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A Posteriori Error Estimates for a Nonlinear Parabolic Equation*

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Abstract. A posteriori error estimates form a reliable basis for adaptive approximation techniques for modeling various physical phenomena. The estimates developed recently in the finite element method of lines for solving a parabolic differential equation are simple, accurate, and cheap enough to be easily computed along with the approximate solution and applied to provide the optimum number and optimum distribution of space grid nodes.
The contribution is concerned with a posteriori error estimates needed for the adaptive construction of a space grid in solving an initial-boundary value problem for a nonlinear parabolic partial differential equation by the method of lines. Under some conditions, it adds some more statements to the results of [2] in the semidiscrete case. Full text of the contribution will appear as a paper [4].

AMS Subject Classification. 65M15, 65M20

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1 A Nonlinear Model Problem

The principal ideas of semidiscrete a posteriori error estimation for nonlinear parabolic partial differential equations can be demonstrated with the help of a simple initial-boundary value one-dimensional model problem. We consider the nonlinear equation

$$\frac{\partial u}{\partial t}(x,t) - \frac{\partial}{\partial x}\Big(a(u)\frac{\partial u}{\partial x}(x,t)\Big) + f(u) = 0, \quad 0 < x < 1, \quad 0 < t \le T,$$

for an unknown function $u(x,t)$ with the homogeneous Dirichlet boundary conditions

$$u(0,t) = u(1,t) = 0, \quad 0 \le t \le T,$$

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and the initial condition

$$u(x,0) = u_0(x), \quad 0 < x < 1.$$

In the above formulae, $T > 0$ is a fixed number and a, f, and u_0 are smooth functions. Let

$$0 < \mu \le a(s) \le M, \quad s \in R,$$

and let a and f satisfy the global Lipschitz conditions

$$|a(r) - a(s)| \le L|r - s|,$$
$$|f(r) - f(s)| \le L|r - s|, \quad r, s \in R.$$

We employ the usual $L_2(0,1)$ inner product to introduce the *weak solution* $u(x,t) \in H^1([0,T], H_0^1(0,1))$ of the model problem by the identity

$$\Big(\frac{\partial u}{\partial t}, v\Big) + \Big(a(u)\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}\Big) + (f(u), v) = 0$$

holding for almost every $t \in (0,T]$ and all functions $v \in H_0^1$, and the identity

$$\Big(a(u_0)\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}\Big) = \Big(a(u_0)\frac{\partial u_0}{\partial x}, \frac{\partial v}{\partial x}\Big)$$

holding for $t = 0$ and all functions $v \in H_0^1$.

2 Discretization

Finite element solutions of the model problem are constructed from this weak formulation, too. We first introduce a partition

$$0 = x_0 < x_1 < \cdots < x_{N-1} < x_N = 1$$

of the interval $(0,1)$ into N subintervals (x_{j-1}, x_j), $j = 1, \ldots, N$, and then put

$$h_j = x_j - x_{j-1}, \quad j = 1, \ldots, N, \quad \text{and} \quad h = \max_{j=1,\ldots,N} h_j.$$

We further use the notation

$$(v, w)_j = \int_{x_{j-1}}^{x_j} v(x)w(x)\,\mathrm{d}x$$

for the $L_2(x_{j-1}, x_j)$ inner product.

We construct the finite dimensional subspace $S_0^{N,p} \subset H_0^1$ with a piecewise polynomial hierarchical basis of degree $p \ge 1$ in the following way. We put

$$S_0^{N,p} = \Big\{V \mid V \in H_0^1, V(x) = \sum_{j=1}^{N-1} V_{j1}\varphi_{j1}(x) + \sum_{j=1}^{N}\sum_{k=2}^{p} V_{jk}\varphi_{jk}(x)\Big\},$$

where φ_{j1} are the usual piecewise linear shape functions of the finite element method,

$$\begin{aligned}\varphi_{j1}(x) &= (x - x_{j-1})/h_j, \quad x_{j-1} \le x < x_j,\\ &= (x_{j+1} - x)/h_{j+1}, \quad x_j \le x \le x_{j+1},\\ &= 0 \quad \text{otherwise,}\end{aligned}$$

while for $k > 1$,

$$\begin{aligned}\varphi_{jk}(x) &= \frac{\sqrt{2(2k-1)}}{h_j} \int_{x_{j-1}}^{x_j} \mathrm{P}_{k-1}(y)\,\mathrm{d}y, \quad x_{j-1} \le x \le x_j,\\ &= 0 \quad \text{otherwise}\end{aligned}$$

are bubble functions with P_k being the kth degree Legendre polynomial scaled to the subinterval $[x_{j-1}, x_j]$ (see, e.g., [5]).

