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Original Citation:

Nupur, Gupta and Neela, Nataraj

(2011)

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(Submitted)

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An Adaptive Finite Element Method for Laser Surface Hardening of Steel Problem

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Abstract The main focus of this article is on the development of an adaptive finite element method for the laser surface hardening of steel, which is an optimal control problem governed by a dynamical system consisting of a semi-linear parabolic equation and an ordinary differential equation. *A posteriori* error estimators are being calculated, for the variable representing temperature and austenite, using residual method when a continuous piecewise linear discretization has been used for the finite element approximation of space variables and a discontinuous Galerkin method has been used for time and control discretizations. The estimators are used in the implementation and numerical results are obtained.

Keywords: Laser surface hardening of steel problem, Adaptive finite element method, Residual type estimators, *a posteriori* error estimates.

1 Introduction

In this paper, we develop *a posteriori* error estimates for the the approximation of the variables representing temperature and austenite in the optimal control problem describing the laser surface hardening of steel. The purpose of surface hardening is to increase the hardness of the boundary layer of a workpiece by rapid heating and subsequent quenching (see Figure 1). The hardening effect is achieved as the heat treatment leads to a change in micro-structure. A few applications include cutting tools, wheels, driving axles, gears, etc.

The mathematical model for the laser surface hardening of steel has been studied in [13] and [17]. For an extensive survey on mathematical models for laser material treatments, we refer to [26]. In this article, we follow the Leblond-Devaux model [13] which is described below:

Let $\Omega \subset \mathbb{R}^2$, denoting the workpiece, be a convex, bounded domain with piecewise Lipschitz continuous boundary $\partial\Omega$, $Q = \Omega \times I$ and $\Sigma = \partial\Omega \times I$, where $I = (0, T)$, $T < \infty$. The evolution of volume fraction of

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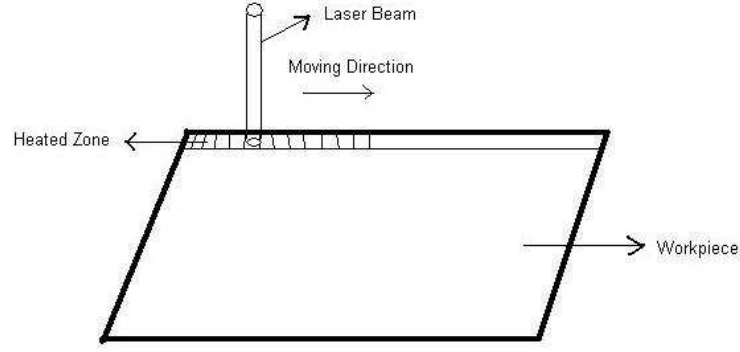


Fig. 1: Laser Hardening Process

austenite $a(t)$ for a given temperature evolution $\theta(t)$ is described by the following initial value problem:

$$\partial_t a = f_+(\theta, a) = \frac{1}{\tau(\theta)} [a_{eq}(\theta) - a]_+ \quad \text{in } Q, \quad (1.1)$$

$$a(0) = 0 \quad \text{in } \Omega, \quad (1.2)$$

where $a_{eq}(\theta(t))$, denoted as $a_{eq}(\theta)$ for notational convenience, is the equilibrium volume fraction of austenite and τ depends only on temperature. The term $[a_{eq}(\theta) - a]_+ = (a_{eq}(\theta) - a)\mathcal{H}(a_{eq}(\theta) - a)$, where \mathcal{H} is the Heaviside function

$$\mathcal{H}(s) = \begin{cases} 1 & s > 0 \\ 0 & s \leq 0, \end{cases}$$

denotes the non-negative part of $a_{eq}(\theta) - a$, that is, $[a_{eq}(\theta) - a]_+ = \frac{(a_{eq}(\theta) - a) + |a_{eq}(\theta) - a|}{2}$.

Neglecting the mechanical effects and using the Fourier law of heat conduction, the temperature evolution can be obtained by solving the non-linear energy balance equation given by

$$\rho c_p \partial_t \theta - \mathcal{K} \Delta \theta = -\rho L a_t + \alpha u \quad \text{in } Q, \quad (1.3)$$

$$\theta(0) = \theta_0 \quad \text{in } \Omega, \quad (1.4)$$

$$\nabla \theta \cdot \mathbf{n} = 0 \quad \text{on } \Sigma, \quad (1.5)$$

where the density ρ , the heat capacity c_p , the thermal conductivity \mathcal{K} and the latent heat L are assumed to be positive constants. The term $u(t)\alpha(x, t)$ describes the volumetric heat source due to laser radiation, $u(t)$ being the time dependent control variable. Since the main cooling effect is the self cooling of the workpiece, homogeneous Neumann conditions are assumed on the boundary. Also, θ_0 denotes the initial temperature.

To maintain the quality of the workpiece surface, it is important to avoid the melting of surface. In the case of laser hardening, it is a quite delicate problem to obtain parameters that avoid melting but nevertheless lead to the right amount of hardening. Mathematically, this corresponds to an optimal control problem in which we minimize the cost functional defined by:

$$J(\theta, a, u) = \frac{\beta_1}{2} \int_{\Omega} |a(T) - a_d|^2 dx + \frac{\beta_2}{2} \int_0^T \int_{\Omega} [\theta - \theta_m]_+^2 dx ds + \frac{\beta_3}{2} \int_0^T |u|^2 ds \quad (1.6)$$

subject to the state equations (1.1) – (1.5) in the set of admissible controls U_{ad} ,

where $U_{ad} = \{u \in U : \|u\|_{L^2(I)} \leq M\}$ is a closed, bounded and convex subset of $U = L^2(I)$, denoting the admissible intensities of the laser, β_1, β_2 and β_3 being positive constants and a_d being the given desired fraction of the austenite. The second term in (1.6) is a penalizing term that penalizes the temperature above the melting temperature θ_m .

The authors of [1] and [17], have regularised the right hand side function in (1.1) and have established results on existence, regularity and stability. This approach seems to be common in all subsequent literature not only for existence results but also for numerical approximations. In [14], the existence of the solution of the original problem has been established. Laser and induction hardening has been used to explain the model and then a finite volume method has been used for the space discretization in [18]. In [19], the optimal control problem is analyzed and error estimates for proper orthogonal decomposition Galerkin method for the state system are derived. Also a penalized problem has been considered for the purpose of numerical simulations. A finite element scheme combined with a nonlinear conjugate gradient method has been used to solve the optimal control problem and a finite element method has been used for the purpose of space discretization in [31]. In [15] (respectively, [16]), *a priori* error estimates are developed for a finite element scheme in which the space discretization is done using conformal finite elements (respectively, discontinuous Galerkin method), whereas the time and control discretizations are based on a discontinuous Galerkin method.

Adaptive Finite Element Methods (AFEMs) are amongst one of the important means to boost the accuracy and efficiency of the finite element discretization. It ensures higher density of nodes in certain areas of computational domain, where it is more difficult to approximate the solution. Estimates obtained are called *a posteriori* error estimates as they depend on the approximate solution and data given, and the refinement/coarsening of meshes is done based on the estimate for the discretization error. *A posteriori* error estimation for finite element methods for two point elliptic boundary value problems began with the pioneering work of Babuška and Rheinboldt [2]. The use of adaptive technique based on *a posteriori* error estimation is well accepted in the context of finite element discretization of partial differential equations, see Bank [3], Becker and Rannacher [4], [7], [8], Eriksson and Johnson [10], [11], Verfurth [30].

Two approaches, namely the *residual* and *dual weighted residual* (DWR) methods based *a posteriori* error estimates have been studied for elliptic, parabolic, non-linear and optimal control problems in literature. While residual based methods are useful in estimating error in L^2 or energy based norms involving local residuals of the computed solution, DWR method is useful in estimating the error bounds not only in energy norm and L^2 norm but also on some quantity of physical interest, like, point value error, point value derivative error, mean normal flux etc. (see [7], [8] and [29]).

For *a posteriori* error estimates for elliptic equations using residual (resp. DWR) method, see [2], [3] and [30] (resp. [4], [7], [8]), just to mention a few. AFEM for linear parabolic problems are also studied in [10], [11] using residual type estimators and in [4] using DWR type estimators, and the references cited therein. In [27], *a priori* and *a posteriori* estimates using DWR method have been developed for the optimal control problem governed by parabolic equations, where laser surface hardening of steel problem is considered as one of the applications. Energy type error estimation for the error in the control, state and adjoint variables using residual method are developed in [21], [23] and [24] in the context of distributed optimal control problems governed by elliptic equation subject to pointwise control constraints. These techniques are also been applied to optimal control problem governed by linear parabolic differential equations, see [22] and [25].

In this article we will discuss residual AFEM for the laser surface hardening of steel. In [15] and [16], *a priori* error estimates are developed for the same problem and non-uniform meshes (more refined near the heated zone and coarse far from the operational area) are used in implementations. Even though it has been observed that non-uniform meshes are helpful in yielding the desired numerical results which justify theoretical

estimates, practically, they are quite expensive as the mesh used for the approximation, chosen a priori, is independent of the approximate solution of the problem. To overcome this, in this article, residual based *a posteriori* estimates has been developed and the refinement of the triangulation near the heating zone is done based on these indicators.

The outline of this article is as follows. Section 1 is introductory in nature. In Section 2, the regularized laser surface hardening of steel problem and its weak formulation are stated. Section 3 gives details of the space, time and control discretizations. In Section 4, *a posteriori* error estimates corresponding to residual approach is developed. In Section 5, adaptive refinement algorithm is described and the results of implementations are presented.

