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THE FINITE ELEMENT METHOD FOR PARABOLIC EQUATIONS
II. A POSTERIORI ERROR ESTIMATION AND ADAPTIVE APPROACH

by

M. Bieterman

and

I. Babuška

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THE FINITE ELEMENT METHOD FOR PARABOLIC EQUATIONS,

II. A POSTERIORI ERROR ESTIMATION AND ADAPTIVE APPROACH

Technical Note BN-984

by

M. Bieterman [1]

and

I. Babuška [2]

1 Laboratory of Applied Studies
Division of Computer Research and Technology
National Institutes of Health
Bethesda, MD 20205

2 Institute for Physical Science and Technology
and Department of Mathematics
University of Maryland
College Park, MD 20742

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Abstract/Summary:

We extend in this paper the analysis of a posteriori estimates of the space discretization error presented in a previous paper [3] for time-independent space meshes. In the context of the model problem studied there, results are given relating the effectivity of the error estimator to properties of the solution, space meshes, and manner in which the meshes change. A procedure based upon this theory is presented for the adaptive construction of time-dependent meshes. The results of some computational experiments show that this procedure is practically very effective and suggest that it can be used to control the space discretization error in more general problems.

1. Introduction

The finite element method of lines (FEMOL) is the numerical procedure used to approximate the solution of time-dependent partial differential equations (PDEs) in which a problem is first reduced, through finite element discretization of the space variables, to that of solving a system of ordinary differential equations (ODEs). Full advantage can then be taken of the efficient and reliable ODE software available to complete the computational procedure.

In order to achieve a given level of accuracy in the FEMOL, it is prudent to refine space meshes in areas of greater solution activity. If this activity is localized in different areas of space at different points of time, it then is desirable to modify the space mesh at various times, and to have decisions concerning such modifications made adaptively by the computer during the solution process. Some of the applications for which this procedure is suitable are continuum models of enzyme-catalyzed chemical reactions, the transmission of electrical nerve impulses, the propagation of flame fronts in combustion, and flow in porous media.

We mention here that the subject of mesh modification in Galerkin procedures other than the FEMOL for the solution of time-dependent PDEs has attracted much recent research.

The use of finite elements both in time and space to modify meshes was analyzed in [11], and schemes implementing versions of this technique can be found in [5] and [6]. The concept of "moving" finite elements which deform continuously in time was introduced in [13], and several interesting experimental results were presented in [10] and [14]. This approach was recently analyzed in [8], where general types of continuous and discontinuous mesh modifications were studied, and certain symmetric a priori error estimates were given.

This paper is a continuation of a previous paper [3], in which for time-independent space meshes we analyzed a posteriori estimators of the space discretization error (i.e. the total error, provided that the resulting ODE system is solved exactly) in the FEMOL solution of parabolic PDEs. An a posteriori estimator based upon computable local residuals was shown to be effective, provided certain conditions on the solution regularity, mesh family, and mesh size were satisfied. Under less restrictive conditions a modification of this principal estimator was shown to be effective.

These results are extended here to the setting of the FEMOL in which the space mesh is allowed to undergo discontinuous transitions during the solution process. An a posteriori estimator analogous to that given in [3, section 5] is shown to be effective in this setting, provided that regularity assumptions on the solution related to those given in [3, section 5] hold, the discrete data at the transition time points are properly chosen, and the mesh transitions satisfy certain conditions.

The principal tool needed in carrying out this extension is the a priori estimate presented in Thm. 3.2. This result requires assumptions related to, but in some ways less restrictive than those given in [8]. In particular, no relations need hold on the locations of points in one mesh to those in the successive mesh. This freedom is desirable when considering adaptive schemes for the construction of such meshes. The result of Thm. 3.2 is also important in that it leads to apparently new optimal order a priori error estimates, one of which is demonstrated in Thm. 3.3.

The a posteriori analysis presented forms the basis of an adaptive scheme given for the control, as well as the estimation of the space discretization error. The isolation of this component of the total error provides insight as to how such estimates and adaptive procedures can be used with state of the art ODE software to estimate and control the total error in the FEMOL.

All results are given here in the context of the model problem studied in [3] (cf. [4] for extensions mentioned in [3]). The full description of this problem, necessary preliminaries, and a discussion of some of the results for changing meshes are given in section 2. Sections 3 and 4 contain the a priori and a posteriori estimates mentioned above. In section 5 under conditions less restrictive than in section 4 it is shown that a modification of our principal estimator, which takes into account the errors introduced by the mesh transitions, is effective. An adaptive scheme is presented in section 6 and applied to examples related to those considered in [3, section 7].

In order to facilitate a first reading of this paper, some basic notions concerning a posteriori error estimates in the setting of changing meshes are presented here, and a description of how these estimates can be used in an adaptive procedure to control the space discretization error is given. The discussion is specifically oriented to the experiments described in section 6, which were directed toward the evaluation of various aspects of a posteriori estimates and adaptive procedures. By reading this description and skipping to section 6, one should obtain a good overview of the motivations behind the somewhat technical development of the theory in sections 2-5 and, more importantly, see how these ideas can be used in practice.

Let $u = u(t,x)$ be the solution of the model problem

$$(1.1)\quad \begin{cases} u_t = f - Lu = f(t,x) + [a(x)u_x]_x - b(x)u; & 0 < x < 1, \\ & 0 < t \le T_{FINAL}, \\ u(t,x) = g(t,x); \qquad x = 0,1, & 0 < t \le T_{FINAL}, \\ u(0,x) = u_0(x); & 0 < x < 1, \end{cases}$$

where $a > 0$, $b \ge 0$, u_0, g, and f are given functions. For simplicity we assume here that these functions are both smooth and compatible, but the theory does not require this.

The FEMOL approximation U of u is the solution of a weak, or integral form of eqs. (1.1), and is defined through the partitioning of the time and space intervals $(0,T_{FINAL})$ and $(0,1)$. The procedure used to create these partitions and obtain U is based upon the attempt to control for each $t \in [0,T_{FINAL}]$

$$(1.2)\quad |||e(t,\cdot)||| \equiv \left\{\int_0^1 a(x)e_x^2(t,x)dx\right\}^{1/2},$$

where $e = u - U$, according to the following principle. For any given $TOL > 0$, the partitions of $(0,1)$ used in the FEMOL should be chosen or modified at various times so that

$$(1.3)\quad |||e(t,\cdot)||| \sim TOL; \quad \forall t \in [0,T_{FINAL}].$$

Required input for the procedure are partitions

(1.4) $\Delta_0 = \{0 = x_0^0 < x_1^0 < \ldots < x_{N_0}^0 = 1\}$

and

(1.5) $\Delta^T = \{0 = T_0 < T_1 < \ldots < T_{M+1} = T_{FINAL}\}$.

The points $\{T_m\}_{m=0,M+1}$ are times when discontinuous mesh changes are permitted, although they need not occur. The first step in the algorithm is the determination of a continuous, piecewise linear function $U(0,\cdot)$ on Δ_0, which is chosen to approximate $u(0,\cdot) = u_0(\cdot)$. The norm $|||e(0,\cdot)|||$ is then estimated by

(1.6) $$E(0) = \left\{\sum_{j=1}^{N_0} \eta_{0j}^2\right\}^{1/2},$$

where the computable local error indicators $\{\eta_{0j}\}_{j=1,N_0}$ are defined by

(1.7) $$\eta_{0j}^2 = \frac{|X_j^0 - X_{j-1}^0|^2}{12a\left(\frac{X_{j-1}^0 + X_j^0}{2}\right)} \int_{x_{j-1}^0}^{x_j^0} (Lu-LU)^2(0,x)dx; \; 1 \le j \le N_0.$$

Based upon the size of each η_{0j}, a decision of whether to accept Δ_0 and $U(0,\cdot)$ or to modify Δ_0 and recompute $U(0,\cdot)$ is made by the computer. Having obtained Δ_0 and $U(0,\cdot)$, the FEMOL solution $U = U(t,x)$ is then uniquely determined as a function which is continuous and piecewise linear in x and smooth in t on each subinterval $[T_m, T_{m+1})$ in the following manner.

For $t \in [T_0, T_1]$, $U(t,\cdot)$ is characterized by the vector of its nodal values $\{U(t,x_j^0)\}_{j=1,N_0-1}$, which is the solution of an $N_0 - 1$ dimensional ODE initial value problem. In order to isolate the space discretization error and means of estimating it, very small error tolerances were used in a time discretization scheme in the computational examples so that these ODEs were essentially solved exactly. The norm $|||e(T_1,\cdot)|||$ is then estimated by

$$E(T_1) = \left\{ \sum_{j=1}^{N_1} \eta_{1j}^2 \right\}^{1/2}, \tag{1.8}$$

where $N_1 \equiv N_0$, $\Delta_1 = \{0 = x_0^1 < x_1^1 < \ldots < x_{N_1}^1 = 1\} \equiv \Delta_0$, and the indicators $\{\eta_{1j}\}_{j=1,N_1}$ are defined by

$$\eta_{1j}^2 = \frac{|x_j^1 - x_{j-1}^1|^2}{12a\left(\frac{x_{j-1}^1 + x_j^1}{2}\right)} \int_{x_{j-1}^1}^{x_j^1} (U_t + LU - f)^2 (T_1, x)\, dx; \tag{1.9}$$

$$1 \le j \le N_1 .$$

Using $\{\eta_{1j}\}_{j=1,N_1}$, a decision of whether or not to accept Δ_1 and $U(T_1,\cdot)$ is then made. If Δ_1 is modified, new initial or transition data $U(T_1,\cdot)$ and $U_t(T_1,\cdot)$, which are continuous and piecewise linear on the new mesh Δ_1, are determined. This process is effected through the solution of linear algebraic equations. The error is again estimated with $E(T_1)$, defined now on the new mesh Δ_1, and the modification process is permitted to occur once more.

For each $m = 1,M$ the process of solving for $t \in [T_m, T_{m+1}]$ an $N_m - 1$ dimensional ODE problem with initial data $\{U(T_m, x_j^m)\}_{j=1,N_m-1}$ is likewise carried out, and the decisions of whether or not to modify the partition

$$(1.10)\quad \Delta_m = \{0 = x_0^m < x_1^m < \ldots < x_{N_m}^m = 1\}$$

are similarly made by the computer after checking the error indicators $\{\eta_{mj}\}_{j=1,N_m}$, defined by

$$(1.11)\quad \eta_{mj}^2 = \frac{|x_j^m - x_{j-1}^m|^2}{12a\left(\frac{x_{j-1}^m + x_j^m}{2}\right)} \int_{x_{j-1}^m}^{x_j^m} (U_t + LU - f)^2 (T_m, x)\,dx;$$

$$1 \le j \le N_m,$$

and the estimator $E(T_m)$ of $|||e(T_m,\cdot)|||$, given by

$$(1.12)\quad E(T_m) = \left\{\sum_{j=1}^{N_m} \eta_{mj}^2\right\}^{1/2}.$$

The quantity $|||e(t,\cdot)|||$ is clearly defined for all $t \in [0, T_{FINAL}]$ and, in an obvious way, the estimator $E(\cdot)$ can be extended to a piecewise smooth function on $[0, T_{FINAL}]$.

In order to assess the performance of $\mathcal{E}(\cdot)$ and the adaptive procedure, we define the effectivity ratio $\Theta(\cdot)$ by

(1.13) $\Theta(t) = \mathcal{E}(t)/E_{TRU}(t); \quad \forall t \in [0,T_{FINAL}]$, where

(1.14) $$E_{TRU}(t) \equiv |||e(t,\cdot)|||.$$

The process of estimating $|||e(\cdot,\cdot)|||$ with $\mathcal{E}(\cdot)$ on $[0,T_{FINAL}]$ is effective if $1/\Theta(t)$ is uniformly bounded on $[0,T_{FINAL}]$, and it is desirable that $\Theta(t)$ would approach 1 for each t, were the procedure repeated with successively smaller input tolerances TOL. This in turn would lead to an effective adaptive procedure, since the decisions at each T_m are made in an attempt to control $\mathcal{E}(T_m)$ so that $\mathcal{E}(t) \sim \text{TOL}$ for each $t \in [0,T_{FINAL}]$.

The theoretical results in sections 4 and 5 related to the effectivity of the estimator $\mathcal{E}(\cdot)$ are given for generally constructed meshes and are asymptotic in nature. In section 6 experiments testing the applicability of these conclusions in the above adaptive procedure are presented and discussed.

2. Preliminaries, Problem Description, and Discussion

Throughout this paper the convention that the variables i, j, ℓ, m, M, n, N, p, and q take only integer values shall be used. We begin by introducing certain notation and concepts needed for the study of the model problem. For more details we refer to [3] and [12].

Let $I = (0,1) \subset \mathbb{R}^1$, $0 \le T_* < T < \infty$, the open interval $J \subset (0,T)$, real $s \ge 0$, and V be an arbitrary Hilbert space.

We denote by $C^0(\bar{J};V)\{H^0(J;V)\}$ the space of functions which are continuous {square integrable} on $\bar{J}$ with range in V, and by $H^s(J;V)$ the corresponding Sobolev space of order s. When $J = I$ and $V = \mathbb{R}^1$ we suppress J and V and denote by H^s the usual Sobolev space of order s on I with norm $\|\cdot\|_s$, and by H_0^1 the subset of functions in H^1 which vanish at 0 and 1. $H^{2s,s}(J) = H^0(J;H^{2s}) \cap H^s(J;H^0)$ is the nonisotropic Sobolev space of order s on $J \times I$ with norm $\|\cdot\|_{2s,s}^J$.

Throughout this paper α and β denote real numbers related to the data of the model problem and satisfy

$$(2.1) \qquad -1 \le \beta \le \alpha; \quad 3 < \alpha \le 4; \quad \beta,\alpha \ne \text{integer} + 1/2.$$

For sufficiently smooth functions a and b on $\bar{I}$ satisfying

$$\left.\begin{array}{ll} (2.2) & 0 < \underline{a} \le a(x) \le \bar{a} < \infty \\ (2.3) & 0 \le b(x) \le \bar{b} < \infty \end{array}\right\} \quad \forall x \in \bar{I},$$

we consider the model problem: Find $u = u(\ ;u_0,f)$ satisfying

$$(2.4)\quad \begin{cases} \frac{\partial u}{\partial t}(t,x) + Lu(t,x) = f(t,x); & t,x \in (0,T) \times I, \\ u(t,0) = 0 = u(t,1); & t \in (0,T), \\ u(0,x) = u_0(x); & x \in I, \end{cases}$$

where L is the positive self-adjoint operator defined by

$$(2.5)\qquad Lu = -(au_x)_x + bu$$

with domain $\mathcal{D}(L) = \{v \in H^2 : v(x)|_{x=0,1} = 0\}$.

