LA-UR-16-27664
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Title: The “2T” ion-electron semi-analytic shock solution for code-comparison with xRAGE: A report for FY16

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Intended for: Report

Issued: 2016-10-05

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1. Introduction

This report documents an effort to generate the semi-analytic "2T" ion-electron shock solution developed in the paper by Masser, Wohlbier, and Lowrie [1], and the initial attempts to understand how to use this solution as a code-verification tool for one of LANL's ASC codes, xRAGE. Most of the work so far has gone into generating the semi-analytic solution. Considerable effort will go into understanding how to write the xRAGE input deck that both matches the boundary conditions imposed by the solution, and also what physics models must be implemented within the semi-analytic solution itself to match the model assumptions inherit within xRAGE. Therefore, most of this report focuses on deriving the equations for the semi-analytic 1D-planar time-independent "2T" ion-electron shock solution, and is written in a style that is intended to provide clear guidance for anyone writing their own solver.

2. Introduction to the physical model and its equations

In this Section, the physical model and subsequent equations used in [1] are collected and briefly compared with the model developed in xRAGE. In contradistinction to the semi-analytic radiative shock solutions by Lowrie and Rauenzahn [2], and Lowrie and Edwards [3], these semi-analytic equations do not need to be nondimensionalized because they do not contain multiple different dimensional scalings (e.g., the speed of sound and the speed of light), and so nondimensionalizing the equations and redimensionalizing them can be done without defining any extra parameters. The ion-electron model presented in [1] assumes that the fluid is a fully-ionized hydrodynamic plasma, with electron heat-conduction ($\kappa_e \partial_x T_e$) and separate temperatures for the electrons (T_e) and ions (T_i), that can be described by Eulerian hydrodynamics in 1D,

$$\partial_t \rho + \partial_x (\rho u) = 0 \,, \tag{1a}$$

$$\partial_t (\rho u) + \partial_x \left(\rho u^2 + p\right) = 0 \,, \tag{1b}$$

$$\partial_t \left(\frac{1}{2}\rho u^2 + \rho e\right) + \partial_x \left[u\left(\frac{1}{2}\rho u^2 + \rho e + p\right)\right] = \partial_x \left(\kappa_e \partial_x T_e\right) \,, \tag{1c}$$

along with an internal energy equation for the electrons, which couples the electron and ion temperatures

$$\partial_t (\rho e) + \partial_x (\rho u e_e) + p_e \partial_x u = \gamma_{ei} (T_i - T_e) + \partial_x \left(\partial_x T_e\right) \,, \tag{1d}$$

where κ_e is the electron thermal-diffusivity, and γ_{ei} is the electron-ion coupling coefficient. All other variables have their standard hydrodynamic meaning. Variables with either a subscripted "e" or "i" represent the "electron" or "ion" component for the given variable, and variables without a subscript represent the material value for the given variable. The material pressure is the sum of the electron and ion pressures, $p = p_e + p_i$, and the material internal energy is the sum of the electron and ion internal energies, $e = e_e + e_i$. For convenience, an ideal-gas equation-of-state (EOS) was used in [1]

$$p = \rho e \,(\gamma - 1) \quad \& \quad e = C_v T \,, \tag{2}$$

Thus, the separate electron and ion internal energies can be determined

$$\begin{aligned} e = C_v T = C_{ve} T_e + C_{vi} T_i = e_e + e_i \,, \\ \Rightarrow e_e = C_{ve} T_e \quad \& \quad e_i = C_{vi} T_i \,, \end{aligned} \tag{3}$$

where $C_{ve} = Z/(Z+1)$, $C_{vi} = 1/(Z+1)$, Z represents the number of electrons in the fully-ionized plasma, and the assumption of an ideal-gas EOS makes the bulk specific heat equal to $C_v = [\gamma(\gamma-1)]^{-1}$. Similarly, the separate electron and ion pressures can be determined

$$\begin{aligned} p = \rho(e_e + e_i)(\gamma-1) = \rho e_e(\gamma-1) + \rho e_i(\gamma-1) = p_e + p_i\,, \\ \Rightarrow p_e = \rho e_e(\gamma-1) \quad \& \quad p_i = \rho e_i(\gamma-1)\,. \end{aligned} \tag{4}$$

Finally, the sound speed can be written as

$$c = \sqrt{\frac{\gamma p}{\rho}} = \sqrt{\gamma(\gamma-1)\,e} = \sqrt{\gamma(\gamma-1)\,C_v T} = \sqrt{T}\,, \tag{5}$$

which motivates the following useful expressions for the local Mach number

$$\mathcal{M}^2 = \frac{u^2}{c^2} = \frac{u^2}{T} = \frac{\mathcal{M}_0^2}{\rho^2 T}\,. \tag{6}$$

The last expression has made use of the definition of the initial Mach number, $\mathcal{M}_0 = \rho u$, which is rederived below.