2 The Regularized Laser Surface Hardening of Steel Problem

For theoretical, as well as computational reasons, the term $[a_{eq} - a]_+$ in (1.1) is regularized and the regularized laser surface hardening problem is given by:

$$\min_{u_\epsilon \in U_{ad}} J(\theta_\epsilon, a_\epsilon, u_\epsilon) \text{ subject to} \quad (2.1)$$

$$\partial_t a_\epsilon = f_\epsilon(\theta_\epsilon, a_\epsilon) = \frac{1}{\tau(\theta_\epsilon)}(a_{eq}(\theta_\epsilon) - a_\epsilon)\mathcal{H}_\epsilon(a_{eq}(\theta_\epsilon) - a_\epsilon) \quad \text{in } Q, \quad (2.2)$$

$$a_\epsilon(0) = 0 \quad \text{in } \Omega, \quad (2.3)$$

$$\rho c_p \partial_t \theta_\epsilon - \mathcal{K} \Delta \theta_\epsilon = -\rho L \partial_t a_\epsilon + \alpha u_\epsilon \quad \text{in } Q, \quad (2.4)$$

$$\theta_\epsilon(0) = \theta_0 \quad \text{in } \Omega, \quad (2.5)$$

$$\frac{\partial \theta_\epsilon}{\partial n} = 0 \quad \text{on } \Sigma, \quad (2.6)$$

where $\mathcal{H}_\epsilon \in C^{1,1}(\mathbb{R})$ is a monotone approximation of the Heaviside function satisfying $\mathcal{H}_\epsilon(x) = 0$ for $x \leq 0$.

We now make the following assumptions [19]:

- (A1) $a_{eq}(x) \in (0, 1)$ for all $x \in \mathbb{R}$ and $\|a_{eq}\|_{C^1(\mathbb{R})} \leq c_a$;
- (A2) $0 < \underline{\tau} \leq \tau(x) \leq \bar{\tau}$ for all $x \in \mathbb{R}$ and $\|\tau\|_{C^1(\mathbb{R})} \leq c_\tau$;
- (A3) $\theta_0 \in H^1(\Omega)$, $\theta_0 \leq \theta_m$ a.e. in Ω , where the constant $\theta_m > 0$ denotes the melting temperature of steel;
- (A4) $\alpha \in L^\infty(Q)$;
- (A5) $u \in L^2(I)$;
- (A6) $a_d \in L^\infty(\Omega)$ with $0 \leq a_d \leq 1$ a.e. in Ω .

Remark 2.1 Now onwards, since the finite element approximation of the regularized problem will be considered in the sequel, for the sake of notational simplicity $(\theta_\epsilon, a_\epsilon, u_\epsilon)$ and f_ϵ will be replaced by (θ, a, u) and f respectively, throughout the paper.

Let $V = H^1(\Omega)$ and $H = L^2(\Omega)$, and (\cdot, \cdot) (resp. $(\cdot, \cdot)_{I, \Omega}$) and $\|\cdot\|$ (resp. $\|\cdot\|_{I, \Omega}$) denote the inner product and norm in $L^2(\Omega)$ (resp. $L^2(I, L^2(\Omega))$). The inner product and norm in $L^2(I)$ are denoted by $(\cdot, \cdot)_{L^2(I)}$ and $\|\cdot\|_{L^2(I)}$, respectively. The weak formulation of the regularized version of laser surface hardening of steel

problem (2.1)-(2.6) is given by:

$$\min_{u \in U_{ad}} J(\theta, a, u) \text{ subject to} \quad (2.7)$$

$$(\partial_t a, w) = (f(\theta, a), w) \quad \forall w \in H, \text{ a.e. in } I, \quad (2.8)$$

$$a(0) = 0, \quad (2.9)$$

$$\rho c_p(\partial_t \theta, v) + \mathcal{K}(\nabla \theta, \nabla v) = -\rho L(\partial_t a, v) + (\alpha u, v) \quad \forall v \in V, \text{ a.e. in } I, \quad (2.10)$$

$$\theta(0) = \theta_0, \quad (2.11)$$

where $(\theta(t), a(t)) \in V \times H$. The following theorem ([31], Theorem 2.1) ensures the existence of a unique solution of the system (2.8)-(2.11).

Theorem 2.1 [31] *Suppose that (A1)-(A6) are satisfied. Then, the system (2.8)-(2.11) has a unique solution*

$$(\theta, a) \in H^{1,1} \times W^{1,\infty}(I; L^\infty(\Omega)),$$

where $H^{1,1} = L^2(I; H^1(\Omega)) \cap H^1(I; L^2(\Omega))$. Moreover, a satisfies

$$0 \leq a < 1 \text{ a.e. in } Q.$$

For existence of the solution of the of the original laser surface hardening of steel problem, we refer to ([14], Theorem 3.2).

Remark 2.2 [31] Using Theorem 2.1, (A1)-(A2) and the definition of the regularized Heaviside function \mathcal{H}_ε , there exists a constant $c_f > 0$ independent of θ and a such that

$$\max(\|f(\theta, a)\|_{L^\infty(Q)}, \|f_a(\theta, a)\|_{L^\infty(Q)}, \|f_\theta(\theta, a)\|_{L^\infty(Q)}) \leq c_f$$

for $(\theta, a) \in L^2(Q) \times L^\infty(Q)$ which satisfy (2.8) - (2.11).

The existence of the optimal control is guaranteed by the following Theorem ([31], Theorem 2.3).

Theorem 2.2 *Suppose that (A1)-(A6) hold true. Then the optimal control problem (2.7)-(2.11) has at least one (global) solution.*

Let $u^* \in U_{ad}$ be a solution of (2.7)-(2.11) and (θ^*, a^*) be the solution of the corresponding state system. In the following lemma, we state the existence and uniqueness result of the corresponding adjoint system.

Lemma 2.1 [31] *Let (A1)-(A6) hold true and $(\theta^*, a^*, u^*) \in X \times Y \times U_{ad}$ be a solution to (2.7)-(2.11). Then there exists a unique solution $(z^*, \lambda^*) \in H^{1,1} \times H^1(I, L^2(\Omega))$ of the corresponding adjoint system defined by:*

$$-(\psi, \partial_t \lambda^*) + (\psi, f_a(\theta^*, a^*)(\rho L z^* - \lambda^*)) = 0 \quad \forall \psi \in H, \text{ a.e. in } I, \quad (2.12)$$

$$\lambda^*(T) = \beta_1(a^*(T) - a_d), \quad (2.13)$$

$$-\rho c_p(\phi, \partial_t z^*) + \mathcal{K}(\nabla \phi, \nabla z^*) + (\phi, f_\theta(\theta^*, a^*)(\rho L z^* - \lambda^*)) = \beta_2(\phi, [\theta^* - \theta_m]_+) \quad (2.14)$$

$$\forall \phi \in V, \text{ a.e. in } I,$$

$$z^*(T) = 0. \quad (2.15)$$

Moreover, z^* satisfies the following variational inequality

$$\left(\beta_3(u^* - u_d) + \int_{\Omega} \alpha z^* dx, p - u^* \right)_{L^2(I)} \geq 0 \quad \forall p \in U_{ad}. \quad (2.16)$$

3 Discretizations

In this section, we describe a temporal discretization using a discontinuous Galerkin finite element method and a space discretization using continuous piecewise polynomials. The control is being discretized using piecewise constants in each discrete interval $I_n, n = 1, 2, \dots, N$.

Time Discretization

In order to discretize (2.7)-(2.11) in time, we consider the following partition of I :

$$0 = t_0 < t_1 < \dots < t_N = T.$$

Set $I_1 = [t_0, t_1]$, $I_n = (t_{n-1}, t_n]$, $k_n = t_n - t_{n-1}$, for $n = 2, \dots, N$ and $k = \max_{1 \leq n \leq N} k_n$. We define the spaces

$$X_k^q = \{\phi : I \rightarrow V; \phi|_{I_n} = \sum_{j=0}^q \psi_j t^j, \psi_j \in V\}, \quad q \in \mathbb{N}, \quad (3.1)$$

$$Y_k^q = \{\phi : I \rightarrow H; \phi|_{I_n} = \sum_{j=0}^q \psi_j t^j, \psi_j \in H\}, \quad q \in \mathbb{N}. \quad (3.2)$$

For a function v in X_k^q or Y_k^q , we use the following notations:

$$v_n = v(t_n), \quad v_n^+ = \lim_{t \rightarrow t_n^+} v(t) \quad \text{and} \quad [v]_n = v_n^+ - v_n.$$

Then the dG(q) discretization of (2.7)-(2.11) reads as:

$$\min_{u_k \in U_{ad}} J(\theta_k, a_k, u_k) \quad \text{subject to} \quad (3.3)$$

$$\sum_{n=1}^N (\partial_t a_k, w)_{I_n, \Omega} + \sum_{n=1}^{N-1} ([a_k]_n, w_n^+) + (a_{k,0}^+, w_0^+) = (f(\theta_k, a_k), w)_{I, \Omega}, \quad (3.4)$$

$$a_k(0) = 0, \quad (3.5)$$

$$\begin{aligned} \rho c_p \sum_{n=1}^N (\partial_t \theta_k, v)_{I_n, \Omega} + \mathcal{K}(\nabla \theta_k, \nabla v)_{I, \Omega} + \rho c_p \sum_{n=1}^{N-1} ([\theta_k]_n, v_n^+) + \rho c_p (\theta_{k,0}^+, v_0^+) \\ = -\rho L(f(\theta_k, a_k), v)_{I, \Omega} + (\alpha u_k, v)_{I, \Omega} + \rho c_p (\theta_0, v_0^+), \end{aligned} \quad (3.6)$$

$$\theta_k(0) = \theta_{h,0} \quad (3.7)$$

for all $(v, w) \in X_k^q \times Y_k^q$ and $\theta_{h,0}$ is suitable approximation of θ_0 .

