MEEN 673 Project

Nonlinear Finite Element Implementation of Time Dependent Radiation Diffusion

Zachary M. Prince

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Dr. J. N. Reddy

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1 Introduction

This purpose of this paper is to detail a project involving the finite element implementation of a nonlinear system of partial differential equations. The project focuses on the evaluation of the time dependent radiation diffusion equation [1, 2]. The implementation involves defining the weak form of the equations, developing the finite element model, and detailing the nonlinear iteration process.

The time dependent radiation diffusion equations are defined in (1). Where E is the photon energy and T is the material temperature.

$$\frac{1}{c}\frac{\partial E}{\partial t} - \nabla \cdot D_r \nabla E = \sigma_a \left(aT^4 - E \right) \tag{1a}$$

$$C_v \frac{\partial T}{\partial t} - \nabla \cdot D_t \nabla T = -c\sigma_a \left(aT^4 - E \right) \tag{1b}$$

C_v is the material specific heat. c is the speed of light (photon). a is the Stephan-Boltzmann constant. D_r is the radiation diffusion coefficient defined by (2). D_t is the material (plasma) conduction diffusion coefficient defined by (3). Finally, σ_a is the photon absorption cross-section defined by (4).

$$D_r(T) = \frac{1}{3\sigma_a} \tag{2}$$

$$D_t(T) = kT^{5/2} \tag{3}$$

$$\sigma_a(T) = \frac{z^3}{T^3} \tag{4}$$

Where k is a constant and z is the atomic mass number of the material.

2 Finite Element Development

2.1 Weak Form

To develop the weak form, (1) is multiplied by test functions (u for the E equation and v for the T equation) and integrated over elements. The result is shown in (5).

$$\int_{\Omega^e} \left\{ \frac{1}{c}\frac{\partial E}{\partial t} u + \nabla u \cdot D_r \nabla E - \sigma_a \left(aT^4 - E \right) u \right\} + q_E = 0 \tag{5a}$$

$$\int_{\Omega^e} \left\{ C_v \frac{\partial T}{\partial t} v + \nabla v \cdot D_t \nabla T + c\sigma_a \left(aT^4 - E \right) v \right\} + q_T = 0 \tag{5b}$$

Where q_E and q_T are boundary contributions dependent on the boundary conditions.

2.2 Finite Element Model

To develop the finite element model, the solutions and test functions are expanded in nodal values and shape function show in (6). These expansions are applied to (5) and shown in (7)

$$E = \sum_{j=1}^{N} \psi_j E_j; \qquad T = \sum_{j=1}^{N} \psi_j T_j; \qquad u = v = \psi_i \tag{6}$$

$$\sum_{j=1}^{N} \int_{\Omega^e} \left\{ \frac{1}{c} \frac{\partial E_j}{\partial t} \psi_i \psi_j + \nabla \psi_i \cdot D_r \nabla \psi_j E_j - \sigma_a \left(a T^3 T_j - E_j \right) \psi_i \psi_j \right\} dxdy + q_E = 0 \tag{7a}$$

$$\sum_{j=1}^{N} \int_{\Omega^e} \left\{ C_v \frac{\partial T_j}{\partial t} \psi_i \psi_j + \nabla \psi_i \cdot D_t \nabla \psi_j T_j + c \sigma_a \left(a T^3 T_j - E_j \right) \psi_i \psi_j \right\} dxdy + q_T = 0 \tag{7b}$$

After applying material definitions from (2)-(4), (7) reduces to the form shown in (8).

$$\sum_{j=1}^{N} \int_{\Omega^e} \left\{ \frac{1}{c} \frac{\partial E_j}{\partial t} \psi_i \psi_j + \nabla \psi_i \cdot \frac{T^3}{3z^3} \nabla \psi_j E_j - z^3 \left(a T_j - \frac{E_j}{T^3} \right) \psi_i \psi_j \right\} dxdy + q_E = 0 \tag{8a}$$

$$\sum_{j=1}^{N} \int_{\Omega^e} \left\{ C_v \frac{\partial T_j}{\partial t} \psi_i \psi_j + \nabla \psi_i \cdot k T^{5/2} \nabla \psi_j T_j + c z^3 \left(a T_j - \frac{E_j}{T^3} \right) \psi_i \psi_j \right\} dxdy + q_T = 0 \tag{8b}$$

The system can now be represented in matrix form shown in (9) with matrix component definitions.