3. Some similarities and distinctions between the this physical model and xRAGE

As described in the xRAGE User's Manual, most EOS data is the for the bulk material properties and does not apply directly to either the EOS for the electrons and ions separately. In this case a "Z-split" EOS can be used in xRAGE. The EOS for the bulk material is assumed to be well represented as functions of the material mass density and the material temperature, such that $e = e(\rho, T)$ and $p = p(\rho, T)$, and for a "Z-split" EOS these relations become

$$e_e = \frac{Z}{Z+1} e(\rho, T_e) \quad \& \quad e_i = \frac{1}{Z+1} e(\rho, T_i) \quad \text{and}\,, \tag{7a}$$

$$p_e = \frac{Z}{Z+1} p(\rho, T_e) \quad \& \quad p_i = \frac{1}{Z+1} p(\rho, T_i)\,. \tag{7b}$$

The separate electron and ion equations for the internal energy (2) and pressure (2), developed above to describe the semi-analytic solution, can also be written in the form of a Z-split EOS

$$e_e = C_{ve} T_e = \frac{C_{ve}}{C_v} C_v T_e = \frac{Z}{Z+1} e(\rho, T_e)\,, \tag{8a}$$

$$p_e = \rho e_e(\gamma-1) = \frac{Z}{Z+1} \rho e(\rho, T_e)(\gamma-1) = \frac{Z}{Z+1} p(\rho, T_e)\,, \tag{8b}$$

$$e_i = C_{vi} T_i = \frac{C_{vi}}{C_v} T_i = \frac{1}{Z+1} e(\rho, T_i)\,, \tag{8c}$$

$$p_i = \rho e_i(\gamma-1) = \frac{Z}{Z+1} \rho e(\rho, T_i)(\gamma-1) = \frac{Z}{Z+1} p(\rho, T_i)\,. \tag{8d}$$

However, in addition to the electron internal energy equation and the electron thermal-diffusivity, xRAGE also solves the ion internal energy equation, includes the ion heat-conduction term where appropriate and thus also defines an ion thermal-diffusivity. It is not clear yet if the semi-analytic solutions presented in [1] can be extended to include these terms. Currently, we are at the initial stages of understanding and building the relevant xRAGE input deck. Other model similarities and distinctions will become evident as the xRAGE code team is consulted more, especially as it applies to the electron thermal-diffusivity and the electron-ion coupling parameter.

4. The equations used and their results

The solution procedure developed here closely follows the method developed by Lowrie and Edwards [3] for obtaining semi-analytic radiative shock solutions, and the primary difference is that a different set of equations representing a different physical model are being solved. The general structure is 1) to determine the downstream post-shock equilibrium state by using the Rankine-Hugoniot conditions which are the conservation of mass, momentum and energy, then 2) linearizing away from these equilibrium states, followed by 3) integrating the pertinent ODE away from the equilibrium state toward the opposite equilibrium state, and finally 4) splicing the solutions together somewhere between the two equilibrium states. Lowrie and Edwards developed the idea of integrating the ODE for the semi-analytic radiative shock problem in Mach space, starting at a position linearized away from the equilibrium points, and integrating toward the middle of the shock where the local Mach number is 1. The method presented by Masser, Wohlbier and Lowrie [1] uses the inverse compression ratio, $\eta = \rho_0/\rho$, as the integration variable, and it is not possible to specify when to stop integrating away from equilibrium, other than do not integrate past the other equilibrium state.

4.1. Solving for the downstream equilibrium values

It is straight-forward to derive the Rankine-Hugoniot conditions for this problem using the conservation equations of mass, momentum and energy. The Rankine-Hugoniot conditions connect the values of the downstream post-shock equilibrium state to the upstream unshocked equilibrium state. The conservation equations of mass, momentum and energy connecting these equilibrium states can be written as

$$\begin{pmatrix} \rho u \\ \rho u^2 + p \\ u\left[\frac{1}{2}\rho u^2 + \rho e + p\right] \end{pmatrix}_0 = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u\left[\frac{1}{2}\rho u^2 + \rho e + p\right] \end{pmatrix}_1 \tag{9}$$