The adjoint system corresponding to (3.3)-(3.7) obtained from Karush-Kuhn-Tucker (KKT) conditions is defined by: find $(z_k^*, \lambda_k^*) \in X_k^q \times Y_k^q$ such that

$$-\sum_{n=1}^N (\psi, \partial_t \lambda_k^*)_{I_n, \Omega} - \sum_{n=1}^{N-1} (\psi_n, [\lambda_k^*]_n) = -(\psi, f_a(\theta_k^*, a_k^*)(\rho L z_k^* - \lambda_k^*))_{I, \Omega}, \quad (3.8)$$

$$\lambda_k^*(T) = \beta_1 (a_k^*(T) - a_d), \quad (3.9)$$

$$\begin{aligned} -\rho c_p \sum_{n=1}^N (\phi, \partial_t z_k^*)_{I_n, \Omega} + \mathcal{K}(\nabla \phi, \nabla z_k^*)_{I, \Omega} - \rho c_p \sum_{n=1}^{N-1} (\phi_n, [z_k^*]_n) = -(\phi, f_\theta(\theta_k^*, a_k^*)(\rho L z_k^* - \lambda_k^*))_{I, \Omega} \\ + \beta_2 (\phi, [\theta_k^* - \theta_m]_+)_{I, \Omega}, \end{aligned} \quad (3.10)$$

$$z_k^*(T) = 0, \quad (3.11)$$

for all $(\psi, \phi) \in X_k^q \times Y_k^q$. Moreover, z_k^* satisfies the following variational inequality

$$\left(\beta_3 u_k^* + \int_{\Omega} \alpha z_k dx, p - u_k^* \right)_{L^2(I)} \geq 0 \quad \forall p \in U_{ad}. \quad (3.12)$$

Space Discretization

We describe a space discretization for (3.3)-(3.7) using a continuous Galerkin finite element method. Let \mathcal{T}_h be an admissible regular triangulation of $\bar{\Omega}$ into triangles/quadrilaterals K . Let the discretization parameter h be defined as $h = \max_{K \in \mathcal{T}_h} h_K$, where h_K is the diameter of K . Let the finite element space $V_h \subset V$ consist of globally continuous functions which when restricted to $K \in \mathcal{T}_h$ are piecewise polynomials.

$$\text{Let } X_{kh}^q = \{ \phi : I \rightarrow V_h; \phi|_{I_n} = \sum_{j=0}^q \psi_j t^j, \psi_j \in V_h \}, \quad q \in \mathbb{N}. \quad (3.13)$$

Then the space-time discretization of (3.3)-(3.7) reads as:

$$\min_{u_{kh} \in U_{ad}} J(\theta_{kh}, a_{kh}, u_{kh}) \quad \text{subject to} \quad (3.14)$$

$$\sum_{n=1}^N (\partial_t a_{kh}, w)_{I_n, \Omega} + \sum_{n=1}^{N-1} ([a_{kh}]_n, w_n^+) + (a_{kh,0}^+, w_0^+) = (f(\theta_{kh}, a_{kh}), w)_{I, \Omega}, \quad (3.15)$$

$$a_{kh}(0) = 0, \quad (3.16)$$

$$\begin{aligned} \rho c_p \sum_{n=1}^N (\partial_t \theta_{kh}, v)_{I_n, \Omega} + \mathcal{K}(\nabla \theta_{kh}, \nabla v)_{I, \Omega} + \rho c_p \sum_{n=1}^{N-1} ([\theta_{kh}]_n, v_n^+) + \rho c_p (\theta_{kh,0}^+, v_0^+) \\ = -\rho L(f(\theta_{kh}, a_{kh}), v)_{I, \Omega} + (\alpha u_{kh}, v)_{I, \Omega} + \rho c_p (\theta_0, v_0^+), \end{aligned} \quad (3.17)$$

$$\theta_{kh}(0) = \theta_{h,0}, \quad (3.18)$$

for all $(v, w) \in X_{kh}^q \times X_{kh}^q$ and $(\theta_{kh}, a_{kh}) \in X_{kh}^q \times X_{kh}^q$.

Remark 3.3 Although, for the computational ease, the finite element space X_{kh}^q has been used to discretize the variables θ and a , where approximation is done using continuous functions, the variable a can also be approximated using discontinuous polynomials.

The adjoint system corresponding to (3.14)-(3.18) is defined by: find $(z_{kh}^*, \lambda_{kh}^*) \in X_{kh}^q \times X_{kh}^q$ such that

$$-\sum_{n=1}^N (\psi, \partial_t \lambda_{kh}^*)_{I_n, \Omega} - \sum_{n=1}^{N-1} (\psi_n, [\lambda_{kh}^*]_n) = -(\psi, f_a(\theta_{kh}^*, a_{kh}^*)(\rho L z_{kh}^* - \lambda_{kh}^*))_{I, \Omega}, \quad (3.19)$$

$$\lambda_{kh}^*(T) = \beta_1 (a_{kh}^*(T) - a_d), \quad (3.20)$$

$$\begin{aligned} -\rho c_p \sum_{n=1}^N (\phi, \partial_t z_{kh}^*)_{I_n, \Omega} + \mathcal{K}(\nabla \phi, \nabla z_{kh}^*)_{I, \Omega} \\ -\rho c_p \sum_{n=1}^{N-1} (\phi_n, [z_{kh}^*]_n) = -(\phi, f_{\theta}(\theta_{kh}^*, a_{kh}^*)(\rho L z_{kh}^* - \lambda_{kh}^*))_{I, \Omega} \end{aligned} \quad (3.21)$$

$$+\beta_2 (\phi, [\theta_{kh}^* - \theta_m]_+)_{I, \Omega}, \quad (3.22)$$

$$z_{kh}^*(T) = 0, \quad (3.23)$$

for all $(\psi, \phi) \in X_{kh}^q \times X_{kh}^q$. Here, z_{kh}^* satisfies the following variational inequality

$$\left(\beta_3 u_{kh}^* + \int_{\Omega} \alpha z_{kh}^* dx, p - u_{kh}^* \right)_{L^2(I)} \geq 0 \quad \forall p \in U_{ad}. \quad (3.24)$$

Complete discretization

In order to completely discretize the problem (2.7)-(2.11), we choose a discontinuous Galerkin piecewise constant approximation of the control variable, u . Let U_d be the finite dimensional subspace of U defined by

$$U_d = \{v_d \in L^2(I) : v_d|_{I_n} = a \text{ constant}\} \quad \forall n = 1, 2, \dots, N.$$

Let $U_{d,ad} = U_d \cap U_{ad}$ and $\sigma = \sigma(h, k, d)$ be the discretization parameter. The completely discretized problem reads as:

$$\min_{u_\sigma \in U_{d,ad}} J(\theta_\sigma, a_\sigma, u_\sigma) \quad \text{subject to} \quad (3.25)$$

$$\sum_{n=1}^N (\partial_t a_\sigma, w)_{I_n, \Omega} + \sum_{n=1}^{N-1} ([a_\sigma]_n, w_n^+) + (a_{\sigma,0}^+, w_0^+) = (f(\theta_\sigma, a_\sigma), w)_{I, \Omega}, \quad (3.26)$$

$$a_\sigma(0) = 0, \quad (3.27)$$

$$\rho c_p \sum_{n=1}^N (\partial_t \theta_\sigma, v)_{I_n, \Omega} + \mathcal{K}(\nabla \theta_\sigma, \nabla v)_{I, \Omega} + \rho c_p \sum_{n=1}^{N-1} ([\theta_\sigma]_n, v_n^+) + \rho c_p (\theta_{\sigma,0}^+, v_0^+) \quad (3.28)$$

$$= -\rho L (f(\theta_\sigma, a_\sigma), v)_{I, \Omega} + (\alpha u_\sigma, v)_{I, \Omega} + \rho c_p (\theta_0, v_0^+),$$

$$\theta_\sigma(0) = \theta_{h,0}, \quad (3.29)$$

for all $(v, w) \in X_{kh}^q \times X_{kh}^q$ and where $(\theta_\sigma, a_\sigma) \in X_{kh}^q \times X_{kh}^q$.

The adjoint system corresponding to (3.25)-(3.29) is defined by: find $(z_\sigma^*, \lambda_\sigma^*) \in X_{kh}^q \times X_{kh}^q$ such that

$$-\sum_{n=1}^N (\psi, \partial_t \lambda_\sigma^*)_{I_n, \Omega} - \sum_{n=1}^{N-1} (\psi_n, [\lambda_\sigma^*]_n) = -(\psi, f_a(\theta_\sigma^*, a_\sigma^*)(\rho L z_\sigma^* - \lambda_\sigma^*))_{I, \Omega}, \quad (3.30)$$

$$\lambda_{\sigma,N}^* = \beta_1 (a_\sigma^*(T) - a_d), \quad (3.31)$$

$$-\rho c_p \sum_{n=1}^N (\phi, \partial_t z_\sigma^*)_{I_n, \Omega} + \mathcal{K}(\nabla \phi, \nabla z_\sigma^*)_{I, \Omega} - \rho c_p \sum_{n=1}^{N-1} (\phi_n, [z_\sigma^*]_n) = -(\phi, f_\theta(\theta_\sigma^*, a_\sigma^*)(\rho L z_\sigma^* - \lambda_\sigma^*))_{I, \Omega} \quad (3.32)$$

$$+ \beta_2 (\phi, [\theta_\sigma^* - \theta_m]_+)_{I, \Omega},$$

$$z_{\sigma,N}^* = 0, \quad (3.33)$$

for all $(\psi, \phi) \in X_{kh}^q \times X_{kh}^q$. Moreover, z_σ^* satisfies the variational inequality,

$$\left(\beta_3 u_\sigma^* + \int_{\Omega} \alpha z_\sigma^* dx, p - u_\sigma^* \right)_{L^2(I)} \geq 0 \quad \forall p \in U_{d,ad}. \quad (3.34)$$

4 A Posteriori Error Estimates

In this section, *a posteriori* error estimates using residual method is developed for the purpose of adaptive refinement. A use of AFEM helps in obtaining meshes which are solution and data dependent.

