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Using Tabular EOS at Low Temperatures

R. A. Managan

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Disclaimer

Using Tabular EOS at Low Temperatures (U)

[1]**Robert A. Managan**
[1]*Lawrence Livermore National Laboratory, Livermore, CA*

Abstract

In multi-physics hydro-codes there are many algorithms that update the internal energy of a zone. It is the job of the equation of state to take this new internal energy and calculate a new temperature. When the physics of the problem requires that the code use separate electron and ion temperatures problems can arise when determining the new temperature. This is due to the fact that in the LEOS tables the electron energy is zero until there are free electrons while the algorithms that couple energy into the electrons generally assume a plasma and don't account for whether the electrons are bound or free.

A new approach for dealing with these issues is presented that avoids discontinuous jumps in the electron temperature. It does this by smoothly switching from a total energy solution to separate temperature updates for electrons and ions. (U)

Introduction

The Livermore Equation of State (LEOS) tables are built with separate tables for the cold, electron, and ion values. These three tables are also combined into a table for the total values. When a multi-physics code is run in a mode that has separate electron and ion temperatures we need to use the separate tables for the EOS. However, most multi–physics codes are based on algorithms that are derived in the plasma physics regime and make different assumptions in the low temperature limit than the EOS tables do. In particular the table's electron energy is zero at low temperatures until there are free electrons, but the radiation–electron coupling transfers energy to the electrons without ionizing them. The result is that once a little energy is put in to the electron field the electron temperature jumps up only to drop the next cycle when the electron energy is coupled to the ions.

The original algorithm for updating the temperature is to iterate on the temperature until the energy we look up matches the energy of the zone. These equations are used in every iteration to solve for the updates to the electron and ion temperatures:

$$E_e = E'_e(T_e) + \frac{\partial E'_e}{\partial T}\Delta T_e \tag{1}$$

$$E_i = E_i'(T_i) + \frac{\partial E_i'}{\partial T}\Delta T_i \tag{2}$$

where E is the zone's internal energy we want to match, E' is the energy evaluated at the current guess for the temperature, and ΔT is the update to the temperature. The iteration proceeds until ΔT becomes small enough.

Take an ignition NIF capsule as an example. It starts at cryogenic temperatures but the simulation is run with separate electron and ion temperatures since that is required when the fuel is burning. Fig. 1 shows the electron temperature for a point in the outer half of the ablator. As the radiation heats the electrons the temperature jumps up to temperatures between 6×10^{-7} to 1×10^{-5} keV and then gets pulled back down by electron-ion coupling. Clearly the simple iteration defined by equations 1 and 2 is inadequate and needs to be improved.

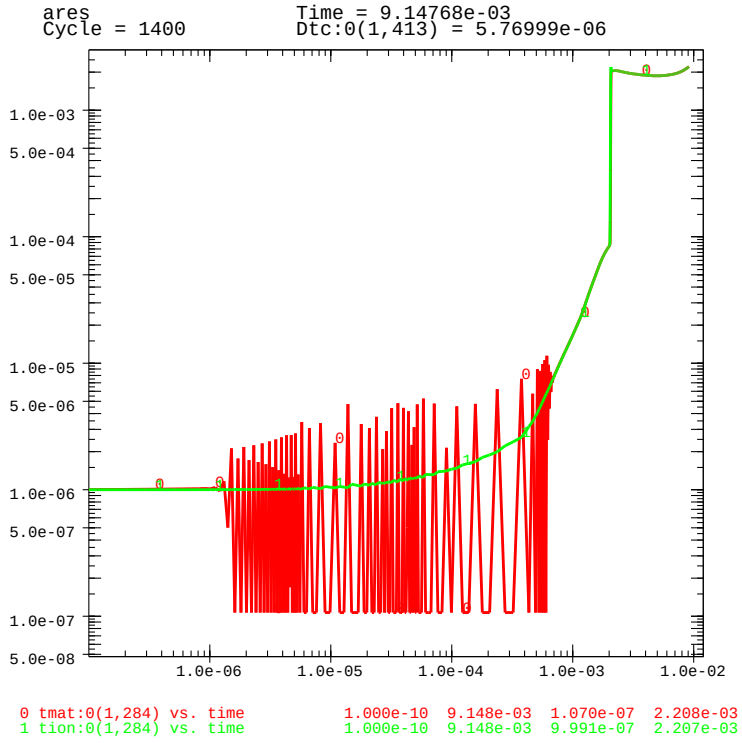

Figure 1: Electron temperature in the outer ablator using the old algorithm.