Variables with a subscripted-"0" take values from the upstream unshocked equilibrium state, and variables with a subscripted-"1" take values from the downstream post-shock equilibrium state. Borrowing a result which is derived in the next subsection, $\mathcal{M}_0 = \rho u$, equality of the first set of expressions is trivial. Using this result in the second line to write $\rho u^2 = \mathcal{M}_0^2/\rho$, along with an expression for the pressure, $p = \rho e\,(\gamma - 1) = \rho T/\gamma = \mathcal{M}_0^2/\rho\mathcal{M}^2$, results in the following expression for the downstream material density

$$\rho_1 = \frac{\rho_0 \mathcal{M}_0^2\left(\gamma\mathcal{M}_1^2 + 1\right)}{\mathcal{M}_1^2\left(\gamma\mathcal{M}_0^2 + 1\right)} \tag{10}$$

Combining these expressions in the equality on the third line results in an expression that is quadratic in $\mathcal{M}_1^2$, and which can be solved to provide

$$\mathcal{M}_1^2 = \frac{\left(\gamma\mathcal{M}_0^4 + 1\right) \pm \sqrt{\left(\gamma\mathcal{M}_0^4 + 1\right)^2 - \left(\gamma\left(2\mathcal{M}_0^2 - 1\right) + 1\right)\mathcal{M}_0^2\left(\left(\gamma - 1\right)\mathcal{M}_0^2 + 2\right)}}{\left[\gamma\left(2\mathcal{M}_0^2 - 1\right) + 1\right]} \tag{11}$$

Interestingly, choosing the positive sign in front of the discriminant yields $\mathcal{M}_1 = \mathcal{M}_0$, and provides a good check for the code generating the semi-analytic solution. Choosing the negative sign in front of the discriminant yields the correct value of the downstream post-shock equilibrium Mach number. Given $\mathcal{M}_1$, ρ_1 can be determined from equation (10), T_1 can be determined from equation (6), and p_1 and e_1 can be determined from equations (2).

4.2. Linearizing away from equilibrium

In equilibrium the ODEs describing the physical model are identically zero, so it is necessary to move to a state near equilibrium before integrating the ODEs. This can be done by solving the linear Taylor-expansion of the ODE to determine the appropriate values at the state $\mathcal{M}_\epsilon = \mathcal{M}_{eq} \pm \epsilon$, where $\epsilon \ll 1$. When leaving

the upstream unshocked state then $\mathcal{M}_\epsilon = \mathcal{M}_{eq} - \epsilon$, and when leaving the downstream postshock state then $\mathcal{M}_\epsilon = \mathcal{M}_{eq} + \epsilon$. Then the expression being solved to determine the value of T_e appropriate to $\mathcal{M}_\epsilon$ is

$$T_e\left(\mathcal{M}_\epsilon\right) = T_{eq} + \left(\mathcal{M}_{eq} - \mathcal{M}_\epsilon\right)\frac{dT_e}{d\mathcal{M}}\,. \tag{12}$$

The expression for $dT_e/d\mathcal{M}$ is derived in the next Subsection.

4.3. The ODEs and some auxiliary equations

It is an important reminder that the equations being solved are time-independent such that all time derivatives in equations (1) above are neglected. As such, integrating the conservation of mass equation (1a) produces the standard definition for the initial Mach number, $\mathcal{M}_0 = \rho u = \rho_0 u_0$. Integrating the conservation of momentum equation (1b) produces an expression for the material density as a function of the local Mach number

$$\rho = \frac{\rho_0 \mathcal{M}_0^2\left(\gamma\mathcal{M}^2 + 1\right)}{\mathcal{M}^2\left(\gamma\mathcal{M}_0^2 + 1\right)}\,, \tag{13}$$

which is the same as the expression for the downstream post-shock density given in equation (10). Integrating the conservation of energy equation (1c) produces an expression for the spatial derivative of the electron energy

$$\frac{dT_e}{dx} = \frac{1}{\kappa_e}\left[\frac{\mathcal{M}_0}{\rho}\left(\frac{\mathcal{M}_0^2}{2\rho} + \frac{\mathcal{M}_0^2}{\left(\gamma-1\right)\rho\mathcal{M}^2}\right) - \frac{\mathcal{M}_0}{\rho_0}\left(\frac{\mathcal{M}_0^2}{2\rho_0} + \frac{1}{\left(\gamma-1\right)\rho_0}\right)\right]\,. \tag{14}$$

Returning to the conservation of momentum equation, allowing the derivative operator to act on the individual terms, and collecting results produces an expression relating $d\rho/dx$ and $d\mathcal{M}/dx$:

$$\frac{d\rho}{dx} = -\frac{2\rho}{\mathcal{M}\left(\gamma\mathcal{M}^2+1\right)}\frac{d\mathcal{M}}{dx}\,. \tag{15}$$