$$\begin{bmatrix} C^{11} & 0 \\ 0 & C^{22} \end{bmatrix} \begin{bmatrix} \dot{E} \\ \dot{T} \end{bmatrix} + \begin{bmatrix} K^{11} & K^{12} \\ K^{21} & K^{22} \end{bmatrix} \begin{bmatrix} E \\ T \end{bmatrix} = \begin{bmatrix} F^1 \\ F^2 \end{bmatrix} \tag{9a}$$

$$C_{ij}^{11} = \int_{\Omega^e} \frac{1}{c} \psi_i \psi_j dxdy \tag{9b}$$

$$C_{ij}^{22} = \int_{\Omega^e} C_v \psi_i \psi_j dxdy \tag{9c}$$

$$K_{ij}^{11} = \int_{\Omega^e} \nabla \psi_i \cdot \frac{T^3}{3z^3} \nabla \psi_j dxdy + \int_{\Omega^e} \frac{z^3}{T^3} \psi_i \psi_j dxdy + q_E(\psi_i, \psi_j) \tag{9d}$$

$$K_{ij}^{12} = -\int_{\Omega^e} z^3 a \psi_i \psi_j dxdy \tag{9e}$$

$$K_{ij}^{21} = -\int_{\Omega^e} \frac{c z^3}{T^3} \psi_i \psi_j dxdy \tag{9f}$$

$$K_{ij}^{22} = \int_{\Omega^e} \nabla \psi_i \cdot k T^{5/2} \nabla \psi_j dxdy + \int_{\Omega^e} c z^3 a \psi_i \psi_j dxdy + q_T(\psi_i, \psi_j) \tag{9g}$$

$$F_i^1 = q_E(\psi_i) \tag{9h}$$

$$F_i^2 = q_T(\psi_i) \tag{9i}$$

2.3 Time Discretization

The time discretization used for this project is defined by (10), where U can be E or T.

$$\frac{U_{s+1}-U_s}{\Delta t} \approx \theta \frac{\partial U_{s+1}}{\partial t} + (1-\theta)\frac{\partial U_s}{\partial t} \tag{10}$$

The finite element model can now be refactored into a new matrix form defined by (11) with coefficient definitions. U^1 and U^2 correspond to E and T, respectively.

$$\begin{bmatrix} \hat{K}^{11} & \hat{K}^{12} \\ \hat{K}^{21} & \hat{K}^{22} \end{bmatrix} \begin{bmatrix} E \\ T \end{bmatrix}_{s+1} = \begin{bmatrix} \hat{F}^1 \\ \hat{F}^2 \end{bmatrix} \tag{11a}$$

$$\hat{K}^{\alpha\beta}_{ij} = \theta \Delta t K^{\alpha\beta}_{ij,s+1} + C^{\alpha\beta}_{ij} \qquad \alpha,\beta = 1,2 \tag{11b}$$

$$\hat{F}^{\alpha}_i = \sum_{\gamma=1}^{2}\sum_{j=1}^{N}\left[C^{\alpha\gamma}_{ij} - (1-\theta)\Delta t K^{\alpha\gamma}_{ij,s}\right] U^{\gamma}_{j,s} + \Delta t\left[\theta F^{\alpha}_{i,s+1} + (1-\theta)F^{\alpha}_{i,s}\right] \qquad \alpha = 1,2 \tag{11c}$$

2.4 Iteration Technique

Two types of iteration processes are necessary to analyze in this project. The first is direct or fixed-point iteration. Where the evaluation of the system described by (11) is iterated, updating E and T into $\hat{K}$, until convergence. The second process is Newton iteration, where the tangent of the residual vector is evaluated. A Newton iteration system can be described by (12). Where T and R correspond to the tangent matrix and residual vector, respectively.

$$\begin{bmatrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{bmatrix} \delta \begin{bmatrix} E \\ T \end{bmatrix}_{s+1} = -\begin{bmatrix} R^1 \\ R^2 \end{bmatrix} \tag{12a}$$

$$R^{\alpha}_i = \sum_{\gamma=1}^{2}\sum_{j=1}^{N} \hat{K}^{\alpha\gamma}_{ij} U^{\gamma}_{j,s+1} - \hat{F}^{\alpha}_i \qquad \alpha = 1,2 \tag{12b}$$

$$T^{\alpha\beta}_{ij} = \frac{\partial R^{\alpha}_i}{\partial U^{\beta}_{j,s+1}} \qquad \alpha,\beta = 1,2 \tag{12c}$$