The Algorithm

The new method uses an interpolating function $f(T) = 2^{-(T/T_0)^2}$ to switch from iterating on the total energy to iterating on the separate electron and ion energies. Currently T_0, the "half-way" temperature, is chosen to be 5×10^{-3} keV a temperature at which all materials have begun to ionize and have non-zero

electron energies. Different forms for the interpolating function or different values of T_0 could be used but this choice appears to be adequate.

The temperature updates are calculated using these effective energies:

$$E_e^* = \frac{E_e + f(T_e)\,(E_i + E_c)}{1 + f(T_e)} \tag{3}$$

$$E_i^* = \frac{f(T_e)E_e + (E_i + E_c)}{1 + f(T_e)} \tag{4}$$

At low temperatures $f(T_e) \simeq 1$ so $E_e^* \simeq E_i^*$ and both are equal to the half of the total internal energy. At high temperatures they are equal to the electron and ion energies respectively, where the ion energy includes the cold energy. For updating temperatures we consider E_e^* as a function only of T_e and E_i^* as a function only of T_i. This results in using these equations to solve for ΔT_e and ΔT_i:

$$\begin{aligned} E_e^* = & \frac{E_e' + f(T_e)\,(E_i' + E_c)}{1 + f(T_e)} + \\ & \frac{1}{1 + f(T_e)} \left\{ \frac{\partial E_e'}{\partial T_e} + \frac{df}{dT_e} \left[E_i' + E_c - \frac{E_e' + f\,(E_i' + E_c)}{1 + f(T_e)} \right] + f(T_e) \frac{\partial E_i'}{\partial T_i} \right\} \Delta T_e \end{aligned} \tag{5}$$

$$\begin{aligned} E_i^* = & \frac{f(T_e)E_e' + E_i' + E_c}{1 + f(T_e)} + \\ & \frac{1}{1 + f(T_e)} \left[f(T_e) \frac{\partial E_e'}{\partial T_e} + \frac{df}{dT_e} \left(E_e' - \frac{f E_e' + E_i' + E_c}{1 + f(T_e)} \right) + \frac{\partial E_i'}{\partial T_i} \right] \Delta T_i \end{aligned} \tag{6}$$

Using equations 3 and 4 we can rewrite these as:

$$\frac{E_e - E_e' + f(T_e)\,(E_i - E_i')}{1 + f} = \frac{1}{1 + f} \left\{ \frac{\partial E_e'}{\partial T_e} + \frac{df}{dT_e} \left[E_i' + E_c - \frac{E_e' + f\,(E_i' + E_c)}{1 + f} \right] + f \frac{\partial E_i'}{\partial T_i} \right\} \Delta T_e$$

$$\frac{f(T_e)(E_e - E_e') + E_i - E_i'}{1 + f} = \frac{1}{1 + f} \left[f \frac{\partial E_e'}{\partial T_e} + \frac{df}{dT_e} \left(E_e' - \frac{f E_e' + E_i' + E_c}{1 + f} \right) + \frac{\partial E_i'}{\partial T_i} \right] \Delta T_i$$

which can be simplified to:

$$\frac{E_e - E_e' + f(T_e)\,(E_i - E_i')}{1 + f(T_e)} = \frac{1}{1 + f(T_e)} \left[\frac{\partial E_e'}{\partial T_e} - \frac{df}{dT_e} \frac{E_e' - (E_i' + E_c)}{1 + f(T_e)} + f(T_e) \frac{\partial E_i'}{\partial T_i} \right] \Delta T_e \tag{7}$$

$$\frac{f(T_e)(E_e - E_e') + E_i - E_i'}{1 + f(T_e)} = \frac{1}{1 + f(T_e)} \left[f(T_e) \frac{\partial E_e'}{\partial T_e} + \frac{df}{dT_e} \frac{E_e' - (E_i' + E_c)}{1 + f(T_e)} + \frac{\partial E_i'}{\partial T_i} \right] \Delta T_i \tag{8}$$

After each iteration E_e' and E_i' are evaluated using the current estimate of T_e and T_i respectively. The right hand sides of equations 7 and 8 are effective electron and ion heat capacities. These are not used elsewhere in the code.