Residual methods are important, when estimating errors in global norms are crucial. We have used residual method to calculate the *a posteriori* error estimates for the temperature θ , austenite a and control u , in $L^\infty(I, L^2(\Omega))$ and $L^2(I)$ norm, respectively. These estimates are then used in the next section for the purpose of numerical experiments. The following results would be necessary for developing the estimates.

– **Average interpolation Operator** [20], [22]: The average interpolation operator $\pi_h : V \rightarrow V_h$ satisfies the following error estimates: for $v \in H^1(\Omega)$,

$$\|v - \pi_h v\|_{H^1(K)} \leq C \sum_{\substack{K' \in \mathcal{T}_h \\ \bar{K} \cap \bar{K}' \neq \emptyset}} h_K^{m-l} |v|_{H^m(K')}, \quad v \in H^m(K'), \quad l = 0, 1, \quad l \leq m \leq 2. \quad (4.1)$$

– **Trace Inequality** [20], [22]: For $\forall v \in H^1(K)$,

$$\|v\|_{L^2(\partial K)} \leq C \left(h_K^{-\frac{1}{2}} \|v\|_K + h_K^{\frac{1}{2}} |v|_{H^1(K)} \right). \quad (4.2)$$

– **Space-time interpolation operator** [20], [22]: Let $\phi_I \in X_{hk}^q$ be the interpolant of ϕ defined by

$$\phi_I|_{\Omega \times I_n} = \pi_{h,n} \pi_n \phi \quad n = 1, 2, \dots, N, \quad (4.3)$$

where $\pi_{h,n}$ is the average interpolation operator satisfying (4.1) and $\pi_n : C(\bar{I}, V) \rightarrow P_q(I_n)$ is the L^2 -projection operator, satisfying

$$\|\phi - \pi_n \phi\|_{I_n, K} \leq C k_n^{q+1} \|\partial_t^{q+1} \phi\|_{I_n, K}. \quad (4.4)$$

Then,

$$\begin{aligned} \|\phi - \phi_I\|_{I_n, K} &\leq \|\phi - \pi_n \phi\|_{I_n, K} + \|\pi_n \phi - \phi_I\|_{I_n, K} \\ &\leq C \left(k_n^{q+1} \|\partial_t^{q+1} \phi\|_{I_n, K} + h_K^2 \|\phi\|_{L^2(I_n, H^2(K))} \right). \end{aligned} \quad (4.5)$$

Now, we state and prove Theorems 4.4 and 4.5 in which the *a posteriori* estimates for the laser surface hardening problem are derived. The development of *a posteriori* estimates for the optimal control problem governed by a non linear system considered is quite technical and the ideas for the proof is motivated by *a posteriori* estimates for optimal control problems governed by linear parabolic problems [22].

Theorem 4.3 *let (θ, a, u) and $(\theta_\sigma, a_\sigma, u_\sigma)$ be respectively the solutions of (2.7)-(2.11) and (3.25)-(3.29) with (z, λ) and $(z_\sigma, \lambda_\sigma)$ as the corresponding adjoint solutions. Then, we have*

$$\|u - u_\sigma\|_{L^2(I)}^2 \leq C \left(\max_{\Omega} |\alpha| \sum_{n=1}^N \sum_{T \in \mathcal{T}_h} \|z_\sigma + \beta_3 u_\sigma\|_{L^2(I_n, K)}^2 + \|z_\sigma - z_{u_\sigma}\|_{L^2(I, \Omega)}^2 \right) \quad \forall k \leq k_\epsilon \text{ where } \epsilon > 0, \quad (4.6)$$

where $(z_{u_\sigma}, \lambda_{u_\sigma})$ is the adjoint solution of (2.7)-(2.11) for control u_σ and k is represented by $\sigma = (h, k, d)$.

Proof: From mean value theorem for $\nu \in (0, 1)$, we have

$$\begin{aligned} (j'(u) - j'(u_\sigma))(u - u_\sigma) &= j''(u + \nu(u - u_\sigma))(u - u_\sigma)^2 \\ &= j''(u)(u - u_\sigma)^2 + j''(u + \nu(u - u_\sigma))(u - u_\sigma)^2 - j''(u)(u - u_\sigma)^2 \\ &\leq j''(u)(u - u_\sigma)^2 - |j''(u + \nu(u - u_\sigma))(u - u_\sigma)^2 - j''(u)(u - u_\sigma)^2|. \end{aligned} \quad (4.7)$$

Function j'' is defined by

$$j''(u)(p_1, p_2) = \beta_3(p_1, p_2) - (\rho Lz - \lambda, f_{\theta, \theta}(\theta, a)\delta\theta\delta\theta + f_{\theta, a}(\theta, a)\delta\theta\delta a + f_{a, a}(\theta, a)\delta a\delta a + f_{a, \theta}(\theta, a)\delta\theta\delta a) \quad (4.8)$$

where $(\delta\theta, \delta a)$ is the solution of the problem, see [19]

$$\begin{aligned}\rho c_p(\partial_t \delta\theta, v) + \mathcal{K}(\nabla \delta\theta, \nabla v) &= -\rho L(\partial_t \delta a, v) + (\alpha \delta u, v), \\ \delta\theta(0) &= 0, \\ (\partial_t \delta a, w) &= (f_\theta(\theta, a)\delta\theta + f_a(\theta, a)\delta a, w), \\ \delta a(0) &= 0.\end{aligned}$$

Using assumptions (A1)-(A2) and by (4.8), we obtain that j is C^2 in $L^2(\Omega)$. Therefore, there exists $\epsilon > 0$ such that,

$$|j''(u + \nu(u - u_\sigma))(u - u_\sigma)^2 - j''(u)(u - u_\sigma)^2| \leq \frac{\delta}{2} \|u - u_\sigma\|_{L^2(I)}^2 \quad \text{if } \|u - u_\sigma\|_{L^2(I)}^2 \leq \epsilon.$$

From [14], we have $u_\sigma \rightarrow u$ in $L^2(I)$, therefore there exists $\epsilon > 0$ such that

$$\|u - u_\sigma\|_{L^2(I)}^2 \leq \epsilon \quad \forall k \leq k_\epsilon.$$

Using (4.9) in (4.7), we obtain

$$(j'(u) - j'(u_\sigma))(u - u_\sigma) \leq j''(u)(u - u_\sigma)^2 - \frac{\delta}{2} \|u - u_\sigma\|_{L^2(I)}^2. \quad (4.9)$$

From second order optimality condition there exists $\delta > 0$ (see [Theorem 3.8, Lemma 4.6, [9]]) such that,

$$j''(u)(u - u_\sigma)^2 \geq \delta \|u - u_\sigma\|_{L^2(I)}^2. \quad (4.10)$$

Using (4.10) in (4.9), (2.16) and (3.34), we obtain

$$\begin{aligned}\frac{\delta}{2} \|u - u_\sigma\|_{L^2(I)}^2 &\leq j'(u)(u - u_\sigma) - j'(u_\sigma)(u - u_\sigma) \\ &\leq j'_\sigma(u_\sigma)(u - u_\sigma) - j'(u_\sigma)(u - u_\sigma) + j'_\sigma(u_\sigma)(u - u_\sigma) \\ &= \left(\int_\Omega \alpha(z_\sigma - z_{u_\sigma}) dx, u - u_\sigma \right)_I + \left(\int_\Omega \alpha z_\sigma dx + \beta_3 u_\sigma, u - u_\sigma \right)_I.\end{aligned}$$

Using Cauchy-Schwartz and Young's inequality with Young's constant as $\delta/4$, we obtain

$$\frac{\delta}{4} \|u - u_\sigma\|_{L^2(I)}^2 \leq C \left(\max_\Omega |\alpha| \sum_{n=1}^N \sum_{T \in \mathcal{T}_h} \|z_\sigma + \beta_3 u_\sigma\|_{L^2(I_n, K)}^2 + \|z_\sigma - z_{u_\sigma}\|_{L^2(I, \Omega)}^2 \right) \quad \forall k \leq k_\epsilon.$$

Theorem 4.4 For a fixed control $u_\sigma \in U_{d,ad}$, let $(\theta_{u_\sigma}, a_{u_\sigma})$ and $(\theta_\sigma, a_\sigma)$ be respectively the solutions of (2.8)-(2.11) and (3.26)-(3.29) with $(z_{u_\sigma}, \lambda_{u_\sigma})$ and $(z_\sigma, \lambda_\sigma)$ as the corresponding adjoint solutions. Then,

$$\|z_{u_\sigma} - z_\sigma\|^2 + \|\lambda_{u_\sigma} - \lambda_\sigma\|^2 \leq C \left(\sum_{j=1}^9 \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{j,n,K}^2 + \|\theta_{u_\sigma} - \theta_\sigma\|^2 \right),$$

where

$$\left. \begin{aligned}\eta_{1,n,K}^2 &= h_K^4 \|r_z(x, t)\|_{I_n, K}^2, \\ r_z(x, t) &= -(\rho c_p \partial_t z_\sigma + \beta_2 [\theta_\sigma - \theta_m]_+ + \mathcal{K} \Delta z_\sigma + \rho c_p \frac{[z_\sigma]_{n-1}}{k_n} - f_\theta(\theta_\sigma, a_\sigma)(\rho L z_\sigma - \lambda_\sigma)) \\ \eta_{2,n,K}^2 &= k_n^2 (\|[\theta_\sigma - \theta_m]_+\|_{I_n, K}^2 + \|\Delta z_\sigma\|_{I_n, K}^2 + \|\rho L z_\sigma - \lambda_\sigma\|_{I_n, K}^2), \\ \eta_{3,n,K}^2 &= h_K^3 \|\mathcal{K}[\nabla z_\sigma] \cdot \mathbf{n}\|_{L^2(I_n, L^2(\partial K))}^2, \quad \eta_{4,n,K}^2 = \|z_\sigma\|_{I_n, K}^2, \\ \eta_{5,n,K}^2 &= k_n \| [z_\sigma]_{n-1} \|_{I_n, K}^2, \quad \eta_{6,n,K}^2 = k_n^2 \|\rho L z_\sigma - \lambda_\sigma\|_{I_n, K}^2, \\ \eta_{7,n,K}^2 &= \|\lambda_\sigma\|_{I_n, K}^2, \quad \eta_{8,n,K}^2 = \|z_\sigma\|_{I_n, K}^2, \quad \eta_{9,n,K}^2 = k_n \|[\lambda_\sigma]_{n-1}\|_{I_n, K}^2.\end{aligned}\right\} \quad (4.11)$$

