ends of the time interval.

$$\chi_l = \tfrac{1}{2}[\chi(T^n_{i,l}, T^n_{e,l}) + \chi(T^{n-1}_{i,l}, T^{n-1}_{e,l})] \tag{3.6}$$

we prefer to calculate χ at the averaged temperatures of this time step:

$$T^{n-(1/2)} = \tfrac{1}{2}(T^{n-1} + T^n), \tag{3.7}$$

$$\chi_l = \chi(T^{n-(1/2)}_{i,l}, T^{n-(1/2)}_{e,l}). \tag{3.8}$$

Let us return now to the solution of Eqs. (3.3), (3.4). We arrange the $2N$ unknown temperatures in the following order:

$$T^n_{i,1}, T^n_{e,1}, T^n_{i,2}, T^n_{e,2}, \ldots, T^n_{i,N}, T^n_{e,N}.$$

For this arrangement the coefficients matrix contains nonzero elements only in the main diagonal, in the two nearest diagonals above it and in the two nearest diagonals below it. This five diagonal matrix can be easily diagonalized by the Gauss elimination procedure.

We write Eqs. (3.3), (3.4) as

$$A_L T_{L-2} + XL_L T_{L-1} + B_L T_L + XR_L T_{L+1} + C_L T_{L+2} = D_L + G_L, \tag{3.9}$$

where $T_{i,l}$ is now called $T_{L=2l-1}$ and $T_{e,l}$ is called $T_{L=2l}$. The exchange terms to the left and right directions XL and XR, respectively are equal to zero or to $EX_l \cdot \delta t$ depending on the pairity of L.

We search for a solution of (3.9) in the form

$$T_L = F_L - E_L T_{L+2} + \beta_L T_{L+1}. \tag{3.10}$$

Inserting (3.10) into (3.9) for T_{L-2}, T_{L-1} we obtain an equation that contains only T_L, T_{L+1} and T_{L+2}, which is now compared to (3.10) to give explicit expressions for F_L, E_L, and β_L:

$$\begin{aligned} E_L &= C_L/Z_L, \\ F_L &= [D_L + G_L - A_L F_{L-2} - (A_L\beta_{L-2} + XL_L) F_{L-1}]/Z_L, \\ \beta_L &= [E_{L-1}(A_L\beta_{L-2} + XL_L) - XR_L]/Z_L, \\ Z_L &= B_L - A_L E_{L-2} + \beta_{L-1}(A_L\beta_{L-2} + XL_L). \end{aligned} \tag{3.11}$$

Expressing this result by the variables of the original ion-electron system we obtain for an odd L

$$T_{i,l} = F_{i,l} - E_{i,L} T_{i,l+1} + \beta_{i,l} T_{e,l} \tag{3.12}$$

with

$$\begin{aligned} Z_{i,l} &= B_{i,l} - A_{i,l} E_{i,l-1} + \beta_{e,l-1} A_{i,l} \beta_{i,l-1}, \\ E_{i,l} &= C_{i,l} / Z_{i,l}, \\ F_{i,l} &= (D_{i,l} + G_{i,l} - A_{i,l} F_{i,l-1} - F_{e,l-1} A_{i,l} \beta_{i,l-1}) / Z_{i,l}, \\ \beta_{i,l} &= (E_{e,l-1} A_{i,l} \beta_{i,l-1} - EX_l \, \delta t) / Z_{i,l}, \end{aligned} \tag{3.13}$$

and for an even L

$$T_{e,l} = F_{e,l} - E_{e,l} T_{e,l+1} + \beta_{e,l} T_{i,l+1}, \tag{3.14}$$

with

$$\begin{aligned} Z_{e,l} &= B_{e,l} - A_{e,l} E_{e,l-1} + \beta_{i,l} (A_{e,l} \beta_{e,l-1} + EX_l \, \delta t), \\ E_{e,l} &= C_{e,l} / Z_{e,l}, \\ F_{e,l} &= [D_{e,l} + G_{e,l} - A_{e,l} F_{e,l-1} - F_{e,l} (A_{e,l} \beta_{e,l-1} + EX_l \, \delta t)] / Z_{e,l}, \\ \beta_{e,l} &= E_{i,l} (A_{e,l} \beta_{e,l-1} + EX_l \, \delta t) / Z_{e,l}. \end{aligned} \tag{3.15}$$

When there is no exchange $EX_l = 0$, all the $\beta_{e,l}$, $\beta_{i,l}$ vanish and this scheme coincides with the original decoupled solution of the Medusa when there is no exchange.