The sum of Eqs. 5 and 6 gives the total energy and guarantees that as the ΔT's go to zero the total energy is preserved. Of course, when $f(T) \to 0$ for large temperatures, the temperature updates are independent

and the same as before. When $f(t) \to 1$ for small temperatures, the two temperature updates are the same and the electron and ion temperatures move up or down together preserving any difference there is between them.

When we apply this method for updating the temperature to the same NIF capsule as in Fig. 1 we get the result in Fig. 2. The oscillations are gone and while a small temperature difference shows up it is never large. Similar results are shown in figures 3 and 4 for a point in the inner half of the ablator.

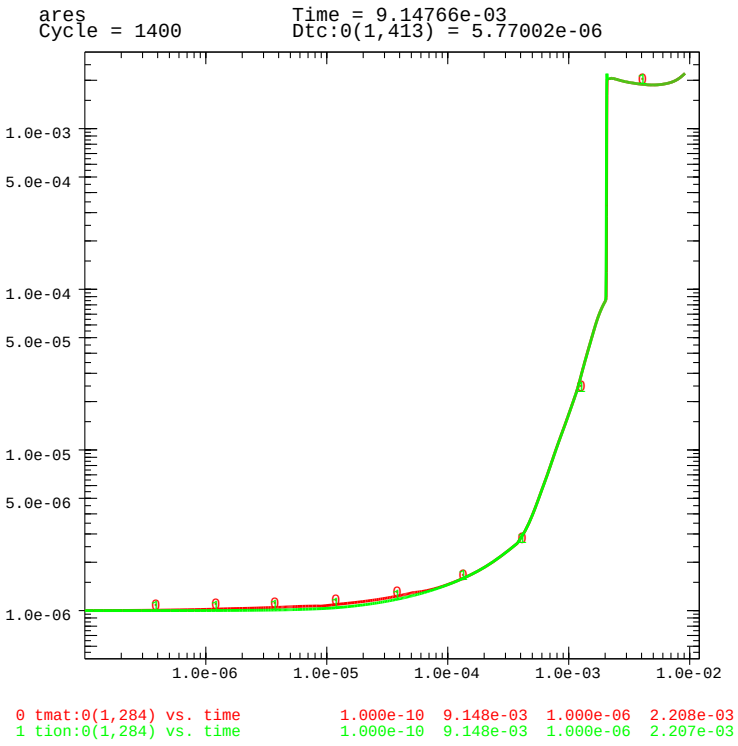

Figure 2: Electron temperature in the outer ablator using the new algorithm.

What did not work

Mathematically the updates for E_e^* and E_i^* should each depend on both ΔT_e and ΔT_i. This gives a two equation system to be solved for the temperature updates ΔT_e and ΔT_i.

$$E_e^* = \frac{E_e' + f(T_e)\,(E_i' + E_c)}{1+f} + \frac{f}{1+f}\frac{\partial E_i}{\partial T_i}\Delta T_i + \frac{1}{1+f}\left\{\frac{\partial E_e}{\partial T_e} + \frac{df}{dT_e}\left[E_i' + E_c - \frac{E_e' + f\,(E_i' + E_c)}{1+f}\right]\right\}\Delta T_e \tag{9}$$