Proof: Consider the auxiliary problem defined by: for given $g \in L^2(I, L^2(\Omega))$, find ϕ such that

$$\rho c_p \partial_t \phi - \mathcal{K} \Delta \phi + \rho L f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) \phi = g \quad \text{in } Q, \quad (4.12)$$

$$\nabla \phi \cdot \mathbf{n} = 0 \quad \text{on } \Sigma, \quad (4.13)$$

$$\phi(0) = 0 \quad \text{in } \Omega, \quad (4.14)$$

where $\nabla \phi \cdot \mathbf{n}$ denotes the outward normal derivative to $\partial \Omega$. Then the solution to (4.12)-(4.14) satisfies (see [12]):

$$\|\phi\|_{L^\infty(I; L^2(\Omega))} \leq C \|g\|_{I, \Omega}, \quad \|\phi\|_{L^2(I; H^1(\Omega))} \leq C \|g\|_{I, \Omega}, \quad (4.15)$$

$$\|\phi\|_{L^2(I; H^2(\Omega))} \leq C \|g\|_{I, \Omega}, \quad \|\partial_t \phi\|_{I, \Omega} \leq C \|g\|_{I, \Omega}. \quad (4.16)$$

Substitute $g = z_\sigma - z_{u_\sigma}$ in (4.12) and consider

$$\begin{aligned} \|z_\sigma - z_{u_\sigma}\|_{I, \Omega}^2 &= \int_0^T (z_\sigma - z_{u_\sigma}, \rho c_p \partial_t \phi - \mathcal{K} \Delta \phi + \rho L f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) \phi) ds \\ &= \sum_{n=1}^N \int_{I_n} \left(-\rho c_p (\partial_t (z_\sigma - z_{u_\sigma}), \phi) + \mathcal{K} (\nabla (z_\sigma - z_{u_\sigma}), \nabla \phi) \right. \\ &\quad \left. + (\rho L f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) (z_\sigma - z_{u_\sigma}), \phi) \right) ds - \rho c_p \sum_{n=1}^N ([z_\sigma]_{n-1}, \phi_{n-1}). \end{aligned} \quad (4.17)$$

Adding and subtracting the terms $(\beta_2 [\theta_\sigma - \theta_m]_+, \phi)$, $(f_\theta(\theta_\sigma, a_\sigma) (\rho L z_\sigma - \lambda_\sigma), \phi)$, $(f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) \lambda_{u_\sigma}, \phi)$, $\rho c_p (\frac{[z_\sigma]_{n-1}}{k_n}, \phi)$ on the right hand side of (4.17) and using (2.12)-(2.15), we obtain

$$\begin{aligned} \|z_\sigma - z_{u_\sigma}\|_{I, \Omega}^2 &= \sum_{n=1}^N \left[\int_{I_n} \left(-\rho c_p (\partial_t z_\sigma, \phi) - (\beta_2 [\theta_\sigma - \theta_m]_+, \phi) + \mathcal{K} (\nabla z_\sigma, \nabla \phi) \right. \right. \\ &\quad \left. \left. + (f_\theta(\theta_\sigma, a_\sigma) (\rho L z_\sigma - \lambda_\sigma), \phi) + \beta_2 ([\theta_\sigma - \theta_m]_+ - [\theta_{u_\sigma} - \theta_m]_+, \phi) \right. \right. \\ &\quad \left. \left. - (\rho c_p \frac{[z_\sigma]_{n-1}}{k_n}, \phi) + \rho c_p (\frac{[z_\sigma]_{n-1}}{k_n}, \phi - \phi_{n-1}) + (f_\theta(\theta_\sigma, a_\sigma) \lambda_\sigma - f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) \lambda_{u_\sigma}, \phi) \right. \right. \\ &\quad \left. \left. + (\rho L (f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) - f_\theta(\theta_\sigma, a_\sigma)) z_\sigma, \phi) \right) ds \right] \end{aligned} \quad (4.18)$$

Adding (3.32), with ϕ replaced by ϕ_I , to the right hand side of (4.18) and then, adding and subtracting $(\rho c_p \frac{[z_\sigma]_{n-1}}{k_n}, \phi_I)$, we have

$$\begin{aligned} \|z_\sigma - z_{u_\sigma}\|_{I, \Omega}^2 &= \sum_{n=1}^N \left[\int_{I_n} \left(-\rho c_p (\partial_t z_\sigma, \phi - \phi_I) - (\beta_2 [\theta_\sigma - \theta_m]_+, \phi - \phi_I) + \mathcal{K} (\nabla z_\sigma, \nabla (\phi - \phi_I)) \right. \right. \\ &\quad \left. \left. + (f_\theta(\theta_\sigma, a_\sigma) (\rho L z_\sigma - \lambda_\sigma), \phi - \phi_I) + (\rho L (f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) - f_\theta(\theta_\sigma, a_\sigma)) z_\sigma, \phi) \right. \right. \\ &\quad \left. \left. + \beta_2 ([\theta_\sigma - \theta_m]_+ - [\theta_{u_\sigma} - \theta_m]_+, \phi) - (\rho c_p \frac{[z_\sigma]_{n-1}}{k_n}, \phi - \phi_I) + (f_\theta(\theta_\sigma, a_\sigma) \lambda_\sigma - f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) \lambda_{u_\sigma}, \phi) \right. \right. \\ &\quad \left. \left. + \rho c_p (\frac{[z_\sigma]_{n-1}}{k_n}, (\phi_I)_{n-1} - \phi_I + \phi - \phi_{n-1}) \right) ds \right] \end{aligned}$$

Integrating the 3^{rd} term on the right hand side by parts and grouping the terms, we obtain

$$\begin{aligned}
& \|z_\sigma - z_{u_\sigma}\|_{I, \Omega}^2 \\
&= \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \left[\int_{I_n} \left(-(\rho c_p \partial_t z_\sigma + \mathcal{K} \Delta z_\sigma - f_\theta(\theta_\sigma, a_\sigma^*)(\rho L z_\sigma - \lambda_\sigma) + \rho c_p \frac{[z_\sigma]_{n-1}}{k_n} + \beta_2 [\theta_\sigma - \theta_m]_+, \phi - \phi_I)_K \right. \right. \\
&\quad + \mathcal{K}([\nabla z_\sigma] \cdot \mathbf{n}, \phi - \phi_I)_{L^2(\partial K)} + \beta_2([\theta_\sigma - \theta_m]_+ - [\theta_{u_\sigma} - \theta_m]_+, \phi)_K + (f_\theta(\theta_\sigma, a_\sigma) \lambda_\sigma - f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) \lambda_{u_\sigma}, \phi)_K \\
&\quad \left. \left. + (\rho L(f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) - f_\theta(\theta_\sigma, a_\sigma)) z_\sigma, \phi)_K + \rho c_p \left(\frac{[z_\sigma]_{n-1}}{k_n}, (\phi_I)_{n-1} - \phi_I + \phi - \phi_{n-1} \right)_K \right) ds \right] \\
&= \mathcal{J}_1 + \mathcal{J}_2 + \mathcal{J}_3 + \mathcal{J}_4 + \mathcal{J}_5 + \mathcal{J}_6, \text{ say,} \tag{4.19}
\end{aligned}$$

Let $r_z(x, t) = -(\rho c_p \partial_t z_\sigma + \mathcal{K} \Delta z_\sigma - f_\theta(\theta_\sigma, a_\sigma)(\rho L z_\sigma - \lambda_\sigma) + \rho c_p \frac{[z_\sigma]_{n-1}}{k_n} + \beta_2 [\theta_\sigma - \theta_m]_+)$. Then

$$\mathcal{J}_1 = \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} (r_z(x, t), \pi_n \phi - \phi_I)_K ds + \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} (r_z(x, t), \phi - \pi_n \phi)_K ds \tag{4.20}$$

Using Cauchy-Schwarz's inequality and (4.1), we obtain

$$\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} (r_z(x, t), \pi_n \phi - \phi_I)_K ds \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} h_K^2 \|r_z(x, t)\|_{I_n, K} \|\phi\|_{L^2(I_n; H^2(K))}. \tag{4.21}$$

Use Cauchy-Schwarz's inequality and definition of the L^2 -projection operator to obtain

$$\begin{aligned}
\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} (r_z(x, t), \phi - \pi_n \phi)_K ds &\leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} k_n (\|\theta_\sigma - \theta_m\|_{I_n, K} + \|\Delta z_\sigma\|_{I_n, K} \\
&\quad + \|\rho L z_\sigma - \lambda_\sigma\|_{I_n, K}) \|\partial_t \phi\|_{I_n, K}, \tag{4.22}
\end{aligned}$$