More generally, the domains of fractional powers of L are Hilbert spaces defined by

$$(2.6)\quad \mathcal{D}(L^{(\beta+1)/2}) = \{v \in H^{\beta+1} : L^p v(x)|_{x=0,1} = 0 \quad \forall p \text{ satisfying } 0 \le p < \beta/2 + 1/4\}.$$

The data u_0 and f in eqs. (2.4) are required to satisfy

$$(2.7)\quad u_0,f \in \mathbb{D}^{\alpha,\beta}(0,T) \equiv \{v,g \in H^{\beta+1} \times H^{\alpha,\alpha/2}(0,T) : M_\beta^{CR}(v,g) = 0\},$$

where with $\sum_{j=p}^{q}{}' \equiv 0$ for $q < p$ and $[\sigma]$ denoting the integral part of any real number σ, M_β^{CR} is defined by

$$(2.8)\quad M_\beta^{CR}(v,g) = \sum_{x=0,1} \sum_{i=0}^{[\beta/2+1/4]}{}' \left| L^i v(x) + \sum_{p=1}^{i}{}' (-1)^p L^{i-p} \frac{\partial^{p-1}}{\partial t^{p-1}} g(0,x) \right|.$$

Setting

(2.9) $\mathcal{H}^{\alpha,\beta}(T_*,T) = \{u \in H^{\alpha+2,(\alpha+2)/2}(T_*,T) : u = u(\ ;v,g)$ solves eqs. (2.4) for some data $v,g \in \mathbb{D}^{\alpha,\beta}(0,T)\}$,

we define for $u(\ ;v,g) \in \mathcal{H}^{\alpha,\beta}(T_*,T)$

$$(2.10)\quad C_\alpha(\beta,T_*,T,u) = \begin{cases} \|v\|_{\beta+1} + \|g\|^{(0,T)}_{\alpha,\alpha/2}\,; & \text{if } T_*=0, \\ (1+T_*^{-(\alpha+1)/2})(M_\alpha^{CR}(0,g)+\|v\|_{\beta+1})+\|g\|^{(0,T)}_{\alpha,\alpha/2}; & \text{if } T_*>0. \end{cases}$$

We have the following useful result.

<u>Theorem 2.1</u> (cf. [3, Thm. 3.4]). Let $u_0, f \in \mathbb{D}^{\alpha,\beta}(0,T)$, with $\beta = \alpha$ if $T_* = 0$, and set $T_* = 0$ if $\beta = \alpha$. Then eqs. (2.4) have a unique solution $u(\ ;u_0,f) \in \mathcal{H}^{\alpha,\beta}(T_*,T)$ and $\exists$ a positive constant C such that

$$\|u\|^{(T_*,T)}_{\alpha+2,(\alpha+2)/2} \le C\,C_\alpha(\beta,T_*,T,u).$$

Using the restriction (2.1) in [3, Thms. 2.1-2.3], we also have

<u>Theorem 2.2</u>. Let $u \in \mathcal{H}^{\alpha,\beta}(T_*,T)$ and $J \subset (T_*,T)$. Then $\exists$ a positive constant C such that for

(2.11) $j = 0$, 1, and 2, $\dfrac{\partial^j u}{\partial t^j} \in H^{(\alpha+2-2j),(\alpha+2-2j)/2}(J) \cap H^0(J;H_0^1)$

and $\left\|\dfrac{\partial^j u}{\partial t^j}\right\|^J_{(\alpha+2-2j),(\alpha+2-2j)/2} \le C\|u\|^J_{\alpha+2,(\alpha+2)/2}$, and

(2.12) for $j = 0$ and 1, $\frac{\partial^j u}{\partial t^j} \in C^0(\bar{J}; H^{\alpha+1-2j} \cap H_0^1)$

$$\text{and} \quad \sup_{t \in \bar{J}} \left\| \frac{\partial^j}{\partial t^j} u(t,\cdot) \right\|_{\alpha+1-2j} \leq C\|u\|^J_{\alpha+2,(\alpha+2)/2}.$$

As in [3], in order to demonstrate the principal a posteriori error estimates in section 4 we require the use of subclasses of $H^{\alpha,\beta}(T_*,T)$, consisting of functions satisfying one or both of the following additional properties.

(2.13) For $\delta_1 > 0$ we say that $u \in H^{\alpha,\beta}(T_*,T)$ satisfies property $I(\delta_1)$ if for each $t \in [T_*,T]$, $\|u_{xx}(t,\cdot)\|_0 > 0$ and

$$\sup_{t \in [T_*,T]} \left\{ \frac{C_\alpha(\beta,T_*,T,u)}{\|u_{xx}(t,\cdot)\|_0} \right\} \leq \delta_1.$$

(2.14) For $\delta_2 > 0$ we say that $u \in H^{\alpha,\beta}(T_*,T)$ satisfies property $II(\delta_2)$ if for each $t \in [T_*,T]$ $\exists$ an open interval $I_t \subset I$ such that

$$g_L(t,u) \equiv \inf_{x \in I_t} \{|u_{xx}(t,x)| \cdot |I_t|^{1/2}\} > 0 \quad \text{and}$$

$$\sup_{t \in [T_*,T]} \frac{g_U(t,u)}{g_L(t,u)} \leq \delta_2, \quad \text{where}$$

$$g_U(t,u) \equiv \sup_{x \in \bar{I}} \{|u_{xx}(t,x)| + |u_{xxx}(t,x)|\}.$$

For $\delta_1 > 0$, $\delta_2 > 0$ we then set

(2.15) $H^{\alpha,\beta}_{\delta_1}(T_*,T) = \{u \in H^{\alpha,\beta}(T_*,T) : u$ satisfies $I(\delta_1)\}$, and

(2.16) $H^{\alpha,\beta}_{\delta_1,\delta_2}(T_*,T) = \{u \in H^{\alpha,\beta}_{\delta_1}(T_*,T) : u$ satisfies $II(\delta_2)\}$.

Our numerical analysis is based upon the following weak form of eqs. (2.4). Find $u : (0,T) \to H^1_0$ satisfying

(2.17) $<u_t(t),\phi> + B(u(t),\phi) = <f(t),\phi>; \quad \forall t,\phi \in (0,T) \times H^1_0,$

(2.18) $$u(0) = u_0,$$

where $<\cdot,\cdot>$ denotes the H^0 inner product on I and the symmetric bilinear form B is defined by

(2.19) $$B(u,v) = <au_x,v_x> + <bu,v>; \qquad \forall u,v \in H^1_0.$$

By (2.2) and (2.3) $\exists$ positive constants C_1, C_2 such that

(2.20) $$C_2\|w\|_1^2 \le \|w\|_E^2 \equiv B(w,w) \le C_1\|w\|_1^2; \qquad \forall w \in H^1_0.$$

Let $\mathcal{T}$ and $\mathcal{P}$ denote the families of mesh partitions of (0,T) and I, respectively. For

$\Delta^T = \{0 = T_0 < T_1 < \cdots < T_{M+1} = T\} \in \mathcal{T}$; $M = M(\Delta^T) \ge 1$, and

$\Delta = \{\Delta_m\}_{m=0,M(\Delta^T)}$, with

$\Delta_m = \{0 = x_0^m < x_1^m < \cdots < x_{N_m}^m = 1\} \in \mathcal{P}$; $m \in [0,M]$, $N_m \ge 2$, we write

$$\left.\begin{aligned}
J_m &= (T_m, T_{m+1}), \quad \bar{J}_m = [T_m, T_{m+1}], \\
{}^cJ_m &= [T_m, T_{m+1}), \quad J_m^c = (T_m, T_{m+1}], \\
\tau_m &= T_{m+1} - T_m, \\
I_j^m &= (x_{j-1}^m, x_j^m), \quad |I_j^m| = x_j^m - x_{j-1}^m, \\
\underline{h}_m &= \min_{1\le j\le N_m} |I_j^m|, \quad h_m = \max_{1\le j\le N_m} |I_j^m|,
\end{aligned}\right\} \quad \begin{aligned} 0 \le m \le M(\Delta^T), \\ 1 \le j \le N_m, \end{aligned}$$

and

$$h = h(\Delta) = \max_{0\le m\le M(\Delta^T)} h_m .$$

For Δ^T and Δ as above, we denote by $\Delta^T \times \Delta$ the partition of $(0,T) \times I$ into the $\sum_{m=0}^{M(\Delta^T)} N_m$ two dimensional subintervals of the form

$$\{J_m \times I_j^m\}_{\substack{m=0,M(\Delta^T) \\ j=1,N_m}} .$$

In general, $\Delta_p \nsubseteq \Delta_q$ for $p \neq q$, but by setting $\Delta_m = \Delta_0$ for $m = 1,M(\Delta^T)$, our results will directly reduce to those shown in [3] for time-independent space meshes.

We say that the family $\mathcal{T} \times \mathcal{P}$ of such Cartesian product partitions of $(0,T) \times I$ is γ-regular, if $\exists\gamma \ge 0$ and $\Lambda_1 > 0$ such that for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$

$$(2.21)\qquad \tau_m \;\geq\; \Lambda_1 h_m^{2\gamma}; \qquad 0 \leq m \leq M(\Delta^T),$$

and that $\mathcal{T} \times \mathcal{P}$ is κ,γ-regular if $\mathcal{T} \times \mathcal{P}$ is γ-regular and $\exists\kappa \geq 1$, $\Lambda_2 > 0$, and $\Lambda_3 > 0$ such that for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$

$$(2.22)\qquad h_p \;\leq\; \Lambda_2 h_q; \qquad 0 \leq p \leq q \leq M(\Delta^T),$$

and

$$(2.23)\qquad \underline{h}_m \;\geq\; \Lambda_3 h_m^{\kappa}; \qquad 0 \leq m \leq M(\Delta^T).$$

(2.24) Unless otherwise specified, throughout the remainder of this paper C shall denote a positive generic constant which depends in general on the functions a and b, the constants Λ_1, Λ_2, Λ_3, and T, but is independent of M, m, τ_m, Δ_m, h_m, T_*, and the functions u_0, f, and u.

For each $\Delta_m \in \mathcal{P}$, $S(\Delta_m) \subset H_0^1$ is the subset of functions whose restrictions to any I_j^m are linear. The operators P_0^m, P_1^m, and L_{Δ_m} mapping H^0, H_0^1, and $S(\Delta_m)$, respectively, to $S(\Delta_m)$ are defined by

$$(2.25)\qquad \left\{\begin{aligned} \langle P_0^m v - v, \phi\rangle &= 0 \\ B(P_1^m v - v, \phi) &= 0 \\ \langle L_{\Delta_m} v, \phi\rangle &= B(v,\phi) \end{aligned}\right\} \quad \forall\phi \in S(\Delta_m).$$

L_{Δ_m} is a positive self-adjoint operator with domain $S(\Delta_m)$ and satisfies

$$(2.26) \qquad L_{\Delta_m}(P_1^m v) = P_0^m(Lv); \qquad \forall v \in \mathcal{D}(L),$$

$$(2.27) \qquad \|L_{\Delta_m}^{-1}\phi\|_0 \le C\|L_{\Delta_m}^{-1}\phi\|_E \le C^2\|\phi\|_0; \qquad \forall \phi \in S(\Delta_m).$$

We have the following approximation results.

Lemma 2.1 (cf. [3, Lemmas 2.1, 2.3]). There exists a positive constant C such that for each $\Delta_m \in \mathcal{P}$

$$(2.28) \qquad \|(I-P_1^m)v\|_s \le Ch_m^{\sigma-s}\|v\|_\sigma; \qquad \forall v \in \mathcal{D}(L^{\sigma/2}),$$
$$0 \le s \le 1 \le \sigma \le 2,$$

$$(2.29) \qquad \|(I-P_0^m)v\|_0 \le Ch_m^{\sigma}\|v\|_\sigma; \qquad \forall v \in \mathcal{D}(L^{\sigma/2}),$$
$$0 \le \sigma \le 2, \quad \sigma \ne 1/2,$$

$$(2.30) \quad \|(I-P_1^m)\frac{\partial^j v}{\partial t^j}\|_{0,0}^{J_m} \le Ch_m^{\sigma}\|v\|_{2\mu,\mu}^{J_m}; \ \forall v \in H^{2\mu,\mu}(J_m) \cap H^0(J_m;H_0^1),$$
$$\mu = j + \sigma/2, \quad j \ge 0, \quad 1 \le \sigma \le 2.$$

For each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$, we define the FEMOL solution

$$U : [0,T) \to \bigcup_{m=0}^{M(\Delta^T)} S(\Delta_m)$$

by

$$(2.31) \qquad U(t) = U^m(t); \quad t \in {}^cJ_m \quad \text{for some} \quad m \in [0,M],$$

where

$$U^0 : \bar{J}_0 \to S(\Delta_0)$$

is defined by

$$(2.32) \quad \langle U_t^0(t),\phi\rangle + B(U^0(t),\phi) = \langle f(t),\phi\rangle; \ \forall t,\phi \in J_0^c \times S(\Delta_0),$$

$$(2.33) \quad U^0(0) = U_0 \equiv \begin{cases} P_1^0 u_0; & \text{if} \quad u_0 \in \mathcal{D}(L), \\ P_0^0 u0; & \text{if} \quad u_0 \notin \mathcal{D}(L), \end{cases}$$

and

$$U^m : \bar{J}_m \to S(\Delta_m) \quad \text{for} \quad 1 \le m \le M(\Delta^T)$$

is defined by

$$(2.34) \quad \langle U_t^m(t),\phi\rangle + B(U^m(t),\phi) = \langle f(t),\phi\rangle; \ \forall t,\phi \in J_m^c \times S(\Delta_m),$$

$$(2.35) \quad U^m(T_m) = L_{\Delta_m}^{-1} P_0^m (f(T_m) - U_t^{m-1}(T_m)).$$

From the definition of L_{Δ_m}, we see that eq. (2.35) is equivalent to

$$B(U^m(T_m),\phi) = \langle f(T_m) - U_t^{m-1}(T_m),\phi\rangle; \qquad \forall \phi \in S(\Delta_m),$$

and it therefore follows from eqs. (2.32), (2.34) and (2.35) that

$$(2.36) \quad \lim_{t \to T_m^+} U_t^m(t) = P_0^m U_t^{m-1}(T_m) \ ; \qquad 1 \le m \le M(\Delta^T).$$

Eqs. (2.31)-(2.35) are equivalent to a sequence of uniquely solvable, iteratively defined ODE initial value problems. At each transition time T_m, the transition data (new initial data) is determined from the solution of an $N_m - 1$ dimensional matrix equation.