Applying the tangent matrix coefficient definition to (9) results in the coefficients described in (13).

$$T^{11}_{ij} = \hat{K}^{11}_{ij} \tag{13a}$$

$$T^{12}_{ij} = \hat{K}^{12}_{ij} + \theta\Delta t\left[\int_{\Omega^e} \frac{T^2_{s+1}}{z^3}\left(\nabla\psi_i \cdot \nabla E_{s+1}\right)\psi_j dxdy - \int_{\Omega^e} \frac{3z^3}{T^4_{s+1}} E_{s+1}\psi_i\psi_j dxdy\right] \tag{13b}$$

$$T^{21}_{ij} = \hat{K}^{21}_{ij} \tag{13c}$$

$$T^{22}_{ij} = \hat{K}^{22}_{ij} + \theta\Delta t\left[\int_{\Omega^e} \frac{5}{2}T^{3/2}_{s+1}\left(\nabla\psi_i \cdot \nabla T_{s+1}\right)\psi_j dxdy + \int_{\Omega^e} \frac{3cz^3}{T^4_{s+1}} E_{s+1}\psi_i\psi_j dxdy\right] \tag{13d}$$

3 Examples

3.1 Quasi-1D Example

The first example comes from [2] which is a two-dimensional problem, but solution is constant in one direction. The material properties, boundary and initial conditions are shown in (14). A 32X32, 64X64, 128X128, and 256X256 mesh was used with linear elements. Reduced Newton-Cotes integration was used for all nonlinear terms, this insured that the temperature would be positive and not confuse the D_t term. Backward Euler discretization ($\theta = 1$) was used with $\Delta t = 0.05$ and simulated 1.5 seconds.

$$z = c = a = C_v = 1.0 \qquad k = 0.1 \tag{14a}$$

$$E(x,y,0) = 1.0 \times 10^{-5} \qquad T(x,y,0) = (E(x,y,0)/a)^{1/4} = 5.62 \times 10^{-5} \tag{14b}$$

$$\frac{1}{4}E - \frac{D_r}{2}\frac{\partial E}{\partial \vec{n}} = 1 \qquad x = 0 \tag{14c}$$

$$\frac{1}{4}E + \frac{D_r}{2}\frac{\partial E}{\partial \vec{n}} = 0 \qquad x = 1 \tag{14d}$$

$$\frac{\partial E}{\partial \vec{n}} = 0 \qquad y = 0, x = 0 \tag{14e}$$

$$\frac{\partial T}{\partial \vec{n}} = 0 \qquad \text{all boundaries} \tag{14f}$$

The results from [2] are shown in Figure 2 and the results of my simulations are in Figure **??**. It is important to note that the paper uses a different definition of σ_a which, in practice, reduces the speed of the thermal wave by approximately half. Therefore their transient lasted 3.0 seconds, but the shapes and magnitudes of the curves are comparable.

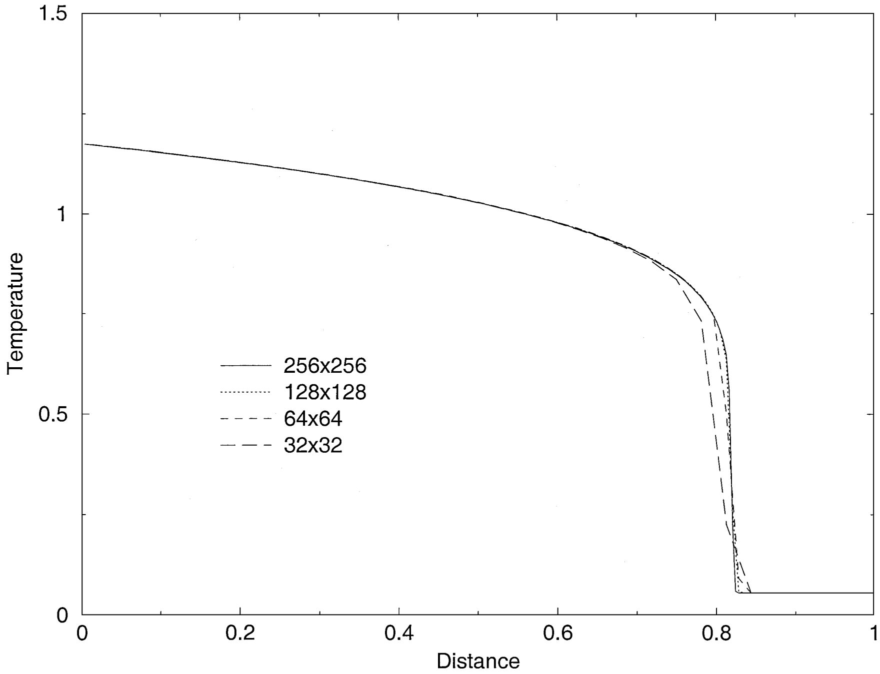

Figure 1: Radiation temperature from [2]