Using (4.21) and (4.22) in (4.20), we obtain

$$\begin{aligned}
\mathcal{J}_1 &\leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \left(h_K^2 \|r_z(x, t)\|_{I_n, K} \|\phi\|_{L^2(I_n; H^2(K))} + k_n (\|\theta_\sigma - \theta_m\|_{I_n, K} + \|\Delta z_\sigma\|_{I_n, K} \right. \\
&\quad \left. + \|\rho L z_\sigma - \lambda_\sigma\|_{I_n, K}) \|\partial_t \phi\|_{I_n, K} \right).
\end{aligned}$$

Using Cauchy-Schwarz's inequality, (4.1) and (4.2), we obtain

$$\mathcal{J}_2 \leq C \left(\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} h_K^{\frac{3}{2}} \|\mathcal{K}[\nabla z_\sigma] \cdot \mathbf{n}\|_{L^2(I_n, L^2(\partial K))} \|\phi\|_{L^2(I_n, H^2(K))} \right)$$

Consider,

$$\mathcal{J}_3 = \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} (\beta_2([\theta_\sigma - \theta_m]_+ - [\theta_{u_\sigma} - \theta_m]_+), \phi)_K ds \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \|\theta_\sigma - \theta_{u_\sigma}\|_{I_n, K} \|\phi\|_{I_n, K}.$$

Using Remark 2.2 and Cauchy-Schwarz's inequality, we obtain

$$\mathcal{J}_4 = \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} \left((f_\theta(\theta_\sigma, a_\sigma) \lambda_\sigma - f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) \lambda_{u_\sigma}, \phi)_K \right) ds \leq \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \|\lambda_\sigma - \lambda_{u_\sigma}\|_{I_n, K} \|\phi\|_{I_n, K}.$$

Repeating similar calculations as for the term \mathcal{J}_4 , we obtain

$$\mathcal{J}_5 = \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} (\rho L(f_\theta(\theta_{u_\sigma}, a_{u_\sigma}) - f_\theta(\theta_\sigma, a_\sigma)) z_\sigma, \phi)_K ds \leq C \left(\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \|z_\sigma\|_{I_n, K} \|\phi\|_{I_n, K} \right).$$

Also, we have

$$\begin{aligned} \mathcal{J}_6 &= \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} \left(\rho c_p \left(\frac{[z_\sigma]_{n-1}}{k_n}, (\phi_I)_{n-1} - \phi_I + \phi - \phi_{n-1} \right)_K \right) ds \\ &\leq C \left(\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} k_n^{\frac{1}{2}} \|[z_\sigma]_{n-1}\|_K \left(\|\partial_t \phi_I\|_{I_n, K} + \|\partial_t \phi\|_{I_n, K} \right) \right). \end{aligned}$$

Now consider the auxiliary problem: for $G \in L^2(I, L^2(\Omega))$, find $\psi \in H^1(I, L^2(\Omega))$ such that

$$\partial_t \psi - f_a(\theta_{u_\sigma}, a_{u_\sigma}) \psi = G \quad \text{in } Q, \quad (4.23)$$

$$\psi(0) = 0 \quad \text{in } \Omega. \quad (4.24)$$

(4.23)-(4.24) has a unique solution and we have (see [12]):

$$\|\psi\|_{L^\infty(I; L^2(\Omega))} \leq C \|G\|_{I, \Omega}, \quad \|\partial_t \psi\|_{I, \Omega} \leq C \|G\|_{I, \Omega}. \quad (4.25)$$

Let $G = \lambda_\sigma - \lambda_{u_\sigma}$ in (4.23) to obtain

$$\begin{aligned} \|\lambda_\sigma - \lambda_{u_\sigma}\|_{I, \Omega}^2 &= \int_0^T (\lambda_\sigma - \lambda_{u_\sigma}, \partial_t \psi - f_a(\theta_{u_\sigma}, a_{u_\sigma}) \psi) ds \\ &= \sum_{n=1}^N \left[\int_{I_n} \left(-(\partial_t(\lambda_\sigma - \lambda_{u_\sigma}), \psi) - (f_a(\theta_\sigma, a_\sigma)(\lambda_\sigma - \lambda_{u_\sigma}), \psi) \right) ds \right. \\ &\quad \left. - ([\lambda_\sigma]_{n-1}, \psi_{n-1}) \right]. \end{aligned} \quad (4.26)$$

Adding (3.30), with ψ replaced by ψ_I , to the right hand side of the (4.26), we obtain

$$\begin{aligned} \|\lambda_\sigma - \lambda_{u_\sigma}\|_{I, \Omega}^2 &= \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \left[\int_{I_n} \left((r_\lambda(x, t), \psi - \psi_I)_K - ((f_a(\theta_{u_\sigma}, a_{u_\sigma}) - f_a(\theta_\sigma, a_\sigma)) \lambda_\sigma, \psi)_K \right. \right. \\ &\quad \left. \left. - (\rho L (f_a(\theta_\sigma, a_\sigma) - f_a(\theta_{u_\sigma}, a_{u_\sigma})) z_\sigma, \psi)_K - (\rho L f_a(\theta_{u_\sigma}, a_{u_\sigma})(z_\sigma - z_{u_\sigma}), \psi)_K \right. \right. \\ &\quad \left. \left. + \left(\frac{[\lambda_\sigma]_{n-1}}{k_n}, (\psi_I)_{n-1} + \psi - \psi_I - \psi_{n-1} \right)_K \right) ds \right] \\ &= \mathcal{J}_7 + \mathcal{J}_8 + \mathcal{J}_9 + \mathcal{J}_{10} + \mathcal{J}_{11}, \quad \text{say} \end{aligned} \quad (4.27)$$

where $r_\lambda(x, t) = -\partial_t \lambda_\sigma + f_a(\theta_\sigma, a_\sigma)(\rho L z_\sigma - \lambda_\sigma) - \frac{[\lambda_\sigma]_{n-1}}{k_n}$. Using Remark 2.2, Cauchy Schwarz inequality, (4.5) and proceeding in a similar way as (4.21) and (4.22), we obtain

$$\mathcal{J}_7 = \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} (r_\lambda(x, t), \psi - \psi_I)_K ds \leq C \left(\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} k_n \|\rho L z_\sigma - \lambda_\sigma\|_{I_n, K} \|\partial_t \psi\|_{I_n, K} \right) \quad (4.28)$$

$$\mathcal{J}_8 = \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} ((f_a(\theta_{u_\sigma}, a_{u_\sigma}) - f_a(\theta_\sigma, a_\sigma)) \lambda_\sigma, \psi)_K ds \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \|\lambda_\sigma\|_{I_n, K} \|\psi\|_{I_n, K}. \quad (4.29)$$

Similarly,

$$\mathcal{J}_9 \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \|z_\sigma\|_{I_n, K} \|\psi\|_{I_n, K} \quad (4.30)$$

and

$$\mathcal{J}_{10} \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \|z_\sigma - z_{u_\sigma}\|_{I_n, K} \|\psi\|_{I_n, K}. \quad (4.31)$$

$$\mathcal{J}_{11} \leq C \left(\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} k_n^{\frac{1}{2}} \|\lambda_\sigma\|_{n-1} \|K\| (\|\partial_t \psi_I\|_{I_n, K} + \|\partial_t \psi\|_{I_n, K}) \right). \quad (4.32)$$

Now adding (4.19) and (4.27), using estimates for \mathcal{J}_1 to \mathcal{J}_{11} and then using (4.15)-(4.16) with $g = z_{u_\sigma} - z_\sigma$, (4.25) with $G = \lambda_{u_\sigma} - \lambda_\sigma$ and Young's inequality, with Young's constants chosen appropriately, we obtain

$$\|z_\sigma - z_{u_\sigma}\|_{I, \Omega}^2 + \|\lambda_\sigma - \lambda_{u_\sigma}\|_{I, \Omega}^2 \leq C \left(\sum_{i=1}^9 \eta_{i,n,K}^2 + \|\theta_\sigma - \theta_{u_\sigma}\|_{I, \Omega}^2 \right), \quad (4.33)$$

where $\eta_{i,n,k}, i = 1, \dots, 11$ are defined in (4.11). This completes the proof. \square

Theorem 4.5 For a fixed control $u_\sigma \in U_{d,ad}$, let $(\theta_{u_\sigma}, a_{u_\sigma})$ and $(\theta_\sigma, a_\sigma)$ be respectively the solutions of (2.8)-(2.11) and (3.26)-(3.29). Then,

$$\|\theta_{u_\sigma} - \theta_\sigma\|^2 + \|a_{u_\sigma} - a_\sigma\|^2 \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \left(\sum_{j=10}^{13} \eta_{j,n,K}^2 + \eta_{a,n,K}^2 \right),$$

where

$$\left. \begin{aligned} \eta_{10,n,K}^2 &= h_K^4 \|r_\theta(x, t)\|_{I_n, K}^2, \\ r_\theta(x, t) &= \rho c_p \partial_t \theta_\sigma - \alpha u_\sigma + \rho L f(\theta_\sigma, a_\sigma) - \mathcal{K} \Delta \theta_\sigma + \rho c_p \frac{[\theta_\sigma]_n}{k_n}, \\ \eta_{11,n,K}^2 &= k_n^2 \|\rho L f(\theta_\sigma, a_\sigma) - \mathcal{K} \Delta \theta_\sigma\|_{I_n, K}^2, \\ \eta_{12,n,K}^2 &= h_K^3 \|\mathcal{K}[\nabla \theta_\sigma] \cdot \mathbf{n}\|_{L^2(I_n, L^2(\partial K))}^2, \quad \eta_{13,n,K}^2 = k_n \|\theta_\sigma\|_n^2, \\ \eta_{a,n,K}^2 &= k_n^2 \|f(\theta_\sigma, a_\sigma)\|_{I_n, K}^2 + k_n \|[a_\sigma]_n\|_K^2. \end{aligned} \right\} \quad (4.34)$$