Remarks. In the case of pure mesh derefinement, i.e. $\Delta_m \subset \Delta_{m-1}$ for some $m \geq 1$, then $S(\Delta_m) \subset S(\Delta_{m-1})$ and we have from eqs. (2.34) and (2.35) that

$$U^m(T_m) = P_1^m U^{m-1}(T_m). \tag{2.37}$$

In the case of pure mesh refinement, i.e. $\Delta_m \supset \Delta_{m-1}$, then $S(\Delta_m) \supset S(\Delta_{m-1})$ and it follows that

$$\begin{cases} P_1^{m-1} U^m(T_m) = U^{m-1}(T_m), \quad \text{and} \\ \lim\limits_{t \to T_m^+} U_t^m(t) = U_t^{m-1}(T_m). \end{cases} \tag{2.38}$$

For $u \in \mathcal{H}^{\alpha,\beta}(T_*,T)$ and each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ we define

$$P_1(t) = P_1^m; \qquad t \in {}^cJ_m \text{ for some } m \in [0,M], \tag{2.39}$$

$$e(t) = u(t) - U(t); \qquad t \in [0,T), \tag{2.40}$$

$$\rho(t) = P_1(t)u(t) - u(t); \qquad t \in [T_*,T), \tag{2.41}$$

$$\theta(t) = P_1(t)u(t) - U(t); \qquad t \in [T_*,T). \tag{2.42}$$

We shall use the following notational convention. For $1 \leq m \leq M$,

$$(2.43)\quad \begin{cases} w(T_m^+) \equiv \lim\limits_{t\to T_m^+} w(t) & \text{and} \\ w(T_m^-) \equiv \lim\limits_{t\to T_m^-} w(t) \end{cases}$$

for any function w such that these limits exist.

In section 3 it will be shown with $\gamma < 1$ and certain $\alpha = \alpha(\gamma)$, that if $u \in H^{\alpha,\beta}(T_*,T)$ and $T \times P$ is a κ,γ-regular mesh family, then the choice (2.35) of discrete transition data yields an a priori estimate of the form

$$(2.44)\qquad \|\theta(t)\|_E + \|e_t(t)\|_0 = O(h_m^\sigma) \quad \text{as} \quad h_m \to 0;$$

$\forall t \in [T_*,T_{m+1})$, each $m \in [0,M]$, *and some* $\sigma(\gamma,\alpha) > 1$. The result (2.44) and the restriction (2.23) for certain κ will lead to statements in section 4 about the effectivity of estimating $\|e\|_E$ on $[T_*,T)$ with an a posteriori estimator $E(\cdot)$.

We note that in the FEMOL, the γ-regularity restriction (2.21) on $T \times P$ is apparently necessary, not only for effective error estimation but also convergence. We refer to the counterexample in [8, section 4] in which a sequence of meshes satisfying $\tau_m = o(h_m^4)$ as $h_m \to 0$ led to convergence to the wrong solution of the heat equation in $\mathbb{R}^1$.

We next remark that in order for the estimator $E(\cdot)$ to perform well on $[T_*,T)$, $T \times P$ must satisfy a restriction like (2.22). If, for example, a sequence of partitions of

$(0,T) \times I$ was used for which $\Delta^T = \{0 < T/2 < T\}$ and Δ_0 remained fixed, while $h_1 \to 0$, then for $T/2 \le t < T$ we would have $E(t) = O(h_1)$ as $h_1 \to 0$, while $\|e(t)\|_E \ge C > 0$ in general.

The restrictions (2.22) and (2.23) would not be needed if our only interest were in obtaining a priori error estimates. If $T \times P$ is γ-regular with $\gamma \le 1$, $u \in H^{\alpha,\beta}(T_*,T)$ for certain $\alpha = \alpha(\gamma)$, and the discrete transition data choice (2.35) is made, then in section 3 we shall show estimates of the form

$$(2.45) \qquad \left.\begin{cases} \|e(t)\|_E = O(h) \\ \|e(t)\|_0 = O(h^{2-\gamma}) \end{cases}\right\} \quad \text{as } h \to 0; \quad \forall t \in [T_*,T).$$

More generally, by replacing $\{S(\Delta_m)\}_{m=0,M}$ in the FEMOL with $\{S^i(\Delta_m)\}_{m=0,M}$, where for $i \ge 1$ $S^i(\Delta_m) \subset H_0^1$ denotes a closed subspace possessing the approximation properties of the C^0 piecewise i-degree polynomials on Δ_m, it can be shown (cf. [4]) that

$$(2.46) \qquad \left.\begin{cases} \|e(t)\|_E = O(h^i) \\ \|e(t)\|_0 = O(h^{i+1-\gamma}) \end{cases}\right\} \quad \text{as } h \to 0; \quad \forall t \in [T_*,T).$$

We note that an estimate of the form

$$(2.47) \qquad \|e(t)\|_0 + \left\{\int_0^t \|e(s)\|_E^2 \, ds\right\}^{1/2} = O(h^i) \quad \text{as } h \to 0$$

follows from a recent result given in [8], where with a different choice of transition data and a 1-regular family $T \times P$, it was also assumed that $\{S^i(\Delta_{m-1}) \cap S^i(\Delta_m)\}_{m=1,M}$ has certain approximation properties, which is a restriction on the locations of points in any mesh to those of points in the successive mesh.

For computational reasons, in the adaptive scheme proposed in section 6 it is assumed that each partition Δ_m is obtained from the previous partition Δ_{m-1} through a combination of refinement and derefinement, but the theory permits for instance meshes which satisfy

$$0 < x_1^m < x_1^{m-1} < \cdots < x_{N_m-1}^m < x_{N_{m-1}-1}^{m-1} < 1, \tag{2.48}$$

in which case $S(\Delta_{m-1}) \cap S(\Delta_m) = \{0\}$.

3. A Priori Estimates

Let $u(\ ;u_0,f)$ be the solution of eqs. (2.4), for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ let U be the FEMOL solution defined by eqs. (2.31)-(2.35), and e,ρ, and θ be as defined in (2.40)-(2.42). The following theorem is a direct consequence of the result in [3,Thm.4.1].

Theorem 3.1. Let $u(\ ;u_0,f) \in H^{\alpha,\beta}(T_*,T)$, where α and β satisfy (2.1). Then $\exists$ a positive constant C such that for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ with $T_1 > T_*$ and all $t \in {}^cJ_0 \cap [T_*,T)$

$$(3.1)\quad \|\theta(t)\|_E + \|e_t(t)\|_0 \le Ch_0^{\alpha-2}C_\alpha(\beta,T_*,T,u).$$

By using Thm. 3.1, the transition data choice (2.35), and the embedding results in Thm. 2.2 on each subinterval $J_m \subset (T_*,T)$, we will exploit the local time character of the error and be able to show

Theorem 3.2. Let $u(\ ;u_0,f) \in H^{\alpha,\beta}(T_*,T)$, where α and β satisfy (2.1), and $\mathcal{T} \times \mathcal{P}$ be a κ,γ-regular family. Then $\exists$ a positive constant C such that for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ with $T_1 > T_*$, each $m \in [0,M]$, and all $t \in {}^cJ_m \cap [T_*,T)$

$$(3.2)\quad \|\theta(t)\|_E + \|e_t(t)\|_0 \le Ch_m^{\alpha-2-\gamma}C_\alpha(\beta,T_*,T,u).$$

Proof. Since $\gamma \ge 0$, the result (3.2) for $m = 0$

follows directly from Thm. 3.1, and it therefore suffices to demonstrate (3.2) for arbitrary m satisfying $1 \le m \le M$.

Suppose we have shown that positive constants C_0 and C_1 (independent of m) exist such that for all $t \in {}^cJ_m$

$$(3.3) \quad \|e_t(t)\|_0 \le \|e_t(T_m^-)\|_0 + C_1 h_m^{\alpha-2}\|u\|^{J_m}_{\alpha+2,(\alpha+2)/2}, \quad \text{and}$$

$$(3.4) \quad \|\theta(t)\|_E \le C_0\{\|e_t(T_m^-)\|_0 + C_1 h_m^{\alpha-2}\|u\|^{J_m}_{\alpha+2,(\alpha+2)/2}\}.$$

We then claim that for all $t \in {}^cJ_m$

$$(3.5) \quad \|e_t(t)\|_0 \le \|e_t(T_1^-)\|_0 + C_1 \sum_{j=1}^{m} h_j^{\alpha-2}\|u\|^{J_j}_{\alpha+2,(\alpha+2)/2}, \quad \text{and}$$

$$(3.6) \quad \|\theta(t)\|_E \le C_0\{\|e_t(T_1^-)\|_0 + C_1 \sum_{j=1}^{m} h_j^{\alpha-2}\|u\|^{J_j}_{\alpha+2,(\alpha+2)/2}\}.$$

If $m = 1$ there is nothing to show, as (3.5) and (3.6) are then just (3.3) and (3.4). If $m \ge 2$ we can estimate the first terms on the right hand sides of (3.3) and (3.4) by following with m replaced by $m - 1$ the same steps which led to (3.3), since by the notational convention (2.43)

$$(3.7) \qquad \|e_t(T_m^-)\|_0 = \lim_{\substack{t\to T_m \\ t\in J_{m-1}}} \|e_t(t)\|_0.$$

Repeating this argument a total of $m - 1$ times yields (3.5) and (3.6).

As eq. (3.7) also holds for $m = 1$, we have by Thm. 3.1 that $\exists$ a positive constant C such that

$$\|e_t(T_1^-)\|_0 \le C h_0^{\alpha-2-\gamma} \; C_\alpha(\beta, T_*, T, u). \tag{3.8}$$

Combining (3.5), (3.6), and (3.8), it follows that $\exists$ a positive constant C (independent of m) such that for all $t \in {}^cJ_m$

$$\|\theta(t)\|_E + \|e_t(t)\|_0 \le C \left\{ h_0^{\alpha-2-\gamma} C_\alpha(\beta, T_*, T, u) + \sum_{j=1}^{m} h_j^{\alpha-2-\gamma} \cdot \left(h_j^{2\gamma}/\tau_j \right)^{1/2} \tau_j^{1/2} \|u\|_{\alpha+2,(\alpha+2)/2}^{J_j} \right\}. \tag{3.9}$$

Using $m \le M$ and the κ,γ-regularity conditions (2.21) and (2.22), (3.9) becomes

$$\|\theta(t)\|_E + \|e_t(t)\|_0 \le C h_m^{\alpha-2-\gamma} \left\{ C_\alpha(\beta, T_*, T, u) + \sum_{j=1}^{M} \tau_j^{1/2} \|u\|_{\alpha+2,(\alpha+2)/2}^{J_j} \right\} \tag{3.10}$$

by the M-dimensional Cauchy-Schwarz inequality

$$\leq Ch_m^{\alpha-2-\gamma}\left\{C_\alpha(\beta,T_*,T,u) + \left(\sum_{j=1}^{M}\tau_j\right)^{1/2} \cdot \left(\sum_{j=1}^{M}(\|u\|_{\alpha+2,(\alpha+2)/2}^{J_j})^2\right)^{1/2}\right\}$$

$$= Ch_m^{\alpha-2-\gamma}\left\{C_\alpha(\beta,T_*,T,u) + (T-T_1)^{1/2} \cdot \|u\|_{\alpha+2,(\alpha+2)/2}^{(T_1,T)}\right\}$$

$$\leq Ch_m^{\alpha-2-\gamma}\left\{C_\alpha(\beta,T_*,T,u) + \|u\|_{\alpha+2,(\alpha+2)/2}^{(T_*,T)}\right\}$$

by Thm. 2.1

$$\leq Ch_m^{\alpha-2-\gamma}C_\alpha(\beta,T_*,T,u),$$

which is the desired result (3.2).