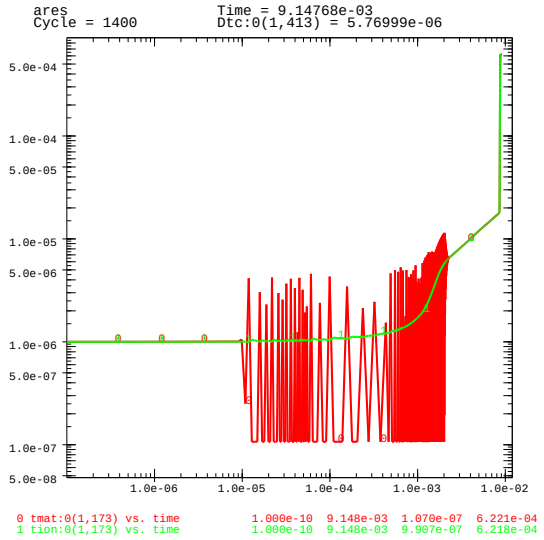

Figure 3: Electron temperature in the inner ablator using the old algorithm.

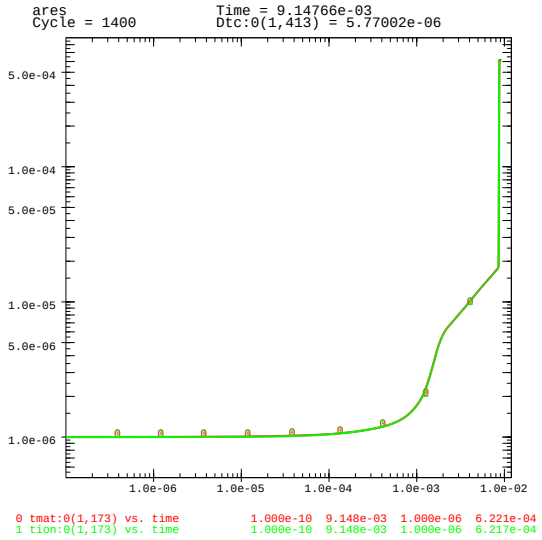

Figure 4: Electron temperature in the inner ablator using the new algorithm.

$$E_i^* = \frac{f(T_e)E_e' + E_i' + E_c}{1+f} + \frac{1}{1+f}\frac{\partial E_i}{\partial T_i}\Delta T_i + \frac{1}{1+f}\left[f(T_e)\frac{\partial E_e}{\partial T_e} + \frac{df}{dT_e}\left(E_e' - \frac{fE_e' + E_i' + E_c}{1+f}\right)\right]\Delta T_e \tag{10}$$

Using equations 3 and 4 and simplifying, equations 9 and 10 can be rewritten as:

$$\frac{E_e - E_e' + f(T_e)\left(E_i - E_i'\right)}{1+f} = \frac{f}{1+f}\frac{\partial E_i}{\partial T_i}\Delta T_i + \frac{1}{1+f}\left\{\frac{\partial E_e}{\partial T_e} + \frac{df}{dT_e}\frac{E_i' + E_c - E_e'}{1+f}\right\}\Delta T_e \tag{11}$$

$$\frac{f(T_e)(E_e - E_e') + E_i - E_i'}{1+f} = \frac{1}{1+f}\frac{\partial E_i}{\partial T_i}\Delta T_i + \frac{1}{1+f}\left[f(T_e)\frac{\partial E_e}{\partial T_e} + \frac{df}{dT_e}\frac{E_e' - E_i' - E_c}{1+f}\right]\Delta T_e \tag{12}$$

This version of the algorithm suffers from an instability similar to the original algorithm since $\frac{\partial E_e}{\partial T_e} = 0$ at low temperatures when $E_e \equiv 0$ because there are no free electrons. When coupled with the fact that $\frac{df}{dT_e} \to 0$ at low temperatures the coefficient of $\Delta T_E \to 0$ leaving the system of equations ill defined.

Conclusion

A new method for updating the temperature from the internal energy when there are separate electron and

ion temperatures has been described. At low temperatures this method uses a total energy update that applies equal increments to the electron and ion temperatures. At high temperatures the electron and ion temperatures are updated independently based on the electron and ion internal energies. The method switches between these two limits with a smooth interpolation function. Using this method has removed one source of numerical noise from calculations of NIF implosions.

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