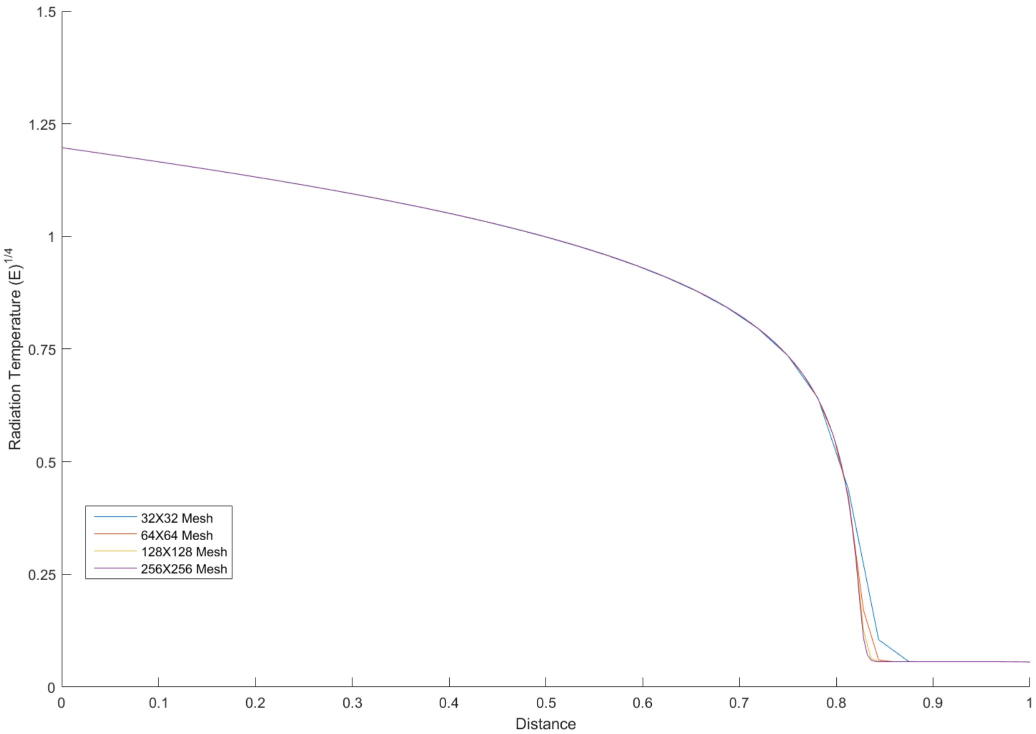

Figure 2: Radiation temperature for Example 1

3.2 Two Dimensional Example

This next example is exactly the same as the first to the first, except there is an opacity step in the middle of the domain. This is implemented by varying z in the domain, shown by (15).

$$z = \begin{cases} Z & 1/3 \leq x, y \leq 2/3 \\ 1.0 & \text{otherwise} \end{cases} \tag{15}$$

Two cases were run: $Z = 2.5$ and $Z = 10.0$. The material temperature for the cases are shown in Figure 3 and Figure 4 as contour plots, respectively.