Proof: Consider the problem: for a given $g \in L^2(I, L^2(\Omega))$, find $v \in H^1(\Omega)$ such that

$$-\rho c_p \partial_t v - \mathcal{K} \Delta v + \rho L F v = g_1 \quad \text{in } Q, \quad (4.35)$$

$$\partial v \cdot \mathbf{n} = 0 \quad \text{on } \Sigma \quad (4.36)$$

$$v(T) = 0 \quad \text{in } \Omega, \quad (4.37)$$

where

$$F = \begin{cases} -\frac{f(\theta_{u_\sigma}, a_{u_\sigma}) - f(\theta_\sigma, a_\sigma)}{\theta_\sigma - \theta_{u_\sigma}} & \text{whenever } \theta_\sigma \neq \theta_{u_\sigma} \\ f_\theta(\theta_\sigma, a_\sigma) & \theta_\sigma = \theta_{u_\sigma}. \end{cases}$$

Moreover, we have (see [12]):

$$\|v\|_{L^\infty(I; L^2(\Omega))} \leq C \|g_1\|_{I, \Omega}, \quad \|v\|_{L^2(I; H^1(\Omega))} \leq C \|g_1\|_{I, \Omega}, \quad (4.38)$$

$$\|v\|_{L^1(I; H^2(\Omega))} \leq C \|g_1\|_{I, \Omega}, \quad \|\partial_t v\|_{I, \Omega} \leq C \|g_1\|_{I, \Omega}. \quad (4.39)$$

Put $g_1 = \theta_\sigma - \theta_{u_\sigma}$ in (4.35) and consider

$$\begin{aligned} \|\theta_\sigma - \theta_{u_\sigma}\|_{I, \Omega}^2 &= \int_0^T (\theta_\sigma - \theta_{u_\sigma}, -\rho c_p \partial_t v - \mathcal{K} \Delta v + \rho L F v) ds \\ &= \sum_{n=1}^N \int_{I_n} \left((\rho c_p \partial_t (\theta_\sigma - \theta_{u_\sigma}), v) + \mathcal{K} (\nabla (\theta_\sigma - \theta_{u_\sigma}), \nabla v) \right. \\ &\quad \left. - (\rho L (f(\theta_{u_\sigma}, a_{u_\sigma}) - f(\theta_\sigma, a_\sigma)), v) + \rho c_p \left(\frac{[\theta]_n}{k_n}, v_n \right) \right) ds. \end{aligned} \quad (4.40)$$

Replacing v by v_I in (3.29) and adding to the right hand side of (4.40), we obtain

$$\begin{aligned} \|\theta_\sigma - \theta_{u_\sigma}\|_{I,\Omega}^2 &= \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} \left((\rho c_p \partial_t \theta_\sigma - \alpha u_\sigma + \rho Lf(\theta_\sigma, a_\sigma) - \mathcal{K} \Delta \theta_\sigma, v - v_I)_K \right. \\ &\quad \left. + \mathcal{K}(\nabla \theta_\sigma \cdot \mathbf{n}, v)_{L^2(\partial K)} + \rho c_p \left(\frac{[\theta_\sigma]_n}{k_n}, v_n - (v_I)_n \right)_K \right) ds \end{aligned}$$

Letting $r_\theta(x, t) = \rho c_p \partial_t \theta_\sigma - \alpha u_\sigma + \rho Lf(\theta_\sigma, a_\sigma) - \mathcal{K} \Delta \theta_\sigma + \rho c_p \frac{[\theta_\sigma]_n}{k_n}$ and adding, subtracting $(\rho c_p \frac{[\theta_\sigma]_n}{k_n}, v - v_I)$ to the right hand side of the above equation, we obtain

$$\begin{aligned} \|\theta_\sigma - \theta_{u_\sigma}\|_{I,\Omega}^2 &= \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} \left((r_\theta(x, t), v - v_I)_K + \mathcal{K}(\nabla \theta_\sigma \cdot \mathbf{n}, v)_{L^2(\partial K)} \right. \\ &\quad \left. - \rho c_p \left(\frac{[\theta_\sigma]_n}{k_n}, (v_I)_n + v - v_I - v_n \right)_K \right) ds \\ &= \mathcal{J}_1 + \mathcal{J}_2 + \mathcal{J}_3, \text{ say} \end{aligned} \tag{4.41}$$

Using Cauchy-Schwarz inequality, (4.1), (4.38)-(4.39) with $g_1 = \theta_\sigma - \theta_{u_\sigma}$ and proceeding in a similar way as (4.21) and (4.22), we obtain

$$\mathcal{J}_1 \leq \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \left(h_K^2 \|r_\theta(x, t)\|_{I_n, K}^2 + k_n \|\rho Lf(\theta_\sigma, a_\sigma) - \mathcal{K} \Delta \theta_\sigma\|_{I_n, K}^2 \right) \|\theta_\sigma - \theta_{u_\sigma}\|_{I_n, K}$$

Repeating the same steps used in the calculation of the term \mathcal{J}_2 in Theorem 4.3, we obtain

$$\mathcal{J}_2 \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \left(h_K^{\frac{3}{2}} \|\mathcal{K}[\nabla \theta_\sigma] \cdot \mathbf{n}\|_{L^2(I_n, L^2(\partial K))} \right) \|\theta_\sigma - \theta_{u_\sigma}\|_{I_n, K}$$

Also,

$$\mathcal{J}_3 \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} k_n^{\frac{1}{2}} \|[\theta_\sigma]_n\|_{I_n, K} \|\theta_\sigma - \theta_{u_\sigma}\|_{I_n, K}.$$

Using the estimates for \mathcal{J}_1 to \mathcal{J}_3 in (4.41) and Young's inequality, we obtain

$$\|\theta_\sigma - \theta_{u_\sigma}\|_{I,\Omega}^2 \leq C \left(\sum_{i=10}^{13} \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{i,n,K}^2 + \mu_3 \|\theta_\sigma - \theta_{u_\sigma}\|_{I,\Omega}^2 \right), \tag{4.42}$$

where $\eta_{i,n,K}$, $i = 10, 11, 12, 13$ are defined by (4.34). Choosing Young's constant in (4.42) such that $C\mu_3 < 1$, we have

$$\|\theta_\sigma - \theta_{u_\sigma}\|_{I,\Omega}^2 \leq C \left(\sum_{i=10}^{13} \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{i,n,K}^2 \right). \tag{4.43}$$

Now we proceed to estimate $\|a_{u_\sigma} - a_\sigma\|$.

Consider the problem: given $g \in L^2(\Omega)$, find w such that

$$-\partial_t w = F_1 w + G_1 \quad \text{in } Q, \tag{4.44}$$

$$w(T) = 0, \tag{4.45}$$

where

$$F_1 = \begin{cases} \frac{f(\theta_\sigma, a_\sigma) - f(\theta_{u_\sigma}, a_{u_\sigma})}{a_\sigma - a_{u_\sigma}} & \text{whenever } a_{u_\sigma} \neq a_\sigma \\ f_a(\theta_\sigma, a_\sigma) & a_{u_\sigma} = a_\sigma. \end{cases}$$

Moreover, we have:

$$\|w\|_{L^\infty(I; L^2(\Omega))} \leq C \|G_1\|_{I, \Omega}, \quad \|\partial_t w\|_{I, \Omega} \leq C \|G_1\|_{I, \Omega}. \quad (4.46)$$

Substitute $G_1 = a_\sigma - a_{u_\sigma}$ in (4.44), use Cauchy-Schwarz's inequality, Young's inequality, (4.4) and (4.46) to obtain

$$\begin{aligned} \|a_\sigma - a_{u_\sigma}\|_{I, \Omega}^2 &= \int_0^T (a_\sigma - a_{u_\sigma}, -\partial_t w - F_1 w) ds \\ &= \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} \left((\partial_t((a_\sigma - a_{u_\sigma}), w)_K - (F_1(a_\sigma - a_{u_\sigma}), w)_K + \left(\frac{[a_\sigma]_n}{k_n}, w_n\right)) \right) ds \\ &= \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \int_{I_n} \left((\partial_t a_\sigma - f(\theta_\sigma, a_\sigma) + \frac{[a_\sigma]_n}{k_n}, w - w_I)_K \right. \\ &\quad \left. + \left(\frac{[a_\sigma]_n}{k_n}, (w_I)_n - w + w_I - w_n\right) \right) ds \\ &\leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \left(k_n^2 \|f(\theta_\sigma, a_\sigma)\|_{I_n, K} + k_n \|[a_\sigma]_n\|_K^2 \right) + \mu_4 \|a_{u_\sigma} - a_\sigma\|_{I, \Omega}^2, \\ &\leq C \left(\sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{a, n, K}^2 + \mu_4 \|a_{u_\sigma} - a_\sigma\|_{I, \Omega}^2 \right). \end{aligned}$$

Choose Young's constant such that $C\mu_4 < 1$ to obtain

$$\|a_{u_\sigma} - a_\sigma\|^2 \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{a, n, K}^2, \quad (4.47)$$

where $\eta_{a, n, K}^2$ is defined in (4.34). Adding (4.43) and (4.47), we obtain the required result. This completes the proof. \square

Remark 4.4 The *a posteriori* error estimates obtained in Theorem 4.4 can be divided into errors due to space and time discretizations, that is,

$$\begin{aligned} \|\theta^*(u_\sigma^*) - \theta_\sigma^*\|_{I, \Omega}^2 + \|z^*(u_\sigma^*) - z_\sigma^*\|_{I, \Omega}^2 + \|a^*(u_\sigma^*) - a_\sigma^*\|_{I, \Omega}^2 + \|\lambda^*(u_\sigma^*) - \lambda_\sigma^*\|_{I, \Omega} \\ \leq \eta_h + \eta_k, \end{aligned}$$

where η_h and η_k are the errors occurred due to space and time discretizations and are given by

$$\begin{aligned} \eta_k &= C \left(\sum_{i=2,5,6,9,11,13} \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{i, n, K}^2 + \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{a, n, K}^2 \right), \\ \eta_h &= C \sum_{i=1,3,4,7,8,10,12} \sum_{n=1}^N \sum_{K \in \mathcal{T}_h} \eta_{i, n, K}^2. \end{aligned}$$

Remark 4.5 Note that a $\text{cg}(1)\text{dg}(0)$ space-time discretization yields us the *a posteriori* error estimates. Higher order polynomial approximation help to obtain better estimates in Theorems 4.3 and 4.4, provided we have higher regularity assumptions on the solution.