The simultaneous solution is thus obtained as follows:

First, we cancel the original exchange term appearing in the Medusa in the D_e, D_i source terms. Then we correct for the coefficients B and G using Eq. (3.5) or (3.5′) according to the degree of implicity used. Using (3.5′) is recommended and then only B_e, B_i have to be modified. Now we calculate the terms in (3.13) and (3.15) in increasing order of l, while for $l = 1$ we have

$$\begin{aligned} Z_{i,1} &= B_{i,1}; & E_{i,1} &= C_{i,1} / Z_{i,1}, \\ F_{i,1} &= (D_{i,1} + G_{i,1}) / Z_{i,1}; & \beta_{i,1} &= -EX_1 \, \delta t / Z_{i,1}, \end{aligned} \tag{3.16}$$

$$\begin{aligned} Z_{e,1} &= B_{e,1} + EX_1 \, \delta t \beta_{i,1}; & E_{e,1} &= C_{e,1} / Z_{e,1}, \\ F_{e,1} &= (D_{e,1} + G_{e,1} - F_{i,1} EX_1 \, \delta t) / Z_{e,1}; & \beta_{e,1} &= E_{i,1} EX_1 \, \delta t / Z_{e,1}. \end{aligned} \tag{3.17}$$

The temperatures are finally obtained in decreasing order of l from eqs. (3.14) and (3.12) with

$$T_{e,N} = F_{e,N}; \qquad T_{i,N} = F_{i,N} + \beta_{i,N} T_{e,N}. \tag{3.18}$$

The boundary conditions (3.16)–(3.18) apply for a system that is thermally isolated with $A_{i,1} = A_{e,1} = C_{i,N} = C_{e,N} = 0$. If for example we allow heat flux from the right boundary coming from a heat source of temperature T_{N+1}, we can still use the same expressions but with the modification

$$\begin{aligned} D_{i,N} &\rightarrow Di,N - C_{i,N} T_{i,N+1}, \\ D_{e,N} &\rightarrow D_{e,N} - C_{e,N} T_{e,N+1} + \beta_{e,N} Z_{e,N} T_{i,N+1}. \end{aligned} \tag{3.19}$$

We conclude this section with a final remark about the accuracy obtained by the proposed procedure. With this stable scheme it is possible to start the calculations at the required room temperature (having an appropriate equation of state in this region). With such low temperatures the exchange rate ($\sim T_e^{-1.5}$) is extremely large. Thus it may happen that the extra term $\chi_l\, \delta t$ in Eq. (3.5′) is several orders of magnitude larger than the original B term. In a 32 bit computer like the one at the University of Alberta the final temperatures, obtained after back and forth sweeps of length $2N$ with many adding and subtractions of large terms, are slowly changing in time due to round of errors. We strongly recommend to make the sweeps of Eqs. (3.12)–(3.15) with double precision. This of course should be followed by calculating (3.5′) too with double precision, and this can be done most conveniently by executing (3.5′) within the Gauss elimination subroutine. When we did this the obtained temperatures were exact and the solution was stable even for extremely high exchange rates.

4. Discussion and Results

The simultaneous solution of the ions and electrons temperature was introduced into the Medusa code and several test cases of its applicability were performed. We find that it is now possible to largely increase the time steps and yet obtain convergence. If before we had, in some problems, to restrict the allowed changes in temperatures in a cell to 2% per time step, we are now able to work with 25% change per step. This becomes really important when one wishes to start the simulation with the experimental initial room temperature.