Returning to the conservation of energy equation, allowing the derivative operator to act on the individual terms on the left-hand side, and collecting results produces a simplified expression for the electron thermal diffusivity:

$$\frac{d}{dx}\left(\kappa_e\frac{dT_e}{dx}\right) = -\frac{2\mathcal{M}_0^3\left(\mathcal{M}^2-1\right)}{\left(\gamma-1\right)\rho^2\mathcal{M}^3\left(\gamma\mathcal{M}^2+1\right)}\frac{d\mathcal{M}}{dx}\,. \tag{16}$$

Considering the electron internal energy equation (1d), it is convenient to rewrite $\gamma_{ei}\left(T_i - T_e\right)$ in terms of $T = T\left(T_e, \mathcal{M}\right)$ and T_e. Returning to equations (2), T_i can be solved for in terms of T and T_e

$$T_i = \left(Z+1\right)T - ZT_e \tag{17}$$

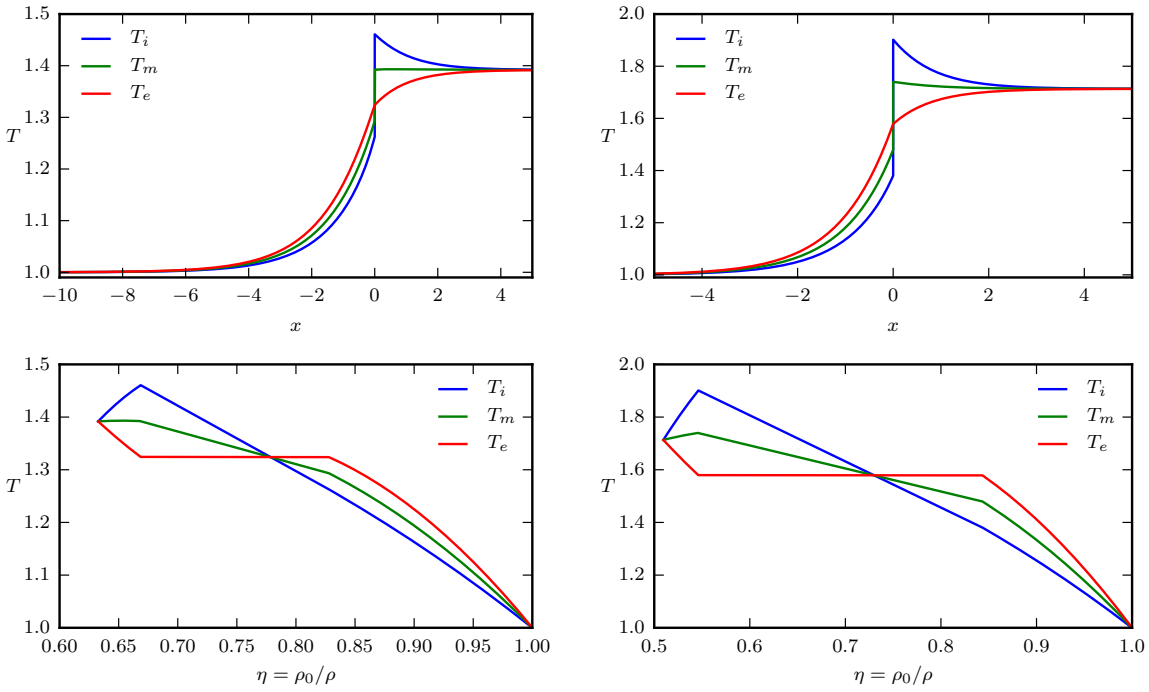
so that

$$T_i - T_e = \left(Z+1\right)\left(T - T_e\right)\,. \tag{18}$$

The electron internal energy equation (**??**) consists of four terms, and the two terms on the right-hand side have already been written as functions of T_e and $\mathcal{M}$, and the two terms on the left-hand side may similarly be written as functions of T_e and $\mathcal{M}$:

$$\frac{d}{dx}\left(\rho u e_e\right) = \mathcal{M}_0 C_{ve}\frac{dT_e}{dx}\,, \tag{19}$$

$$p_e\frac{du}{dx} = \frac{2C_{ve}\mathcal{M}_0 T_e\left(\gamma-1\right)}{\mathcal{M}\left(\gamma\mathcal{M}^2+1\right)}\frac{d\mathcal{M}}{dx} \tag{20}$$



(a) An electron-ion shock for $\mathcal{M}_0 = 1.4$ and $Z = 1$, using constant values for γ_{ei} and κ_{ei} as specified in [1].