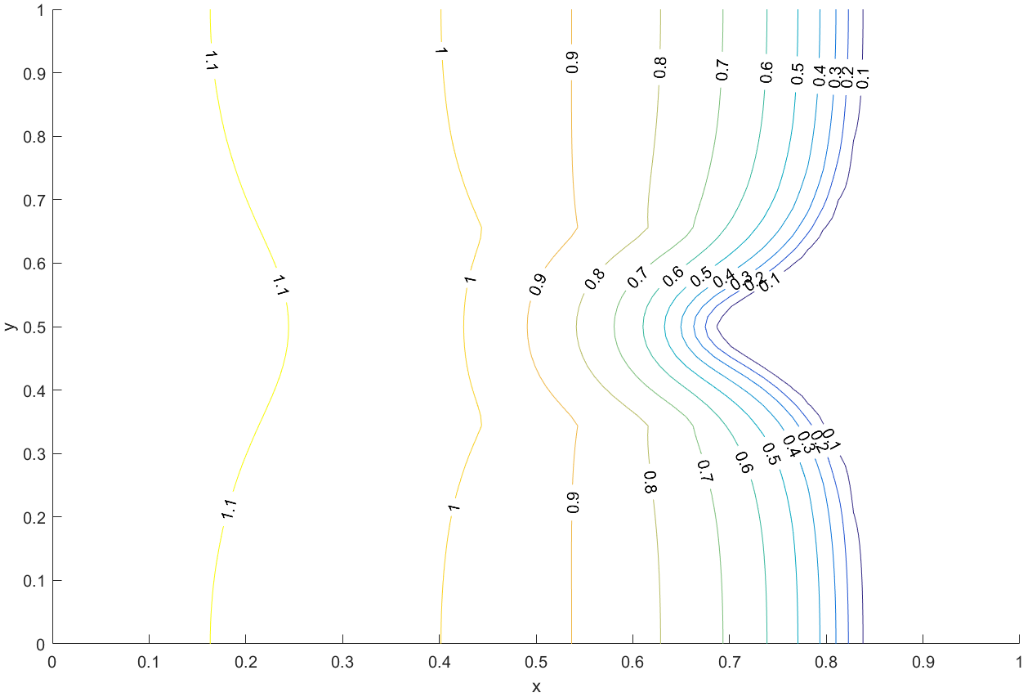

Figure 3: Material temperature for Example 2 ($Z = 2.5$)

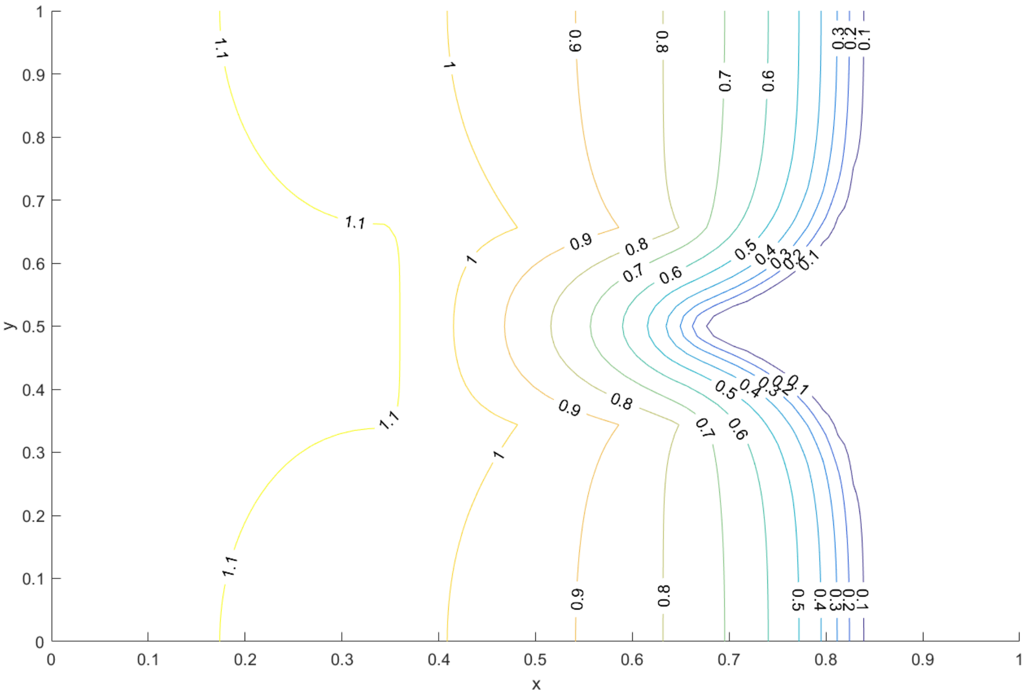

Figure 4: Material temperature for Example 2 ($Z = 10.0$)

References

[1] W. R. D.A. Knoll and G. Olson. An effcient nonlinear solution method for non-equilibrium radiation diffusion. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 63:15–29, 1999.

[2] D. K. V.A Mousseau and W. Rider. Physics-based preconditioning and the newtonkrylov method for non-equilibrium radiation diffusion. *Journal of Computational Physics*, 160:743–765, 2000.