We shall now demonstrate (3.3) and (3.4), first for $t = T_m$ and then for $t \in J_m$. We have by (2.43) and observation (2.36) that

$$(3.11) \quad e_t(T_m) = u_t(T_m) - P_0^m U_t^{m-1}(T_m)$$

$$= P_0^m \lim_{t\to T_m^-}(u_t(t)-U_t(t)) + (I-P_0^m)u_t(T_m)$$

$$= P_0^m e_t(T_m^-) + (I-P_0^m)u_t(T_m).$$

Hence, by the definition of $P_0^m\colon H^0 \to S(\Delta_m)$ and the triangle inequality

$$(3.12) \quad \|e_t(T_m)\|_0 \leq \|e_t(T_m^-)\|_0 + \|(I-P_0^m)u_t(T_m)\|_0$$

by (2.1) and (2.29)

$$\leq \|e_t(T_m^-)\|_0 + Ch_m^{\alpha-2} \sup_{t\in J_m} \|u_t(t)\|_{\alpha-2}$$

by (2.12)

$$\leq \|e_t(T_m^-)\|_0 + Ch_m^{\alpha-2} \|u\|^{J_m}_{\alpha+2,(\alpha+2)/2}.$$

By (2.43), (2.17), (2.35), and (3.11) we have that

$$(3.13) \quad \theta(T_m) = -L^{-1}_{\Delta_m} P_0^m e_t(T_m) = -L^{-1}_{\Delta_m} P_0^m e_t(T_m^-).$$

Therefore by (2.27) and the definition of P_0^m

$$(3.14) \qquad \|\theta(T_m)\|_E \leq C\|e_t(T_m^-)\|_0.$$

Now, it follows from the t-independence of the operator L and subtraction of eq. (2.34) from eq. (2.17) that for $j = 0$ or 1

$$(3.15) \quad \left\langle \frac{\partial^{j+1}}{\partial s^{j+1}} \theta(s), \phi \right\rangle + B\left(\frac{\partial^j}{\partial s^j} \theta(s), \phi\right) = \left\langle \frac{\partial^{j+1}}{\partial s^{j+1}} \rho(s), \phi \right\rangle ;$$

$$\forall s,\phi \in J_m \times S(\Delta_m).$$

With $\phi = 2\theta_s(s)$ and $j = 0$, eq. (3.15) becomes

$$(3.16) \quad 2\|\theta_s(s)\|_0^2 + \frac{d}{ds} \|\theta(s)\|_E^2 = 2\left\langle \rho_s(s), \theta_s(s) \right\rangle .$$

For arbitrary $t \in J_m$, integration of eq. (3.16) on (T_m, t) and application of the Cauchy-Schwarz inequality yield

$$(3.17)\quad \|\theta(t)\|_E^2 \le \|\theta(T_m)\|_E^2 + 2\int_{T_m}^{t} \|(P_1^m - I)u_s(s)\|_0 \cdot \|\theta_s(s)\|_0 ds$$

$$- 2\int_{T_m}^{t} \|\theta_s(s)\|_0^2 ds$$

$$\le \|\theta(T_m)\|_E^2 + \frac{1}{2}\int_{T_m}^{t} \|(P_1^m - I)u_s(s)\|_0^2 ds.$$

Hence, $\exists$ a positive constant C such that

$$(3.18)\quad \|\theta(t)\|_E \le \|\theta(T_m)\|_E + C\|(P_1^m - I)u_t\|_{0,0}^{J_m}$$

by (2.1), (2.11), and (2.30) $\le \|\theta(T_m)\|_E + Ch_m^{\alpha-2}\|u\|_{\alpha+2,(\alpha+2)/2}^{J_m}.$

Now, by the definitions (2.39) - (2.42)

$$(3.19)\quad e_t(t) = -\rho_t(t) + \theta_t(t); \qquad \forall t \in J_m.$$

Setting $\phi = 2\theta_s(s)$ in eq. (3.15) with $j = 1$, we get

$$(3.20)\quad \frac{d}{ds}\|\theta_s(s)\|_0^2 + 2\|\theta_s(s)\|_E^2 = 2\left\langle \rho_{ss}(s), \theta_s(s)\right\rangle.$$

As in (3.17) and (3.18), integration of eq. (3.20) on (T_m, t) for $t \in J_m$ yields

$$(3.21)\quad \|\theta_t(t)\|_0 \le \|\theta_t(T_m)\|_0 + C\|(P_1^m - I)u_{tt}\|_{0,0}^{J_m}$$

$$\le \|\theta_t(T_m)\|_0 + Ch_m^{\alpha-2}\|u\|_{\alpha+2,(\alpha+2)/2}^{J_m}.$$

By (3.19), (3.21), and the triangle inequality we have for $t \in J_m$

$$(3.22)\quad \|e_t(t)\|_0 \le \|e_t(T_m)\|_0 + \|\rho_t(t)\|_0 + \|\rho_t(T_m)\|_0 + Ch_m^{\alpha-2}\|u\|^{J_m}_{\alpha+2,(\alpha+2)/2}$$

$$\le \|e_t(T_m)\|_0 + 2\sup_{s\in\bar{J}_m}\|(I-P_1^m)u_s(s)\|_0 + Ch_m^{\alpha-2}\|u\|^{J_m}_{\alpha+2,(\alpha+2)/2}$$

by (2.1), (2.12), and (2.28)

$$\lesssim \|e_t(T_m)\|_0 + Ch_m^{\alpha-2}\|u\|^{J_m}_{\alpha+2,(\alpha+2)/2}.$$

Combining (3.12), (3.14), (3.18), and (3.22) completes the proof of (3.3), (3.4), and hence, Thm. 3.2 .

We now show the a priori estimates mentioned in section 2.

Theorem 3.3. Let $u(\ ;u_0,f) \in H^{\alpha,\beta}(T_*,T)$, where α and β satisfy (2.1), and $T \times P$ be a γ-regular family with $\gamma \le \alpha - 3$. Then $\exists$ a positive constant C such that for each $\Delta^T \times \Delta \in T \times P$ with $T_1 > T_*$ and all $t \in [T_*,T)$

$$(3.23)\quad \|e(t)\|_E \le Ch(\Delta)C_\alpha(\beta,T_*,T,u)$$

and

(3.24) $\|e(t)\|_0 \le Ch^{\alpha-2-\gamma}(\Delta)C_\alpha(\beta,T_*,T,u)$.

<u>Proof</u>. Let $t \in {}^cJ_m \cap [T_*,T)$ for any $m \in [0,M]$. Then

(3.25) $\|e(t)\|_E = \|-\rho(t)+\theta(t)\|_E \le \|(P_1^m-I)u(t)\|_E + \|\theta(t)\|_E$

by (2.12) and (2.28) $\le Ch(\Delta) \sup_{s\in[T_*,T)} \|u(s)\|_2 + \|\theta(t)\|_E$

by (2.1), (2.12), and Thm. 2.1 $\le Ch(\Delta)C_\alpha(\beta,T_*,T,u) + \|\theta(t)\|_E$.

Similarly,

(3.26) $\|e(t)\|_0 \le Ch^2(\Delta)C_\alpha(\beta,T_*,T,u) + \|\theta(t)\|_0$

by (2.27) $\le Ch^2(\Delta)C_\alpha(\beta,T_*,T,u) + C\|\theta(t)\|_E$.

Examination of the proof of Thm. 3.2 shows that the κ,γ-regularity condition (2.23) was not used, and that (2.22) was only used in obtaining (3.10) from (3.9). Therefore, replacing h_m with $h(\Delta)$ in (3.10) yields

(3.27) $\|\theta(t)\|_E \le Ch^{\alpha-2-\gamma}(\Delta)C_\alpha(\beta,T_*,T,u)$.

Since $\gamma \le \alpha - 3$ by assumption, combining (3.25), (3.26), and (3.27) yields the desired results (3.23) and (3.24).

<u>Remarks</u>. If $\alpha = 4$, the results (3.23) and (3.24) become

(3.28) $h^{-(1-\gamma)}\|e(t)\|_0 + \|e(t)\|_E \le Ch\mathcal{C}_\alpha(\beta,T_*,T,u); \quad \forall t \in [T_*,T),$

and if $\beta = 4$ and $T_* = 0$ (smooth and compatible data), (3.23) and (3.24) become

(3.29) $h^{-(1-\gamma)}\|e(t)\|_0 + \|e(t)\|_E \le Ch\|u\|_{6,4}^{(0,T)}$

$$\le Ch\{\|u_0\|_5+\|f\|_{4,2}^{(0,T)}\}; \quad \forall t \in [0,T).$$

The estimate of $\|e\|_E$ is of optimal order in h, while the estimate of $\|e\|_0$ is only of optimal order when the number of mesh changes is finite ($\gamma=0$), a result given in [7] with a different choice of data at the transition times.

4. *A Posteriori Error Estimates*

We begin this section by extending the notions of upper and asymptotically exact estimators presented in [3] to the setting of time-dependent space meshes.

For $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ with $T_1 > T_*$, let

(4.1) $g\colon \Delta^T \times \Delta \to g^\Delta = \{g^{\Delta_m}\}_{m=0,M(\Delta^T)}$, and

(4.2) $\phi\colon \Delta^T \times \Delta \to \phi^\Delta = \{\phi^{\Delta_m}\}_{m=0,M(\Delta^T)}$, with

(4.3) $g^{\Delta_m} \in C^0({}^cJ_m \cap [T_*,T);\ H^0)$

(4.4) $\phi^{\Delta_m} \in C^0({}^cJ_m \cap [T_*,T);\ S(\Delta_m))$ $\Bigg\}$ $m \in [0,M]$, and

$$\Phi \in C^0([T_*,T);\ H_0^1).$$

We say that a quantity $E(\cdot,g,\phi)$ is an <u>upper estimator</u> for $\|\Phi-\phi\|_E$ on $[T_*,T)$ if $\exists$ positive constants C_1,C_2,h^* such that

(4.5) for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ with $T_1 > T_*$ and $h(\Delta) \le C_1h^*$,

(4.6) $\|\Phi(t)-\phi^\Delta(t)\|_E \le C_2E(t,g^\Delta,\phi^\Delta);\ \forall t \in [T_*,T)$,

where C_1 and C_2 are as in (2.24) and h^* depends in general on the solution class in which Φ resides (i.e.g. on $\alpha,\beta,\delta_1,\delta_2$) and on the family $\mathcal{T} \times \mathcal{P}$ (i.e.g. on κ,γ).

If under the same hypotheses $\exists$ a number $\sigma > 0$ such that

$$(4.7)\quad \|\Phi(t)-\phi^{\Delta}(t)\|_E = E(t,g^{\Delta},\phi^{\Delta})(1+O(h^{\sigma})) \quad \text{as} \quad h \to 0;$$

$$\forall t \in [T_*,T),$$

where the constant in $O(h^{\sigma})$ is as in (2.24), then we say that $E(\cdot,g,\phi)$ is an asymptotically exact estimator for $\|\Phi-\phi\|_E$ on $[T_*,T)$.

Let $u(\ ;u_0,f)$ be the solution of eqs. (2.4) and for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ let U denote the FEMOL solution defined by eqs. (2.31)-(2.35). We now define our principal a posteriori estimator for $\|u-U\|_E$.

For each $m \in [0,M]$ and $t \in {}^cJ_m \cap [T_*,T)$, the local indicators $\{\eta_{mj}\}_{j=1,N_m}$ are defined by

$$(4.8)\quad \eta^2_{mj}(t,f-U_t,U) = \frac{|I^m_j|^2}{12a\left(\frac{x^m_{j-1}+x^m_j}{2}\right)}\int_{I^m_j}(U_t+LU-f)^2(t,x)dx,$$

and the associated estimator $\mathcal{E}$ by

$$(4.9)\quad \mathcal{E}(t,f-U_t,U) = \left\{\sum_{j=1}^{N_m} \eta^2_{mj}(t,f-U_t,U)\right\}^{1/2}.$$

$\mathcal{E}(\cdot,f-U_t,U)$ is a piecewise smooth function on $[T_*,T)$, is based upon local computable residuals, and

$$(4.10)\quad \mathcal{E}(t,f-U_t,U) = O(h(\Delta)) \quad \text{as} \quad h(\Delta) \to 0; \quad \forall t \in [T_*,T).$$

Under suitable hypotheses, by applying Thm. 3.2 and results shown in [3] for time-independent space meshes to each of the subintervals ${}^cJ_m \cap [T_*,T)$, we shall be able to show that $E(\cdot,f-U_t,U)$ is an upper or asymptotically exact estimator for $\|u-U\|_E$ on $[T_*,T)$. The hypotheses leading to these results are among the following:

(4.11) $u \in H^{\alpha,\beta}(T_*,T)$, where α and β satisfy (2.1),

(4.12) $u \in H^{\alpha,\beta}_{\delta_1}(T_*,T)$; $\delta_1 > 0$ and $T \times P$ is κ,γ-regular, with $T_1 > T_*$ for each $\Delta^T \times \Delta \in T \times P$,

(4.13) $u \in H^{\alpha,\beta}_{\delta_1,\delta_2}(T_*,T)$; $\delta_1 > 0$, $\delta_2 > 0$,

(4.14) $\kappa + \gamma < \alpha - 2$ ($\Rightarrow \gamma \in [0,1)$ and $\kappa \in [1,2)$ by (2.1)).

As in [3], the results are demonstrated by comparing $\|e\|_E$ to $\|\rho\|_E$ and $E(\cdot,f-U_t,U)$ to $E(\cdot,f-u_t,P_1u)$, where $E(\cdot,f-u_t,P_1u)$ is defined as in (4.9), with $U_t(t)$ and $U(t)$ replaced by $u_t(t)$ and $P_1(t)u(t)$.

We have the following sequence of lemmas.

<u>Lemma 4.1</u> (cf. [3,Lemma 5.1]). There exists a positive constant C such that for each $\Delta^T \times \Delta \in T \times P$ and $t \in {}^cJ_m \cap [T_*,T)$; any $m \in [0,M]$

$$|E(t,f-U_t,U) - E(t,f-u_t,P_1u)| \leq Ch_m\{\|\theta(t)\|_E + \|e_t(t)\|_0\}.$$

Lemma 4.2 (cf. [3,Lemma 5.2]). Assume (4.11). Then $E(\cdot,f-u_t,P_1u)$ is an upper estimator for $\|\rho\|_E$ on $[T_*,T)$, with $h^* = 1$.

Lemma 4.3 (cf. [3,Lemma 5.3]). Assume (4.11), (4.12), and the result of Lemma 4.2. Then $\exists$ a positive constant C such that for each $\Delta^T \times \Delta \in T \times P$ and $\tau \in {}^cJ_m \cap [T_*,T)$; any $m \in [0,M]$

$$E(t,f-u_t,P_1u) \geq \frac{Ch_m^\kappa}{\delta_1} C_\alpha(\beta,T_*,T,u).$$

Lemma 4.4 (cf. [3,Lemma 5.4]). Assume (4.11)-(4.14). Then $E(\cdot,f-u_t,P_1u)$ is an asymptotically exact estimator for $\|\rho\|_E$ on $[T_*,T)$, with $\sigma = 1 - \kappa/2$ and $h^* = \delta_2^{-1/\sigma}$.

The following results can now be shown.

Theorem 4.1. Assume (4.11), (4.12), and (4.14). Then $E(\cdot,f-U_t,U)$ is an upper estimator for $\|u-U\|_E$ on $[T_*,T)$, with $h^* = \delta_1^{-1/\mu}$, where $\mu = (\alpha-2-\kappa-\gamma)/2$.

Theorem 4.2. Assume (4.11)-(4.14). Then $E(\cdot,f-U_t,U)$ is an asymptotically exact estimator for $\|u-U\|_E$ on $[T_*,T)$, with $\sigma = \mu$ and $h^* = \min\{\delta_1^{-1/\mu},\delta_2^{-2/(2-\kappa)}\}$, where $\mu = (\alpha-2-\kappa-\gamma)/2$.