We say that a function $\bar{U}(x,t)$ is the *semidiscrete finite element approximate solution* of the model problem if it belongs, as a function of the variable t, into $H^1([0,T], S_0^{N,p})$, if the identity

$$\Big(\frac{\partial \bar{U}}{\partial t}, V\Big) + \Big(a(\bar{U})\frac{\partial \bar{U}}{\partial x}, \frac{\partial V}{\partial x}\Big) + (f(\bar{U}), V) = 0$$

holds for each $t \in (0,T]$ and all functions $V \in S_0^{N,p}$, and if the identity

$$\Big(a(u_0)\frac{\partial \bar{U}}{\partial x}, \frac{\partial V}{\partial x}\Big) = \Big(a(u_0)\frac{\partial u_0}{\partial x}, \frac{\partial V}{\partial x}\Big)$$

holds for $t = 0$ and all functions $V \in S_0^{N,p}$. The procedure for constructing the approximate solution

$$\bar{U}(x,t) = \sum_{j=1}^{N-1} \bar{U}_{j1}(t)\varphi_{j1}(x) + \sum_{j=1}^{N}\sum_{k=2}^{p} \bar{U}_{jk}(t)\varphi_{jk}(x)$$

described above is the *method of lines*. It transforms the solution of the original initial-boundary value problem for a parabolic partial differential equation into an initial value problem for a system of ordinary differential equations for the unknown functions $\bar{U}_{jk}(t)$ that, in practice, is solved by proper numerical software.

3 A Posteriori Semidiscrete Error Indicators

Let

$$e(x,t) = u(x,t) - \bar{U}(x,t)$$

be the error of the semidiscrete approximate solution. We employ the finite dimensional subspace

$$\hat{S}_0^{N,p+1} = \Big\{\hat{V} \mid \hat{V} \in H_0^1, \hat{V}(x) = \sum_{j=1}^{N} \hat{V}_j \varphi_{j,p+1}(x)\Big\}$$

of piecewise polynomial bubble functions of degree $p+1$ equal to zero at the grid points x_j to construct error indicators. We say that a function $\bar{E}(x,t) = \bar{E}_{\mathrm{PN}} \in H^1([0,T], \hat{S}_0^{N,p+1})$ is a *parabolic nonlinear a posteriori semidiscrete error indicator* if the identities

$$\Big(\frac{\partial \bar{E}}{\partial t}\ ,\ \hat{V}\Big)_j + \Big(a(\bar{U}+\bar{E})\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j$$
$$= -(f(\bar{U}+\bar{E}), \hat{V})_j - \Big(\frac{\partial \bar{U}}{\partial t}, \hat{V}\Big)_j - \Big(a(\bar{U}+\bar{E})\frac{\partial \bar{U}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j$$

hold for $j = 1, \ldots, N$, all $t \in (0,T]$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$, and if the identities

$$\Big(a(u_0)\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j = \Big(a(u_0)\frac{\partial (u_0 - \bar{U})}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j$$

hold for $j = 1, \ldots, N$, $t = 0$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$. Note that the special choice of the bubble function space $\hat{S}_0^{N,p+1}$ results in an uncoupled system of ordinary differential equations. On each interval (x_{j-1}, x_j), the error indicator

$$\bar{E}(x,t) = \sum_{j=1}^{N} \bar{E}_j(t)\varphi_{j,p+1}(x)$$

is computed independently of the other intervals. The indicator thus has a local character and its computation is rather cheap.

When $\bar{E}$ is neglected in the argument of the functions a and f we say that a function $\bar{E}(x,t) = \bar{E}_{\mathrm{PL}} \in H^1([0,T], \hat{S}_0^{N,p+1})$ is a *parabolic linear a posteriori semidiscrete error indicator* if the identities

$$\Big(\frac{\partial \bar{E}}{\partial t}, \hat{V}\Big)_j + \Big(a(\bar{U})\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j = -(f(\bar{U}), \hat{V})_j - \Big(\frac{\partial \bar{U}}{\partial t}, \hat{V}\Big)_j - \Big(a(\bar{U})\frac{\partial \bar{U}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j$$

hold for $j = 1, \ldots, N$, all $t \in (0,T]$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$, and if the identities

$$\Big(a(u_0)\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j = \Big(a(u_0)\frac{\partial (u_0 - \bar{U})}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j$$

hold for $j = 1, \ldots, N$, $t = 0$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$. The practical computation of the linear error indicator is thus easier.

The task to compute error indicators can be simplified if the derivative $\partial \bar{E}/\partial t$ is neglected. The corresponding a posteriori semidiscrete error indicator is then called (linear or nonlinear) elliptic indicator since the resulting uncoupled algebraic system does not depend on t. Moreover, the practical computation of such an elliptic indicator need not be carried out for each t but only when required. We thus say that the function $\bar{E}(x,t) = \bar{E}_{\mathrm{EN}}$ that maps $[0,T]$ into $\hat{S}_0^{N,p+1}$ is an *elliptic nonlinear a posteriori semidiscrete error indicator* if the identities

$$\Big(a(\bar{U}+\bar{E})\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j = -(f(\bar{U}+\bar{E}), \hat{V})_j - \Big(\frac{\partial \bar{U}}{\partial t}, \hat{V}\Big)_j - \Big(a(\bar{U}+\bar{E})\frac{\partial \bar{U}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\Big)_j$$

hold for $j = 1, \ldots, N$, all $t \in (0, T]$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$, and if the identities

$$\left(a(u_0)\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\right)_j = \left(a(u_0)\frac{\partial (u_0 - \bar{U})}{\partial x}, \frac{\partial \hat{V}}{\partial x}\right)_j$$

hold for $j = 1, \ldots, N$, $t = 0$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$.