(b) An electron-ion shock for $\mathcal{M}_0 = 1.7$ and $Z = 1$, using constant values for γ_{ei} and κ_{ei} as specified in [1].

Using equations (16) and (18) - (20) in the electron internal energy equation (**??**) produces an expression for $d\mathcal{M}/dx$:

$$\frac{d\mathcal{M}}{dx} = \frac{\gamma_{ei}\left(Z+1\right)\left(T-T_e\right) - \mathcal{M}_0 C_{ve}\frac{dT_e}{dx}}{\frac{2\mathcal{M}_0}{\mathcal{M}(\gamma\mathcal{M}^2+1)}\left[\frac{\mathcal{M}_0^2(\mathcal{M}^2-1)}{(\gamma-1)\rho^2\mathcal{M}^2} + C_{ve}T_e\left(\gamma-1\right)\right]} \tag{21}$$

Finally, equations (14) and (21) form an expression for $dT_e/d\mathcal{M}$,

$$\frac{dT_e}{d\mathcal{M}} = \frac{dT_e}{dx}\frac{dx}{d\mathcal{M}} \tag{22}$$

which can be integrated in Mach space from the state $\mathcal{M}_\epsilon$ toward $\mathcal{M} = 1$, for both the upstream unshocked region and the downstream post-shock region. If this shock is continuous then the results from the two sides will not overlap but the values at their endpoints will be close. If the shock is discontinuous then the results will overalp and must be connected appropriately, which is the subject of the next subsection.

4.4. Connecting the upstream and downstream shock regions

As stated in [1], at a shock discontinuity the jump in T_e is proportional to the jump in T_i according to the following relationship

$$\Delta T_e \sim \frac{m_e}{m_i}\Delta T_i\,, \tag{23}$$

which can be derived by considering that the dominant effect of a discontinuous shock is to transform kinetic energy, $\frac{1}{2}mu^2$, into thermal energy, $k_B T$, and by noticing that separate velocities for electrons and

ions have not been described herein so they are expected to slow down by the same amount when crossing the discontinuous shock. Since the mass ratios is at most 1/2000 in the case of hydrogen, ΔT_e will usually be negligibly small such that T_e can be assumed to be continuous across the shock discontinuity. This difference at the shock discontinuity, where ΔT_e is considered to be negligibly small while ΔT_i remains finite, motivates the idea that the electron-ion coupling, γ_{ei}, is also negligible at the shock discontinuity. It is worth noting that while T_e is assumed to be continuous across the shock discontinuity dT_e/dx is not.

The electron internal energy equation is related to the electron entropy equation,

$$\frac{DS_e}{Dt} = \gamma_{ei}\left(T_i - T_e\right) + \partial_x\left(\kappa_e \partial_x T_e\right) , \tag{24}$$

where

$$S_e = C_{ve} \log\left(p_e/\rho^\gamma\right) \tag{25}$$

is appropriately the electron entropy for an electron ideal-gas with a gamma-law EOS, and $D/Dt = \partial_t + u\partial_x$ is the material or substantive derivative. Comparing the electron internal energy equation (**??**) and the electron entropy equation (24) it can be seen that $\rho u T_e \left(dS_e/dx\right) = d\left(\rho u e_e\right)/dx + p_e du/dx$. In the case of negligible electron-ion coupling the following expression holds across the shock discontinuity:

$$\rho u T_e \frac{dS_e}{dx} = \frac{d}{dx}\left(\kappa_e \frac{dT_e}{dx}\right) . \tag{26}$$

As a reminder, at the shock discontinuity T_e is continuous while dT_e/dx is discontinuous, so the expression above can be rewritten as

$$\frac{d}{dx}\left[\rho u T_e S_e - \kappa_e \frac{dT_e}{dx}\right] = 0 , \tag{27}$$

and integrated across the shock discontinuity, which is assumed to be infinitesinally thin, so that the following expression must be continuous

$$\rho u T_e S_e - \kappa \frac{dT_e}{dx} . \tag{28}$$

Results from the semi-analyic solution method described herein are presented in Figures 4.3.

5. Continuing work

The primary thrust for future work will be to develop an input deck for xRAGE that runs this electron-ion steady-state shock problem and to modify the solution method so as to match the physical assumptions made by xRAGE. This will require considerable effort and consultation with the xRAGE code-development team. A secondary thrust is to investigate how the solution method responds when solving the model equations in a coordinate bases that is different than $(T_e, \mathcal{M})$; in [1] the coordinate bases is (T_e, η). Currently, the $(T_e, \mathcal{M})$ coordinate bases is not producing continuous shock solutions which were presented in [1].

6. References

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