Proof of Thms. 4.1 and 4.2. We follow closely the steps used in [3,Thms. 5.1, 5.2]. Assume (4.11), (4.12), and (4.14), let $\Delta^T \times \Delta \in T \times P$, and let $t \in {}^cJ_m \cap [T_*,T)$ for some $m \in [0,M]$. To simplify notation we suppress t and also write

$$(4.15) \quad \begin{cases} E_1 = E(t,f-U_t,U), \\ E_2 = E(t,f-u_t,P_1u), \\ C_\alpha = C_\alpha(\beta,T_*,T,u). \end{cases}$$

By Lemma 4.3 we may write

$$(4.16) \quad 1 - \frac{|E_1-E_2|}{E_2} \le \frac{E_1}{E_2} \le 1 + \frac{|E_1-E_2|}{E_2},$$

which after application of Lemma 4.1 and, again, Lemma 4.3 becomes

$$(4.17) \quad 1 - \frac{C\delta_1 h_m^{1-\kappa}}{C_\alpha}\{\|\theta\|_E+\|e_t\|_0\} \le \frac{E_1}{E_2} \le 1 + \frac{C\delta_1 h_m^{1-\kappa}}{C_\alpha}\{\|\theta\|_E+\|e_t\|_0\}.$$

By (4.11), (4.12), and (4.14) we may apply the result of Thm. 3.2 to (4.17). In view of the definition of μ, we get

$$(4.18) \quad 1 - C\delta_1 h_m^{2\mu+1} \le \frac{E_1}{E_2} \le 1 + C\delta_1 h_m^{2\mu+1}.$$

Now, from the definition of ρ, we may apply the triangle inequality to $e = -\rho + \theta$ and get

$$(4.19) \qquad \|\rho\|_E \le \|e\|_E \le \|\rho\|_E + \|\theta\|_E,$$

which by Lemma 4.3 and Thm. 3.2 becomes

$$(4.20) \quad \mathcal{E}_2 \frac{\|\rho\|_E}{\mathcal{E}_2} \le \|e\|_E \le \mathcal{E}_2 \left\{ \frac{\|\rho\|_E}{\mathcal{E}_2} + C\delta_1 h_m^{2\mu} \right\}.$$

Setting $h^* = \delta_1^{-1/\mu}$, we see in (4.18) that $\exists$ a positive constant C_1 such that for $h_m \le h \le C_1 h^*$

$$(4.21) \qquad \mathcal{E}_2 = \mathcal{E}_1 (1 + O(h^{\mu+1})) \quad \text{as} \quad h \to 0,$$

and therefore from (4.20) that

$$(4.22) \quad \|e\|_E = \mathcal{E}_1 \frac{\|\rho\|_E}{\mathcal{E}_2} (1 + O(h^{\mu})) \quad \text{as} \quad h \to 0.$$

By Lemma 4.2, the result of Thm. 4.1 follows immediately from (4.22). By assuming (4.13) we have Lemma 4.4, which applied to (4.22) yields the result of Thm. 4.2, since $0 < \mu \le 1 - \kappa/2 \le 1/2$.

5. A Posteriori Error Estimates Revisited

In this section we show how the estimator $E(\cdot,f-U_t,U)$ can be modified to take more fully into account the evolutionary nature of eqs. (2.4) and the errors introduced by the discontinuities in the data at the transtion time points. Under less restrictive conditions than (4.11) - (4.14), this modification is shown to be an upper estimator for $\|u - U\|_E$ on $[0,T)$.

We assume that

(5.1) $$u_0 \in \mathcal{D}(L) \quad \text{and}$$

(5.2) $$f,\ f_t \in C^0([0,T);\ H^0),$$

from which it follows that $u(;u_0,f) \in C^0([0,T);\ \mathcal{D}(L))$ and $u_t \in C^0([0,T);\ H^0)$. Define

(5.3) $$\hat{c} = \underline{a}\pi^2(\underline{a} \text{ as in } (2.2)) \le \inf_{\substack{\varphi\neq 0\\ \varphi\in H_0^1}} \frac{\|\varphi\|_E^2}{\|\varphi\|_0^2}.$$

For each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ and $t \in {}^cJ_m$; any $m \in [0,M]$, we define

(5.4) $$E(t,f - U_t,U) = \sum_{i=1}^{4} E_i(t,\Delta^T \times \Delta), \quad \text{where}$$

(5.5) $$E_1(t,\Delta^T \times \Delta) = E(t,f - U_t,U),$$

(5.6) $E_2(t,\Delta^T \times \Delta)$ =

$$e^{-\hat{c}(t-T_m)/2} \sum_{j=0}^{m} h_j \left\{ \int_{J_j \cap (0,t)} e^{-\hat{c}(T_m-s)} E^2(s,f_s-U_{ss},U_s)ds \right\}^{1/2},$$

(5.7) $E_3(t,\Delta^T \times \Delta)$ =

$$e^{-\hat{c}(t-T_m)/2} \cdot \begin{cases} 0 & ; m = 0, \\ h_m \|J_m\|_0 + \sum_{j=1}^{m-1}{}' \, h_j^2 e^{-\hat{c}(T_m-T_j)/2} \|J_j\|_0 & ; m \geq 1, \end{cases}$$

(5.8) $E_4(t,\Delta^T \times \Delta)$ =

$$e^{-\hat{c}t/2} \cdot E(0,U_t(0) + Lu_0 - f(0),0) \cdot \begin{cases} 1 & ; t = 0 \\ \min(1,h_0/t^{1/2}) & ; t > 0, \end{cases}$$

where $E(s,f_s - U_{ss},U_s)$ is defined as in (4.8) and (4.9) with f, U_s, U replaced by f_s, U_{ss}, U_s, and

(5.9) $$J_j \equiv U_t(T_j) - U_t(T_j^-); \qquad 1 \leq j \leq M.$$

By assumptions (5.1), (5.2), and the definitions (2.31)-(2.35), and (2.43) we see that $E(t,f - U_t,U)$ is well-defined and computable, given U.

We show the following result.

<u>Theorem 5.1</u>. Assume (5.1), (5.2), and that $T \times P$ is γ-regular with $\gamma \leq 1$. Then $E(\cdot,f - U_t,U)$ is an upper estimator for $\|u - U\|_E$ on $[0,T)$, with $h^* = 1$.

Proof. We must show that there exists a positive constant C such that for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ and all $t \in {}^cJ_m$; any $m \in [0,M]$

$$\|u(t) - U(t)\|_E \le C\, E(t, f - U_t, U). \tag{5.10}$$

As in [3, Thm. 6.1], to this end we decompose the error $e = u - U$ as

$$e = e^1 + e^2, \quad \text{where} \tag{5.11}$$

$$e^1 = v - U, \tag{5.12}$$

$$e^2 = u - v, \tag{5.13}$$

and for each $t \in [0,T)$, $v(t) \in \mathcal{D}(L)$ is defined as the unique solution of

$$Lv(t) = (f - U_t)(t). \tag{5.14}$$

By (5.1), (5.2), (2.43), and the t-independence of the operator L, we have that v_t satisfies

$$Lv_t(t) = (f_t - U_{tt})(t);\ \forall t \in [0,T), \quad \text{and} \tag{5.15}$$

$$\frac{\partial^j}{\partial t^j} v(t) \in C^0({}^cJ_m; \mathcal{D}(L));\ \text{for } j = 0 \text{ and } 1 \text{ and all } m \in [0,M]. \tag{5.16}$$

From eqs. (2.17), (2.18), (2.31)-(2.35), and the definitions (2.39) and (2.43) we have that

(5.17) $P_1(t) \frac{\partial^j}{\partial t^j} v(t) \;=\; \frac{\partial^j}{\partial t^j} U(t); \; \forall t \in [0,T), \; j = 0$ and 1.

It follows directly from results shown in [3, Thm. 6.1] that $\exists$ a positive constant C such that

(5.18) $$\|e^2(T_1^-)\|_E = \lim_{\substack{t \to T_1 \\ t \in J_0}} \|e^2(t)\|_E \le C\{E_2(T_1, \Delta^T \times \Delta) + E_4(T_1, \Delta^T \times \Delta)\},$$

and more generally that

(5.19) the desired result (5.10) holds when $m = 0$.

In view of the definitions (5.4)-(5.8), (5.11), and the observations (5.18) and (5.19), the demonstration of (5.10) will be completed by showing that for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$ and $t \in {}^cJ_m; \; 1 \le m \le M$

(5.20) $$\|e^1(t)\|_E \;\le\; C \, \mathcal{E}(t, f - U_t, U), \quad \text{and}$$

(5.21) $$\|e^2(t)\|_E \;\le\; C\{e^{-\hat{c}(t-T_1)/2} \|e^2(T_1^-)\|_E + E_2(t, \Delta^T \times \Delta) + E_3(t, \Delta^T \times \Delta)\}.$$

In view of the result in [1, Thm. 7.2], as applied in [3, (6.22)], we have the estimate (5.20) by (5.2), (5.12), (5.14), and (5.17) with $j = 0$.

In order to show (5.21), we subtract eqs. (2.34), (2.35) from eqs. (2.17), (2.18) and get from (5.12), (5.13), and (2.43) that for any m satisfying $1 \le m \le M$,

$$(5.22)\quad \langle e_s^2(s),\varphi\rangle + B(e^2(s),\varphi) = -\langle e_s^1(s),\varphi\rangle;\ \forall s,\varphi \in J_m \times H_0^1,$$

$$(5.23)\qquad e^2(T_m) = e^2(T_m^-) + v(T_m^-) - v(T_m).$$

It follows from (5.9), (5.14), (2.43), and (2.36) that

$$(5.24)\quad B(v(T_m^-) - v(T_m),\varphi) = \begin{cases} \langle J_m,\varphi\rangle; & \forall\varphi \in H_0^1, \\ 0 \quad ; & \forall\varphi \in S(\Delta_m), \end{cases}$$

and so by the approximation result (2.28) and a duality argument there exists a positive constant C such that

$$(5.25)\qquad \|v(T_m^-) - v(T_m)\|_0 \le Ch_m\|v(T_m^-) - v(T_m)\|_E$$

$$\le C^2h_m^2\|J_m\|_0.$$

From (5.23), (5.25), and the triangle inequality it therefore follows that

$$(5.26)\qquad \|e^2(T_m)\|_E \le \|e^2(T_m^-)\|_E + Ch_m\|J_m\|_0, \quad \text{and}$$

$$(5.27)\qquad \|e^2(T_m)\|_0 \le \|e^2(T_m^-)\|_0 + Ch_m^2\|J_m\|_0.$$

We now note from (5.17) with $j = 1$ that

$$B(e_s^1(s),\varphi) = 0;\quad \forall s,\varphi \in J_m \times S(\Delta_m).$$

Hence , it follows by using a duality argument and the definition of $E(\cdot,f_s - U_{ss},U_s)$, as the definition of $E(\cdot,f - U_s,U)$ was used in showing (5.20), that for some positive constant C

$$(5.28) \qquad \|e_s^1(s)\|_0 \le Ch_m E(s, f_s - U_{ss}, U_s); \quad \forall s \in J_m.$$

As in [3, (6.23), (6.24)], we get from (5.28) and energy arguments in eqs. (5.22), (5.23) that

$$(5.29) \quad \|e^2(t)\|_E \le$$

$$e^{-\hat{c}(t-T_m)/2} \cdot \min\left(2^{1/2}\|e^2(T_m)\|_E, \frac{h_m}{(t-T_m)^{1/2}}\|e^2(T_m)\|_0\right)$$

$$+ Ch_m e^{-\hat{c}(t-T_m)/2} \cdot \left\{\int_{T_m}^t e^{-\hat{c}(T_m-s)} E^2(s, f_s - U_{ss}, U_s)\,ds\right\}^{1/2}; \quad \forall t \in J_m.$$

It can similarly be shown that

$$(5.30) \quad \|e^2(t)\|_0 \le$$

$$e^{-\hat{c}(t-T_m)/2} \cdot \left(\|e^2(T_m)\|_0 + Ch_m \left\{\int_{T_m}^t e^{-\hat{c}(T_m-s)} \cdot E^2(s, f_s - U_{ss}, U_s)\,ds\right\}^{1/2}\right); \qquad \forall t \in {}^cJ_m$$

by (5.27)

$$\le e^{-\hat{c}(t-T_m)/2} \cdot \left(\|e^2(T_m^-)\|_0 + Ch_m^2\|J_m\|_0 + Ch_m \left\{\int_{T_m}^t e^{-\hat{c}(T_m-s)} \cdot E^2(s, f_s - U_{ss}, U_s)\,ds\right\}^{1/2}\right); \qquad \forall t \in {}^cJ_m.$$

Combining (5.26) and (5.29), we get

$$(5.31)\quad \|e^2(t)\|_E \le$$

$$e^{-\hat{c}(t-T_m)/2}\cdot\left(2^{1/2}\|e^2(T_m^-)\|_E + Ch_m\|J_m\|_0 + Ch_m\left\{\int_{T_m}^{t} e^{-\hat{c}(T_m-s)}\cdot E^2(s,f_s-U_{ss},U_s)ds\right\}^{1/2}\right); \qquad \forall t \in J_m.$$

In view of the definitions (5.6) and (5.7), this is the desired result (5.21) if $m = 1$. If $m \ge 2$, we can estimate $\|e^2(T_m^-)\|_E$ in (5.31) by applying (5.27) and (5.29) with m and t replaced by $m - 1$ and T_m. Using the γ-regularity of the family $T \times P$ in this argument, we get

$$(5.32)\quad \|e^2(t)\|_E \le$$

$$(2/\Lambda_1)^{1/2}\cdot e^{-\hat{c}(t-T_{m-1})/2}\cdot\|e^2(T_{m-1}^-)\|_0$$

$$+ Ce^{-\hat{c}(t-T_m)/2}\cdot(h_m\|J_m\|_0 + h_{m-1}^2 e^{-\hat{c}(T_m-T_{m-1})/2}\|J_{m-1}\|_0)$$

$$+ Ce^{-\hat{c}(t-T_m)/2}\cdot\sum_{j=m-1}^{m} h_j\left\{\int_{J_j\cap(0,t)} e^{-\hat{c}(T_m-s)}\cdot E^2(s,f_s-U_{ss},U_s)ds\right\}^{1/2}; \quad \forall t \in {}^cJ_m,$$

where Λ_1 is as in the γ-regularity definition (2.21). Noting from the definition (5.3) of $\hat{c}$ that

$$(5.33)\qquad \|e^2(T_1^-)\|_0 \le (1/\hat{c}^{1/2})\|e^2(T_1^-)\|_E,$$

we see that the desired result (5.21) follows from (5.32) if $m = 2$. If $m \geq 3$, we can estimate $\|e^2(T_{m-1}^-)\|_0$ in (5.32) by applying (5.30) with m and t replaced by $m-2$ and T_{m-1}. Repeating this argument a total of $m-2$ times, we get from (5.32) and (5.33) that

$$(5.34)\quad \|e^2(t)\|_E \leq$$

$$(2/\hat{c}\Delta_1)^{1/2}\cdot e^{-\hat{c}(t-T_1)/2}\cdot\|e^2(T_1^-)\|_E$$

$$+ Ce^{-\hat{c}(t-T_m)/2}\cdot(h_m\|J_m\|_0 + \sum_{j=1}^{m-1} h_j^2 e^{-\hat{c}(T_m-T_j)/2}\|J_j\|_0)$$

$$+ Ce^{-\hat{c}(t-T_m)/2}\cdot\sum_{j=1}^{m} h_j\left\{\int_{J_j\cap(0,t)} e^{-\hat{c}(T_m-s)}\cdot\right.$$

$$\left.\mathcal{E}^2(s,f_s-U_{ss},U_s)ds\right\}^{1/2};\forall t \in {}^cJ_m.$$

The result (5.21) for $m \geq 3$ follows immediately from (5.34), thus completing the proof of Thm. 5.1.