As an illustration of the problems with the original scheme, and the way it is cured by the simultaneous solution, we describe a very simple test case. A homogeneous confined *Al* plasma is initially composed of 1000 eV electrons and 1 eV ions. There is no laser source, no radiation emission and transport, and no conductivity as the plasma is homogeneous and is not allowed to move. The only relevant process is the equilibration which tends to equate the temperatures to a final value, which is determined by the specific heat ratio between ions and electrons.

In Fig. 1 we plot the temperatures as a function of time (on a logarithmic scale) as obtained by three different calculations. The time steps in each calculation are so determined that the temperature change in each cell will not exceed 25% per time

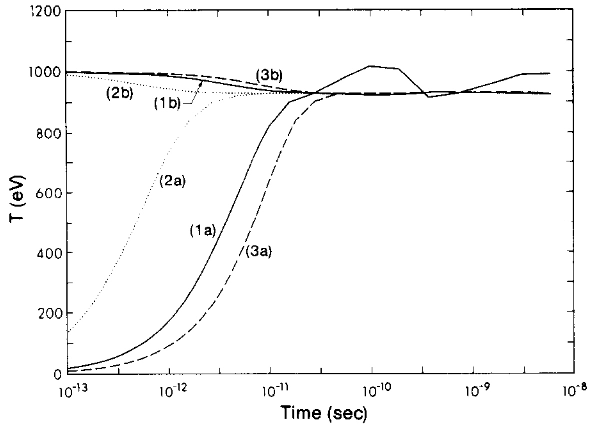

FIG. 1. Temperatures as a function of time for the test case described in Section 4. (a) ions temperature; (b) electrons temperature; (1) (—) nonsimultaneous solution; (2) (···) simultaneous solution with Spitzer's exchange; (3) (---) simultaneous solution with effective exchange rate similar to that of (1).

step. The solid lines (1a) and (1b) represent the ions and electrons temperatures, respectively, as calculated by the original scheme. As the specific heat of the ions is smaller that that of the many free electrons, we get a strong overshoot (of almost 100 eV) of the ion temperature beyond that of the electrons. This is followed by an oscillatory behaviour as a result of other overshootings in the equilibration process. The electron temperature is also oscillating, though this is not clearly seen on the scale of the figure.

The dotted curves (2a), (2b) represent the results of the simultaneous solution when the Spitzer expression for the exchange rate is used. Though the equilibration is much faster, there is no overshooting or oscillations as both the ions and the electrons approach the final temperature.

The different behaviour of the two models is not caused by the numerics, but mainly by the averaging procedure (2.9) used in the original scheme. If this effective reduction of the exchange rates was not performed, the convergence would become even worse. On the other hand, the convergence of the simultaneous solution is not sensitive to the specific form of the exchanged rates, and we are free to choose any model according to physical considerations. The dashed lines (3a), (3b) in Fig. 1 represent a try to imitate the exchange rates used by the Medusa, within the simultaneous solution by defining the effective exchange rate

$$\chi_{eff} = \chi \langle T_i - T_e \rangle / (T_i - T_e), \tag{4.1}$$

where the denominator is taken from the Medusa as in (2.9) and $T_i - T_e$ in the denominator is calculated from a former iteration. As expected the curves (3a), (3b) are close to (2a), (2b), but do not exhibit the oscillatory behaviour, because of the more exact and stable nature of the simultaneous solution.

In conclusion we want to point out that the method can be extended to more complicated plasmas. For example, one can wish to describe relaxation processes between ions, electrons and a radiation field [6]. In this case the five diagonal matrix of Eq. (3.9) is replaced by a seven diagonal matrix, the diagonalization of which in the Gauss elimination procedure is also straightforward, with somewhat more lengthy algebra. In this case the overshooting problem can become a severe limitation, when a relatively low temperature radiation field, which has a very low specific heat, tries to raise the temperature of the electrons with higher specific heat, a situation that might cause an overshooting of the radiation temperature to negative values.

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