5 Numerical Experiments

In this section, the AFEM algorithm using residual method is presented. We use the error estimates obtained in Theorem 4.4 and Theorem 4.5 for the adaptive refinement. A cg(1)dg(0) approximation has been used for space and time discretizations in the implementation. The control variable is discretized using piece wise constants. The parameters in (2.11) used are given by [31] $\rho c_p = 4.91 \frac{J}{cm^3 K}$, $k = 0.64 \frac{J}{cm^3 K}$ and $\rho L = 627.9 \frac{J}{cm^3 K}$. The regularized monotone function \mathcal{H}_ϵ is chosen as

$$\mathcal{H}_\epsilon(s) = \begin{cases} 1 & s \geq \epsilon \\ 10(\frac{s}{\epsilon})^6 - 24(\frac{s}{\epsilon})^5 + 15(\frac{s}{\epsilon})^4 & 0 < s \leq \epsilon \\ 0 & s \leq 0 \end{cases}$$

where $\epsilon = 0.15$. The initial temperature θ_0 and the melting temperature θ_m are chosen as 20 and 1800, respectively. Pointwise data for $aeq(\theta)$ and $\tau(\theta)$ are given by

θ	730	830	840	930
$aeq(\theta)$	0	0.91	1	1
$\tau(\theta)$	1	0.2	0.18	0.05

The shape function $\alpha(x, y, t)$ is given by $\alpha(x, y, t) = \frac{4k_1 A}{\pi D^2} \exp(-\frac{2(x-vt)^2}{D^2}) \exp(k_1 y)$, where $D = 0.47cm$, $k_1 = 60/cm$, $A = 0.3cm$ and $v = 1cm/s$. Nonlinear conjugate gradient method has been used for implementation and the tolerance is chosen as 10^{-7} .

To start with the adaptivity procedure first the problem is solved on the initial triangulation given by Figure 2. Table 1 shows the convergence of solution as the mesh refinement is performed using a posteriori estimates.

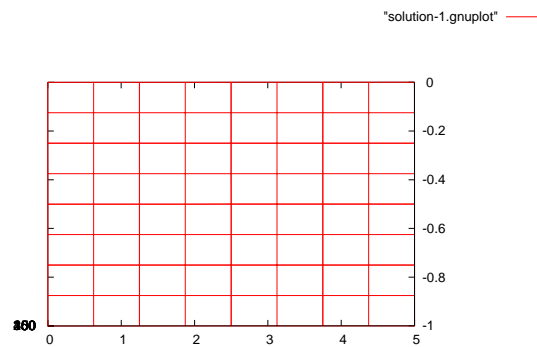


Fig. 2: Initial approximate triangulation

Figure 3 shows the development of meshes over adaptive loop. It depicts that the triangulation gets more and more refined near the zone of heating, which is the boundary area. Figure 4 shows that increment in the mesh size causes the decrease in the error. Figure 5 depicts the austenite value at the final step on the final adaptive mesh using residual type estimator. Figure 6 shows temperature θ on the final mesh. Figure 7 shows the control at the final time $T = 5.25$.

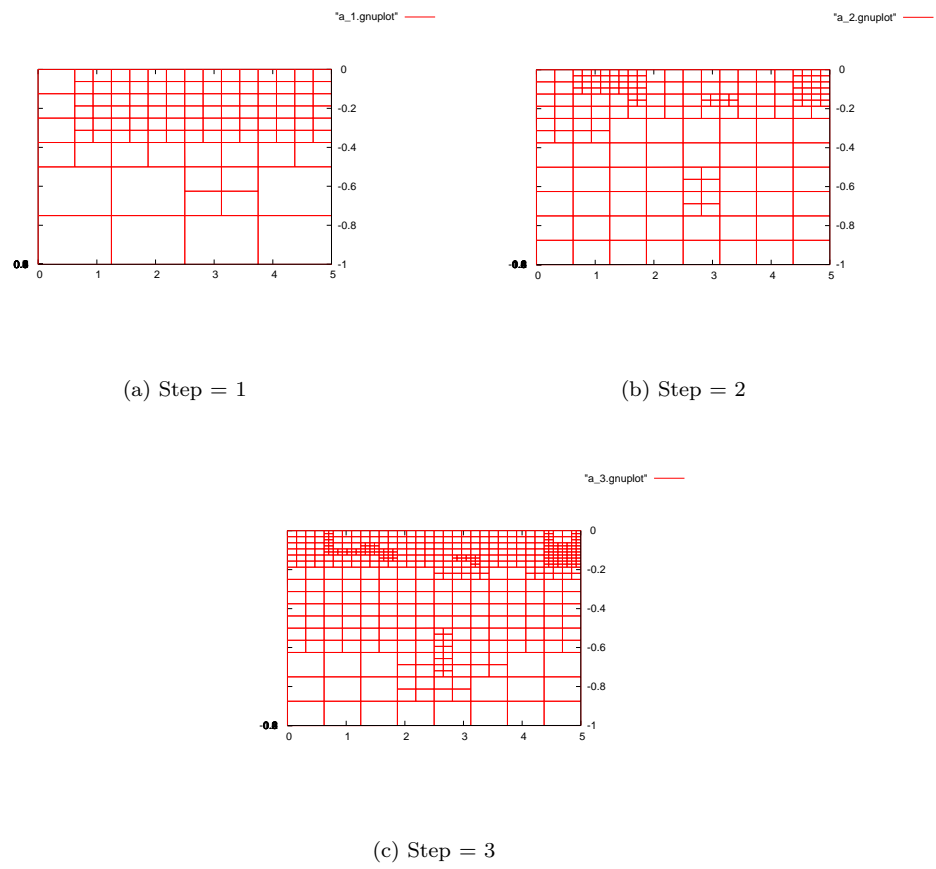


Fig. 3: Adaptive refinement

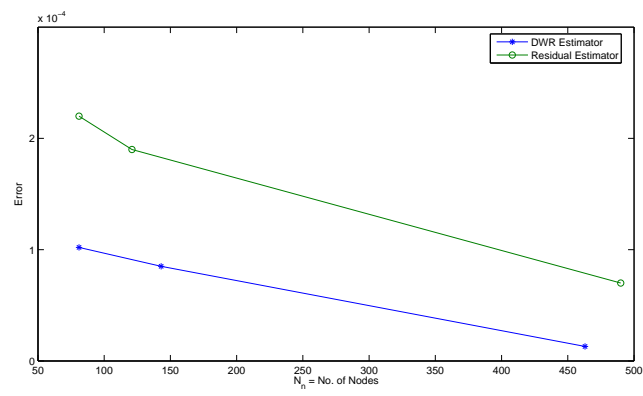


Fig. 4: Error graphs

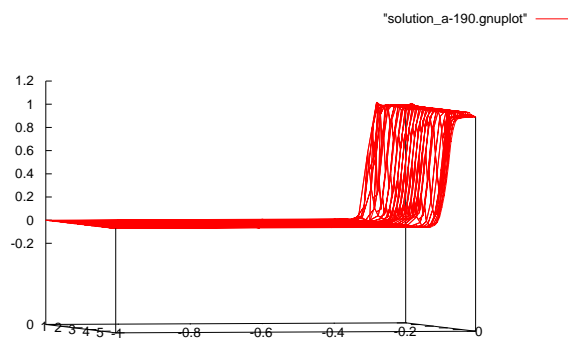
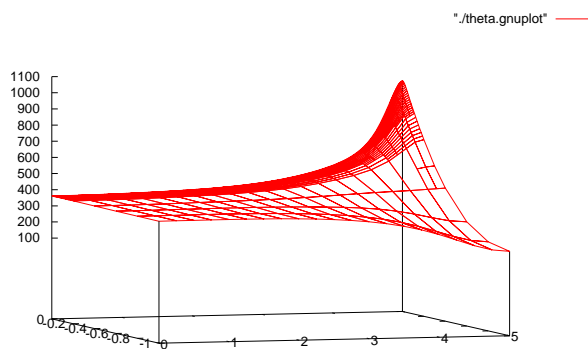
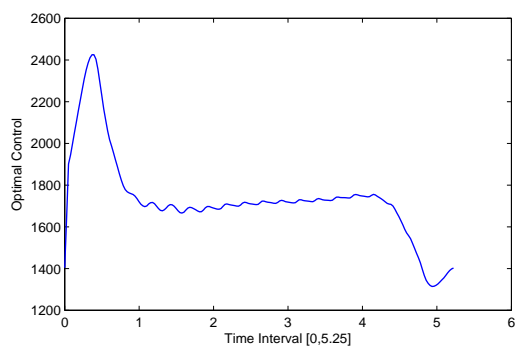
Fig. 5: The volume fraction of the austenite at time $t = T$ Fig. 6: The temperature at time $t = T$ 

Fig. 7: Control

N_n	η_h/J
81	0.00022
143	0.00019
463	0.00007

Table 1: **Error in space for fixed time partition 100**

Conclusion

An adaptive finite element method has helped in obtaining the mesh which depends on approximate solution and data. It has been shown that the mesh obtained using residual type *a posteriori* error estimate has helped in getting a approximate solution to the laser surface hardening of steel problem.

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