We now give conditions, which along with (5.1) and (5.2) are sufficient to show that up to higher order terms in h, $E(\cdot,f-U_t,U) \sim \mathcal{E}(\cdot,f-U_t,U)$.

$$(5.35)\qquad T_* \in (0,T) \quad\text{and}\quad C^* > 0.$$

$$(5.36)\qquad \|u_0\|_2 + \|f(0)\|_0 + \sup_{t\in[0,T]}\|f_t(t)\|_0 \leq C^*.$$

(5.37) $\mathcal{T}\times\mathcal{P}$ is a γ-regular family with $\gamma \in (0,1)$.

(5.38) For each $\Delta^T \times \Delta \in \mathcal{T}\times\mathcal{P}$, $T_1 > T_*$ and $h(\Delta) \leq T_*^{1/2\gamma}$.

The data u_0 and f and family $\mathcal{T} \times \mathcal{P}$ are such that for each $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$

$$(5.39) \quad \sup_{t \in [T_*, T)} \|U_t(t)\|_E + \left(\int_0^T \|U_t(t)\|_E^2 dt\right)^{1/2} + \left(\int_0^T \|U_{tt}(t)\|_0^2 dt\right)^{1/2} \le C^*.$$

We have

Theorem 5.2. Assume (5.1), (5.2), and (5.35)-(5.39). Then

$$(5.40) \quad E(t, f-U_t, U) = \mathcal{E}(t, f-U_t, U) + O(h^{2-\gamma}) \text{ as } h \to 0; \forall t \in [T_*, T),$$

where the constant in the O-term depends on C^*, T, Λ_1 in the γ-regularity definition (2.21), and the functions a and b.

The proof of Thm. 5.2 shall be omitted, as it easily follows by showing

$$(5.41) \quad \mathcal{E}(0, U_t(0) + Lu_0 - f(0), 0) \le Ch\{\|u_0\|_2 + \|f(0)\|_0\},$$

$$(5.42) \quad \|J_m\|_0 \le Ch\|U_t(T_m^-)\|_E; \qquad 1 \le m \le M,$$

$$(5.43) \quad E(s, f_s - U_{ss}, U_s) \le Ch\{\|f_s(s) - U_{ss}(s)\|_0 + \|U_s(s)\|_E\}; \forall s \in [0, T),$$

and applying the Cauchy-Schwarz inequality and γ-regularity of $\mathcal{T} \times \mathcal{P}$ to bound the sums appearing in $E_2(t, \Delta^T \times \Delta)$ and $E_3(t, \Delta^T \times \Delta)$.

Suppose that for $\Delta^T \times \Delta \in \mathcal{T} \times \mathcal{P}$, $M = M(\Delta^T) \ge 3$ and $t \in {}^cJ_M$. Since the terms in E_2, E_3, and E_4 have time decay rates which are pessimistically small for any given problem, in view of Thm. 5.2 one practical implementation of $E(t,f-U_t,U)$ would be to use only $\mathcal{E}(t,f-U_t,U)$, and to monitor the quantities

$$(5.44)\quad \tilde{E}_2(t,\Delta^T\times\Delta) \equiv \sum_{j=M-p}^{M} h_j \left\{\int_{J_j\cap(0,t)} e^{-\hat{c}(t-s)}\cdot \mathcal{E}^2(s,f_s-U_{ss},U_s)ds\right\}^{1/2}$$

and

$$(5.45)\quad \tilde{E}_3(t,\Delta^T\times\Delta) \equiv e^{-\hat{c}(t-T_m)/2} h_m\|J_m\|_0 + \sum_{j=M-p}^{M-1}{}' h_j^2 e^{-\hat{c}(t-T_j)/2}\|J_j\|_0,$$

where $p = 0, 1,$ or 2.

Also, since $\tilde{E}_2$ depends essentially on the past history of the changes in time of the local error indicators $\{\eta_{mj}(t,f-U_t,U)\}$, defined in (4.8), both $\tilde{E}_2$ and $\tilde{E}_3$ can be effectively monitored with a minimal amount of extra computational work.

6. Adaptive Procedure and Computational Examples

In this section we outline many aspects of a general FEMOL procedure in which decisions based upon a posteriori error estimates are used to adaptively construct and modify the space meshes. This procedure is contained in the research program FEMOL1, which was written and implemented on the IBM 370 System in the Division of Computer Research and Technology, NIH. For a discussion of the general capabilities and specific computational aspects of FEMOL1, we refer to [3] and [4]. Most comments on the procedures employed in FEMOL1 shall here be restricted to those related to the adaptivity in our experiments. These experiments were designed for the evaluation of conclusions concerning a posteriori error estimation which are based upon the asymptotic analysis presented in sections 3-5 for general changing meshes. The discussion is primarily oriented to selected examples, in which the exact solutions are those in the examples presented in [3, section 7]. The forms of these solutions are typical of those arising often with systems of linear and nonlinear parabolic equations used in various fields of application.

Before beginning, we mention that in [9] an adaptive procedure in some ways similar to our own was implemented for the FEMOL solution of parabolic PDEs in one and two space dimensions. Using small, uniform time steps in the backward Euler method to integrate the resulting ODE systems, the flexibility of the procedure was compared to that using uniform, time-independent meshes in a few examples.

The model problem considered here is that given in eqs. (1.1), where the functions a, b, and the exact solution u will be specified in each of the examples, and u_0, f, and g are chosen to be the corresponding smooth, compatible data. While the theory in sections 2-5 was presented for the case when the boundary data $g \equiv 0$, it holds more generally for eqs. (1.1).

The notation used here is that of section 1. For further clarity we recall that the norm $|||e(t,\cdot)|||$ of the space discretization error $e = u - U$ was defined in (1.2), the initial mesh Δ_0, error indicators $\{\eta_{0j}\}_{j=1,N_0}$ and estimator $\mathcal{E}(0)$ in (1.4), (1.6), (1.7), and each subsequent mesh Δ_m, corresponding error indicators $\{\eta_{mj}\}_{j=1,N_m}$ and estimator $\mathcal{E}(T_m)$ used in the adaptive procedure in (1.10), (1.11), (1.12).

The evaluation of $\mathcal{E}(\cdot)$ and the adaptive procedure is based upon examining the effectivity ratio $\Theta(\cdot)$ and the true error $E_{TRU}(\cdot)$, defined in (1.13) and (1.14). While the theory in sections 4-5 was presented for the estimation of $\|e(t,\cdot)\|_E$, where $\|\cdot\|_E$ is defined in (2.20), we note that up to higher order terms in the space mesh size, $\|e(t,\cdot)\|_E \sim |||e(t,\cdot)|||$.

The adaptive procedure used in the experiments is that partly described in section 1. More specifically, it is based upon controlling $\|e(t,\cdot)\|$ for all $t \in [0,T_{FINAL}]$ according to the following principle. For any given tolerance $TOL > 0$ and constants C_1, C_2 satisfying

(6.1) $$0 < C_1 \le 1/2 \quad \text{and} \quad 2 \le C_2 < \infty,$$

the space meshes should be modified so that

(6.2) $$\|e(t,\cdot)\| \sim TOL; \quad \forall t \in [0,T_{FINAL}], \quad \text{and}$$

(6.3) $$C_1 \cdot TOL \le \|e(t,\cdot)\| \le C_2 \cdot TOL; \quad \forall t \in [0,T_{FINAL}].$$

That is, it is <u>desirable</u> that $\|e(\cdot,\cdot)\|$ is approximately equal to TOL, but <u>acceptable</u> that (6.3) holds. We now make a number of remarks concerning underlying assumptions used, the goals (6.2) and (6.3), and the computational procedures employed in our experiments to achieve these goals.

(R.1) The adaptive scheme is a "once-through" procedure. If the FEMOL is implemented more than once for a given problem, then no information obtained from a previous implementation is used adaptively in a loop to solve the problem.

(R.2) The <u>primary</u> goal is to <u>control</u> $\|e(\cdot,\cdot)\|$ according to (6.2) and (6.3), and not to minimize it for some fixed number of mesh points, as is often proposed in adaptive schemes.

(R.3) Decisions concerning mesh modifications are based upon achieving (6.2) and (6.3) with $\|e(\cdot,\cdot)\|$ replaced by $E(\cdot)$ and are permitted at each of a collection $\{T_m\}_{m=0,M+1}$ of times, where the partition $\Delta^T = \{0 = T_0 < T_1 < \ldots < T_{M+1} = T_{FINAL}\}$ is given a priori. This choice of possible transition times poses no actual constraint on the procedure, and in practice these points of time could include output target points at which an ODE solver must be restarted.

(R.4) The choice of absolute, and not relative tolerance in (6.2) and (6.3) is made arbitrarily. In most applications the relative tolerance, or a combination of the two has more meaning.

(R.5) In many applications it may be acceptable to abandon (6.2) and place a low priority on achieving the left hand side of (6.3). This is particularly important when considering the computational work involved in mesh modification.

(R.6) TOL is assumed to be time-independent. In applications involving the evolution to a steady state, the transient response of a system to changing loads, or the propagation of a wave through different media, this principle can be modified.

(R.7) As in any adaptive procedure, the achievement of the goals is subject to certain constraints. In our experiments, the number of constraints was kept to a minimum in order to more easily assess the potential of the procedure. The primary constraints were

(6.4) $N_m < N_{max}$; where N_{max} was given a priori,

(6.5) $h \le H$; where h denotes the maximum length of any finite element used and H was given a priori,

and in modifying a partition Δ_m, only combinations of mesh refinement and derefinement were permitted, where

(6.6) no two consecutive nodal points x_{j-1}^m, x_j^m were both allowed to be removed, and

(6.7) no subinterval (x_{j-1}^m, x_j^m) itself was permitted to be refined into more than 2^q subintervals, where the positive integer q was given a priori.

No consideration, however, was given either to the amount of computational work needed to achieve (6.2) and (6.3) or to the question of how best to balance the time and space discretization errors. Because of the complex interaction of the error components in practical computations and the heuristic nature of many work-related constraints, our purpose here is to isolate the space discretization error and examine more clearly the potential of the adaptive procedure. These other important issues will be addressed in the next stage of the analysis. The ODE per step tolerances needed to essentially solve the resulting systems exactly were slightly smaller than those used in the experiments in [3] with time-independent meshes. Because of this stringent requirement and the orientation of our experiments, the amount of CPU time used in the examples is irrelevant and will not be quoted.

Let the parameters TOL, C_1, C_2, H, N_{max}, and q be given. For integers $M \geq 1$ and $N_0 \geq 2$, suppose that the partitions $\Delta^T = \{0 = T_0 < T_1 < \ldots < T_{M+1} = T_{FINAL}\}$ and $\Delta_0 = \{0 = x_0^0 < x_1^0 < \ldots < x_{N_0}^0 = 1\}$ are given, and that the variables m and modflag are initially set equal to zero. The algorithm for the adaptive construction of meshes and the FEMOL solution of eqs. (1.1) can then be summarized as follows.

<u>step 1</u>:

(1) Determine $U(T_m,\cdot)$ and $U_t(T_m,\cdot)$ on Δ_m.

(2) Compute $\{\eta_{mj}\}_{j=1,N_m}$ and $E(T_m)$.

(3) If the exact solution u is available, compute $E_{TRU}(T_m)$ and $\Theta(T_m)$.

(4) Set $\eta^0 = TOL/N_m^{1/2}$, $\eta^- = C_1\eta^0$, and $\eta^+ = C_2\eta^0$.

<u>step 2</u>:

If modflag = 1, set $\Delta_m^* = \Delta_m$; otherwise determine Δ_m^* from Δ_m by checking η_{mj}, for $j = 1, N_m$:

(1) If $j \geq 2$, $|x_j^m - x_{j-2}^m| \leq H$, and $\max\{\eta_{mj-1}, \eta_{mj}\} < \eta^-$, then <u>derefine</u> by removing x_{j-1}^m and marking x_j^m for no removal on the next pass.

(2) If $\eta_{mj} > \eta^{+}$, then refine (x_{j-1}^{m}, x_{j}^{m}) into 2^{p} uniform subintervals, where integer $p \in \{1,\dots,q\}$ approximately solves $2^{p} = \eta_{mj}/\eta^{0}$.

step 3:

If $\Delta_m^{*} \neq \Delta_m$ and Δ_m^{*} defines less than N_{max} subintervals, then set $\Delta_m = \Delta_m^{*}$, modflag = 1, and redo steps 1 and 2.

step 4:

If $m = M + 1$, stop; otherwise determine $U(t,\cdot)$ for $t \in (T_m, T_{m+1}]$ by solving an $N_m - 1$ dimensional ODE system.

step 5:

Set $\Delta_{m+1} = \Delta_m$, $N_{m+1} = N_m$, modflag = 0; and redo steps 1-4 with m replaced by $m + 1$.

In step 1 of each loop of the algorithm, the vector $\{U(T_m, x_j^m)\}_{j=1,N_m-1}$ of nodal values of the FEMOL solution U at $t = T_m$ is determined as the solution of the matrix equation associated with the standard piecewise linear finite element approximation for an elliptic boundary value problem. The way in which the entries of these matrices and the indicators $\{\eta_{mj}\}_{j=1,N_m}$ were computed was different in each of the examples and will be discussed shortly. According to the manner in which $U_t(T_m,\cdot)$ is prescribed (cf. (2.35), (2.36)) after a partition Δ_m is obtained through mesh modification, the computational procedure used in step 1 for $m \geq 1$ to obtain $U_t(T_m,\cdot)$, and hence the right hand side of the matrix equation is the following.

In the event that mesh derefinement has occurred, i.e.g. a point x^m_{j-1} has been removed from the mesh, a system of two linear equations must be solved to determine the values $U_t(T_m,x^m_{j-2})$ and $U_t(T_m,x^m_j)$ on the new mesh, thus determining the function $U_t(T_m,\cdot)$ via L_2-projection. If mesh refinement has occurred, simple linear interpolation is used to determine $U_t(T_m,\cdot)$. While these processes are local, the process for obtaining $U(T_m,\cdot)$ is not, and a full system of $N_m - 1$ linear equations must be solved. The new mass and stiffness matrices are related to the old ones, but to simplify the data structures involved, no advantage is taken of this here and all matrix entries are recomputed after each mesh modification.

In step 2 of every loop of the algorithm the adaptive decision making process takes place. Each indicator η_{mj} is compared to the root mean square of the desired error TOL. The underlying assumption used here is that the best way to achieve (6.2) and (6.3) for all $t \in [T_m,T_{m+1})$ is by constructing Δ_m so that the indicators $\{\eta_{mj}\}_{j=1,N_m}$ are equilibriated. This assumption is based upon the hypotheses which led to Thms. 4.1 and 4.2, and is made in view of results shown in [2], where optimal meshes for elliptic boundary value problems were characterized by asymptotic equality of the error indicators.

The mesh modifications implementing this principle are restricted to being combinations of refinement and derefinement for the sake of computational simplicity. Since each η_{mj} is proportional to $|x_j^m - x_{j-1}^m|$, it is assumed that by removing the nodal point x_{j-1}^m in constructing Δ_{m+1} from Δ_m we will obtain $\eta_{m+1\ n} \sim 2(\eta^2_{m\ j-1} + \eta^2_{mj})^{1/2}$, where $(x_{n-1}^{m+1}, x_n^{m+1}) = (x_{j-2}^m, x_j^m)$. Similarly, by refining any interval (x_{j-1}^m, x_j^m) into the union

$$\bigcup_{n=n_0}^{n_0-1+2^P} (x_{n-1}^{m+1}, x_n^{m+1})$$

of 2^P uniform subintervals, it is assumed that

$$\left\{ \sum_{n=n_0}^{n_0-1+2^P} \eta^2_{m+1\ n} \right\}^{1/2} \sim \eta_{mj}/2^P.$$

These assumptions are based upon asymptotic analysis.

In the actual implementation of step 2 of the algorithm, if the number N_{m+1} of subintervals in a newly constructed partition Δ_{m+1} differs much from the number N_m in Δ_m, then each of the previously computed indicators $\{\eta_{mj}\}_{j=1,N_m}$ is also compared to the values of η^- and η^+ obtained by replacing N_m by N_{m+1}. This is done to avoid a subsequent mesh modification and suggests that the history of the indicators can be used to make the algorithm more efficient.

The conducted experiments consisted of two examples. In all runs the parameter values $C_1 = 1/2$, $C_2 = 2$, $N_{max} = 200$, and $q = 3$ were fixed. The partitions Δ_0 and Δ^T were taken to be uniform and defined by

$$(6.8) \qquad x_j^0 = j/N_0; \quad j = 0, N_0 \quad \text{and}$$

$$(6.9) \qquad T_m = m \cdot DT = m \cdot (T_{FINAL}/M+1); \quad m = 0, M+1.$$

The values of N_0, T_{FINAL}, M, and hence also DT varied in the experiments, as did the parameters TOL and H.

Example 1.

The coefficients a and b and the exact solution u of eqs. (1.1) are as in Example 1 of [3, section 7], namely $a(x) = \cosh(4x-2)$, $b(x) = \sinh(2x)$, and

$$(6.10) \qquad u(t,x) = u^1(t,x) + [1/2 + 1/2 \tanh(10t-11)]u^2(t,x), \text{ where}$$

$$(6.11) \qquad u^1(t,x) = 1 - \exp\{-x^2/(10t+.1)\} \quad \text{and}$$

$$(6.12) \qquad u^2(t,x) = 2\sin(\pi x) + 2\cos(2\pi t)\sin(2\pi x).$$

For $0 \le t \le .9$, u^1 dominates the behavior of u and u decays in t. After undergoing a sharp transition for $.9 < t < 1.1$, u oscillates as its dominant component u^2 (cf. figure 1).

In this example standard two-point Gaussian quadrature was used in the computation of the mass and stiffness matrix entries, load vectors, error indicators, and absolute error E_{TRU}. The parameter values $N_0 = 10$, $T_{FINAL} = 3$, $M = 49 (\Rightarrow DT = .06)$, and $H = .2$ were fixed, and the adaptive FEMOL procedure was implemented twice, with the absolute error tolerance TOL taken to be .530 and .265. These are the mean values about which E_{TRU} oscillated for $1 \leq t \leq 3$ in Example 1 of [3, section 7], using 20 and 40 *uniform*, t-independent finite elements (cf. [3, figure 4], where the corresponding relative error E_{REL} is shown oscillating about .05 and .025).

The numbers of elements used as functions of time for the different values of TOL are shown in figure 2. Because no constraint prohibiting minor mesh modifications was imposed, mesh changes occurred at most of the 50 allowed transition times.

Figure 3 illustrates the effectivity of the adaptive procedure in this example. For each TOL

(6.13) $$1/2 \cdot TOL \leq E_{TRU}(t) \leq 2 \cdot TOL; \quad 1 \leq t \leq 3.$$

For $0 < t < 1$, the imposition of the maximum mesh size constraint limited the flexibility of the procedure, and therefore $E_{TRU}(t) << TOL$.

The effectivity of the estimator $\mathcal{E}(\cdot)$ for meshes changing according to the adaptive procedure is illustrated in figure 4. For each TOL

(6.14) $\quad .95 \leq \Theta(t) \leq 1.12; \quad \forall t \in [.9,1.1]$,

(6.15) $\quad .99 \leq \Theta(t) \leq 1.06; \quad \forall t \in [1.1,3]$, and

it appears as though $\Theta(t) \to 1$ as $TOL \to 0$ for most $t \in [1.1,3]$. The fact that $\Theta(t)$ is not as near 1 for $t \in (0,.9)$ is probably due to the flatness of the exact solution $u(t,\cdot)$, which essentially violates an assumption in the theory of section 4.

<u>Example 2</u>.

The exact solution u of eqs. (1.1) is as in Example 2 of [3, section 7], namely

(6.16) $\quad u(t,x) = 1/2 + 1/2 \tanh[2\beta(x - 10t)]; \quad \beta = 20.$

The solution is a wave with approximate front width β^{-1} which moves in the positive x-direction at speed 10, and is as pictured in figures 5(a), (b), (c).

The coefficients a and b of eqs. (1.1) were taken here to be the constant functions $a \equiv 1$ and $b \equiv 0$. This choice was made so that all integrations needed in the computation of the matrix entries, load vectors, error indicators, and E_{TRU} could be performed exactly. Strong pollution effects were observed in the adaptive procedure for this example when two-point Gaussian quadrature was employed. This effect was particularly evident in computing the L_2-projections of U_t needed to determine the initial data U at the transition times, and indicates the care with which numerical integration methods should be chosen when applying the adaptive FEMOL procedure.

The parameter T_{FINAL} was set equal to .04, which is the amount of time needed for the center of the wave to travel from $x = 0$ to $x = .4$. Two implementations of the adaptive scheme, which we shall refer to as Examples 2(a) and 2(b) were carried out. In Example 2(a), the remaining parameters were taken to be $N_0 = 10$, $M = 19 (\Rightarrow DT = .002)$, $H = .1$, and $TOL = .8$. The values taken in Example 2(b) were $N_0 = 20$, $M = 39($ $DT = .001)$, $H = .05$, and $TOL = .1$. The desired absolute errors of .8 and .1 correspond approximately to 16% and 2% errors.

In figure 6(a) the nodal points at every fifth transition time in the first half of the interval (0,1) chosen by the adaptive scheme in Example 2(a) are pictured. The total number of nodal points at any time varied between 16 and 18. In figure 6(b) the nodal points at every tenth transition time for Example 2(b) are shown. Between 64 and 70 nodal points were used to partition (0,1) at each time in this example.

As in Example 1, in both Examples 2(a) and 2(b) a mesh change occurred at nearly every allowed transition time. Figures 6(a) and 6(b) clearly illustrate the ability of the adaptive scheme to concentrate nodal points along the characteristic $x = 10t$ of the wave, where all of the activity takes place.

The effectivity of the adaptive procedure is illustrated in figure 7. Here, as also in figure 8, the output time points were chosen to coincide with the allowed transition time points. After the second mesh transition in Example 2(a) E_{TRU} oscillates about the value .55 and we see that

$$(6.17) \qquad 1/2 \cdot TOL \le E_{TRU}(t) \le TOL.$$

Similarly, E_{TRU} oscillates about .08 in Example 2(b) after the second mesh transition and

$$(6.18) \qquad 3/4\ TOL \le E_{TRU}(t) \le 5/4\ TOL.$$

The effectivity of the estimator $\mathcal{E}(\cdot)$ in both Examples 2(a) and 2(b) is illustrated in figure 8. In Example 2(a) at all but one of the 21 time points, Θ satisfies

$$(6.19) \qquad 1 \le \Theta(t) \le 1.1,$$

and at all of the 41 time points in Example 2(b)

$$(6.20) \qquad .95 \le \Theta(t) \le 1.05.$$

The steady decline of Θ as a function of t in Example 2(b) is apparently due to errors introduced by the discontinuous mesh transitions. In repeating Example 2(b) with $H = .1$ instead of .05, we observed a similar decline in the effectivity ratio Θ, but this time to .85. In another experiment with $H = .1$ and $DT = .002$ instead of .001, this decline was slightly alleviated.

These experiments suggest modifying the estimator $\mathcal{E}(\cdot)$, as was proposed in section 5 (cf. (5.45)), when no prior knowledge of the relationship between TOL and H, or TOL and DT is available. We recall that the theory in section 4 concerning the effectivity of $\mathcal{E}(\cdot)$ was based partly upon assumptions related to the ratios of the sizes of elements in each mesh and the distances between mesh transitions.

As was observed in [3] for t-independent meshes, it has been seen in the selected examples presented here that $\mathcal{E}(\cdot)$ is an effective estimator of E_{TRU}. While effectivity ratios anywhere in the range [.1,10] would be quite acceptable in most applications, Θ was very near one for all of the adaptively constructed meshes. In view of the apparently stringent conditions concerning the asymptotic range for mesh sizes, which were given for general changing meshes in the theory of section 4, this is a particularly encouraging result.

The mesh modification scheme presented, in which decisions based upon $\mathcal{E}(\cdot)$ are made adaptively by the computer, was likewise quite effective in our experiments. In each case the goals of the procedure were realized, thus illustrating the robustness of both $\mathcal{E}(\cdot)$ and the adaptive process. These results from the selected examples suggest the method's applicability to more general problems occurring in practice (cf. [4]).

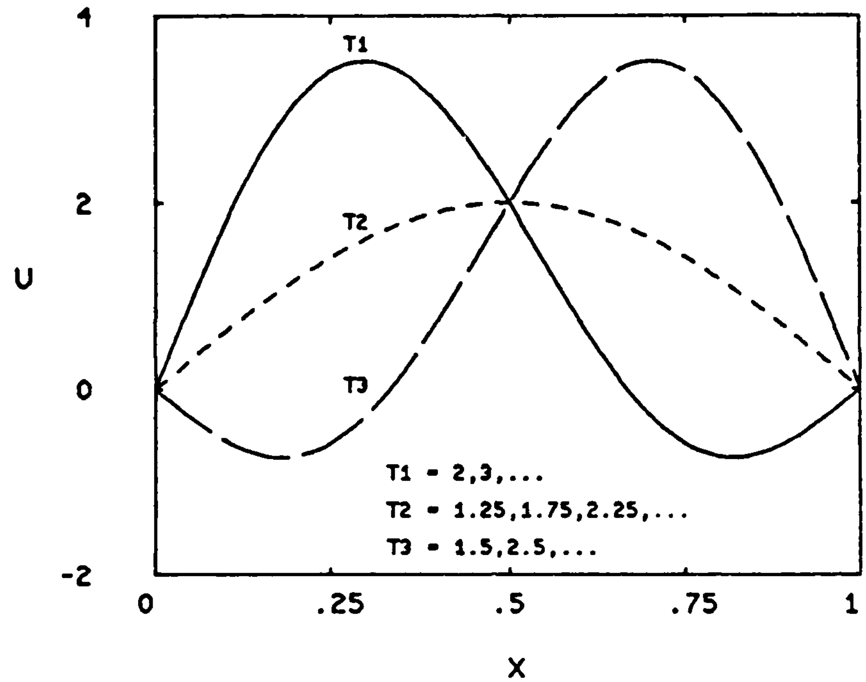

Figure 1. Exact Solution u(T,X) of Example 1 vs. X for various T.

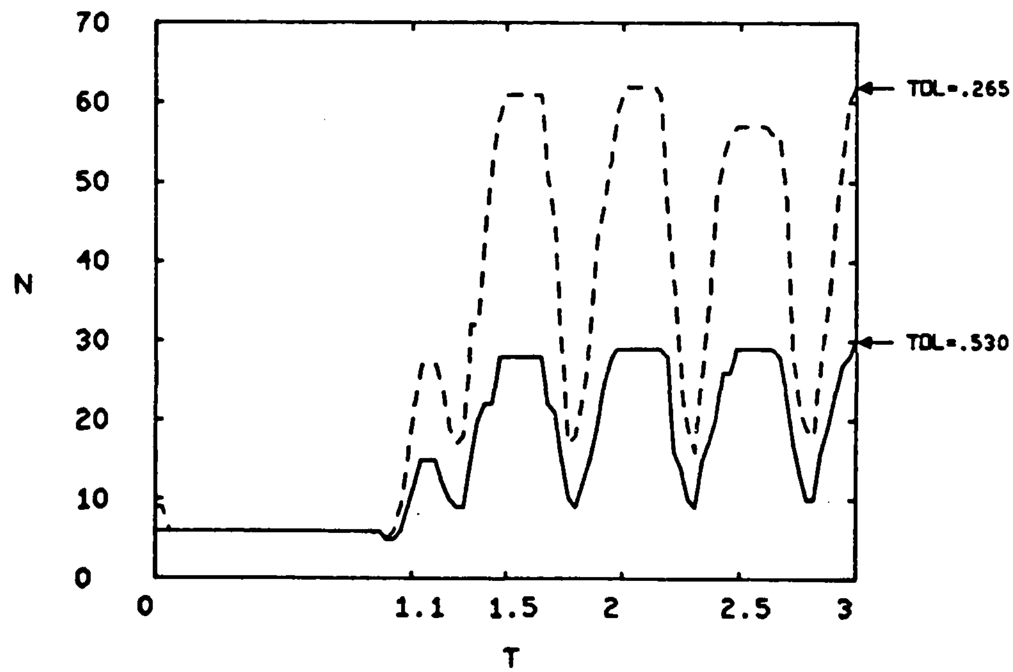

Figure 2. N = Number of Finite Elements in Example 1 vs. T
TOL = Absolute Error Tolerance .

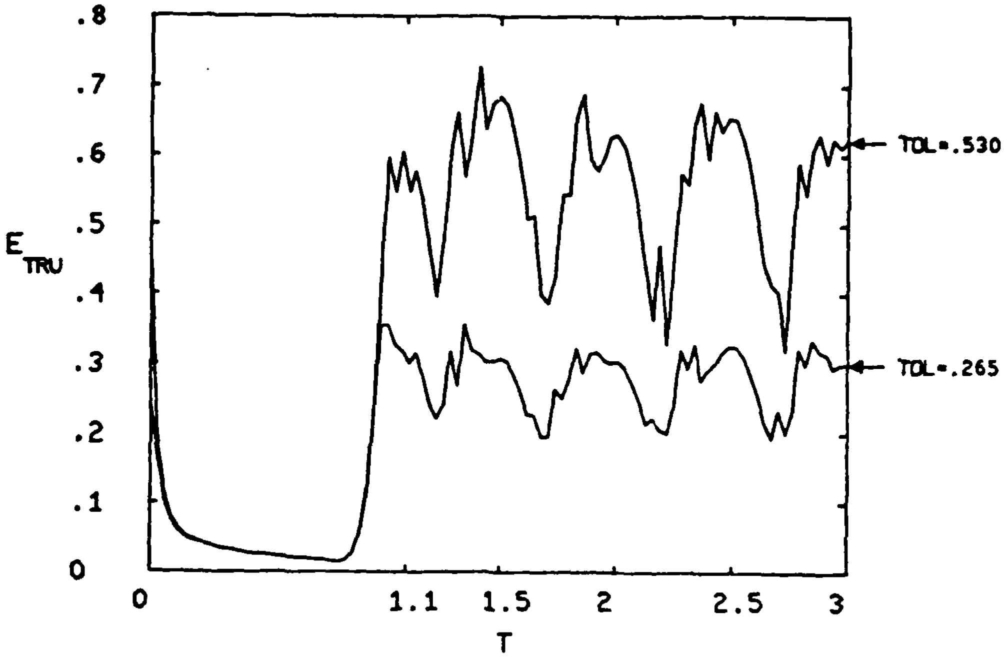

Figure 3. Absolute Error $E_{TRU}(T)$ in Example 1 vs. T
TOL = Absolute Error Tolerance.

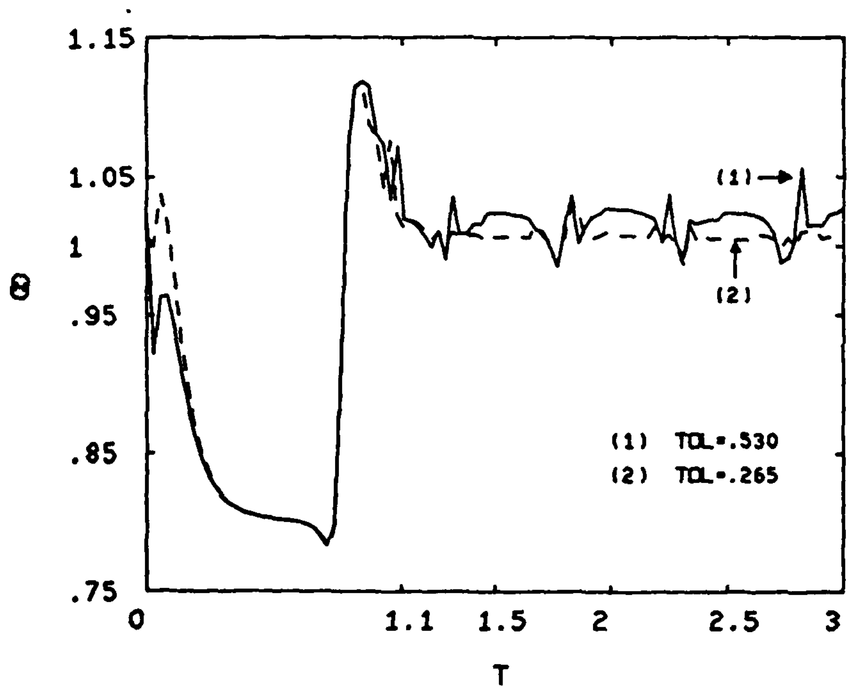

Figure 4. Effectivity Ratio Θ(T) in Example 1 vs. T
TOL = Absolute Error Tolerance.

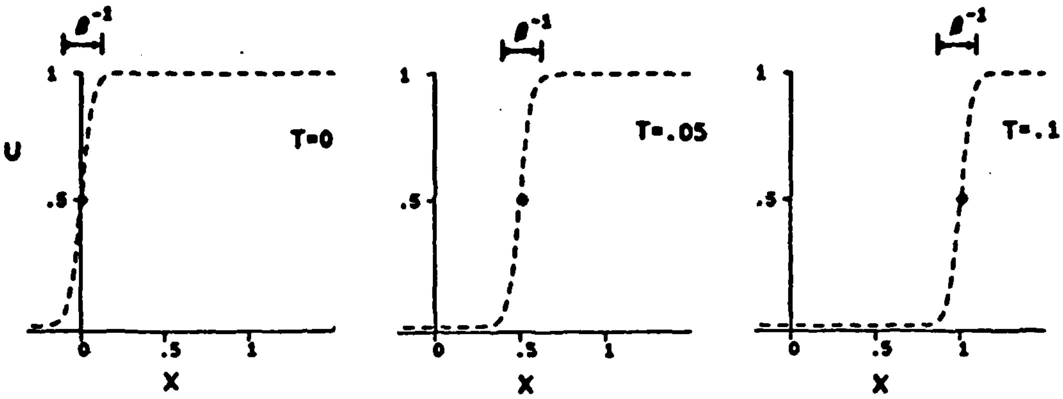

Figure 5(a),(b),(c). Exact Solution u(T,X) of Example 2 vs. X for various T.

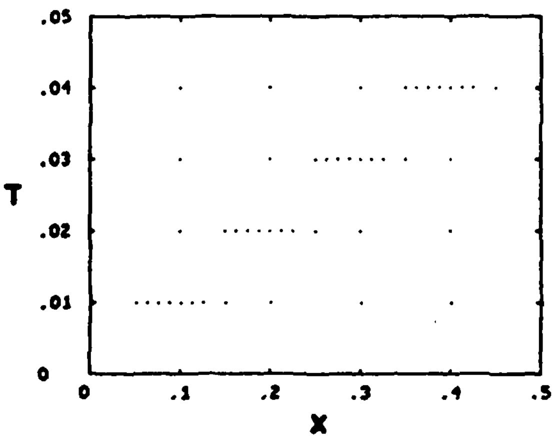

Figure 6(a). Nodal Points in Every 5th Grid in Example 2(a).

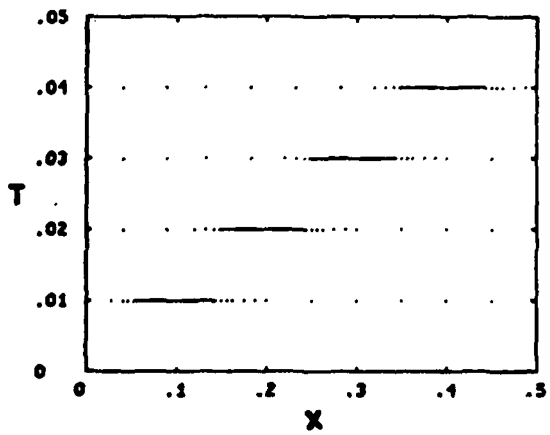

Figure 6(b). Nodal Points in Every 10th Grid in Example 2(b).

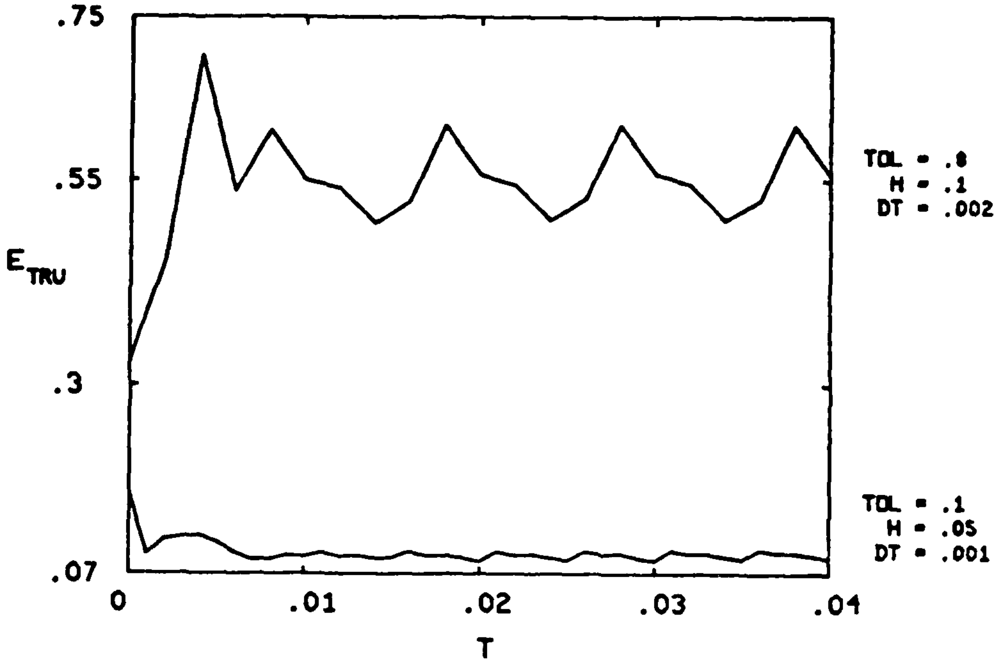

Figure 7. Absolute Error $E_{TRU}(T)$ in Examples 2(a) and 2(b) vs. T .

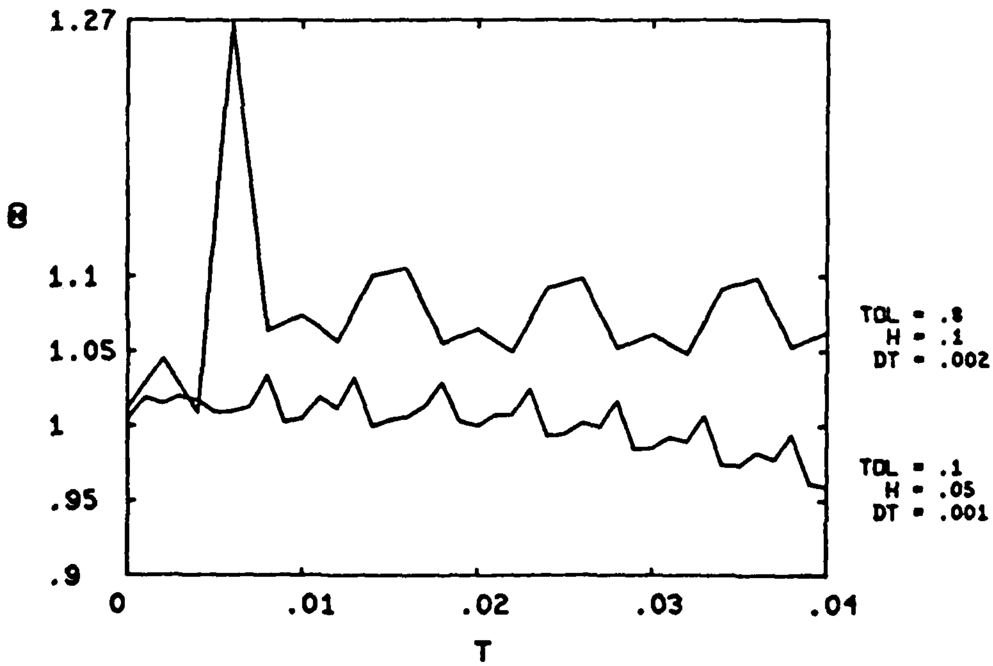

Figure 8. Effectivity Ratio $\Theta(T)$ in Examples 2(a) and 2(b) vs. T.

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