Finally, we say that the function $\bar{E}(x,t) = \bar{E}_{\mathrm{EL}}$ that maps $[0, T]$ into $\hat{S}_0^{N,p+1}$ is an *elliptic linear a posteriori semidiscrete error indicator* if the identities

$$\left(a(\bar{U})\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\right)_j = -(f(\bar{U}), \hat{V})_j - \left(\frac{\partial \bar{U}}{\partial t}, \hat{V}\right)_j - \left(a(\bar{U})\frac{\partial \bar{U}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\right)_j$$

hold for $j = 1, \ldots, N$, all $t \in (0, T]$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$, and if the identities

$$\left(a(u_0)\frac{\partial \bar{E}}{\partial x}, \frac{\partial \hat{V}}{\partial x}\right)_j = \left(a(u_0)\frac{\partial (u_0 - \bar{U})}{\partial x}, \frac{\partial \hat{V}}{\partial x}\right)_j$$

hold for $j = 1, \ldots, N$, $t = 0$ and all functions $\hat{V} \in \hat{S}_0^{N,p+1}$.

To assess properties of the above semidiscrete a posteriori error indicators, we introduce the quantity

$$\Theta = \frac{\|\bar{E}\|_1}{\|e\|_1}$$

called the *effectivity index* of the respective error indicator. The norm used is the $H^1(0,1)$ norm. Then we can prove the following statement.

Theorem 1. *Let $u(x,t) \in H_0^1$ be smooth, let $\bar{U}(x,t) \in S_0^{N,p}$ and $\bar{E} \in \hat{S}_0^{N,p+1}$. Let the norm of the difference between the semidiscrete solution $\bar{U}$ and its elliptic projection is a nondecreasing function of t. Let the same hold for the norm of the difference between the error indicator $\bar{E}$ and its elliptic projection.*

Moreover, let

$$\|e\|_1 \geq Ch^p.$$

Then

$$\lim_{h \to 0} \Theta = 1$$

holds for Θ_{PN}, Θ_{PL}, and Θ_{EL}.

The exact assumptions as well as a complete proof will be published in [4].

4 A Numerical Example

We present numerical results obtained by the finite element method of lines for a nonlinear parabolic initial-boundary value problem (a reaction-diffusion model) with a simple grid adjustment procedures described in [1] (Fig. 1) and [3] (Fig. 2). Both the procedures are based on the equidistribution of error. The example fully confirms the above statement.

The differential equation solved is

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} - D(1+\alpha-u)\exp(-\delta/u) = 0,$$

$$D = R\,\frac{\exp\delta}{\alpha\delta}, \quad 0 < x < 1, \quad 0 < t \le 0.6,$$

$$\alpha = 1, \quad \delta = 20, \quad R = 5,$$

with the boundary conditions

$$\frac{\partial u}{\partial x}(0,t) = 0, \quad u(1,t) = 1, \quad 0 < t \le 0.6,$$

and the initial condition

$$u(x,0) = 1, \quad 0 < x < 1.$$

We used piecewise linear shape functions, i.e. $p = 1$, for the computation of the solution $\bar{U}$ and required a very small error bound in the integration of the corresponding system of ordinary differential equations by a standard differential system solver.

The model describes a single step reaction of a reacting mixture of temperature u in a region $0 < x < 1$. Further, α is the heat release, δ is the activation energy, D is called the Damkohler number, and R is the reaction rate. For small times, the temperature gradually increases from unity with a "hot spot" forming at $x = 0$. At a finite time, ignition occurs and the temperature at $x = 0$ jumps rapidly from near 1 to near $1+\alpha$. A sharp flame front then forms and propagates towards $x = 1$ with velocity proportional to $\frac{1}{2}\exp(\alpha\delta)/(1+\alpha)$. In real problems, α is about unity and δ is large. The flame front thus moves exponentially fast after ignition. The problem reaches a steady state once the flame propagates to $x = 1$.

The trajectories of nodes of the partition of interval $(0,1)$ as constructed by the two procedures mentioned are shown in Figs. 1 and 2. The grid is rather slow and is unable to follow the dynamics of the problem properly. The integration with respect to t requires small time steps and is expensive during this rapid transience as the solution changes rapidly along the grid node trajectories. The problem is very difficult and yet adaptive grid methods are capable of finding a solution with relative ease.

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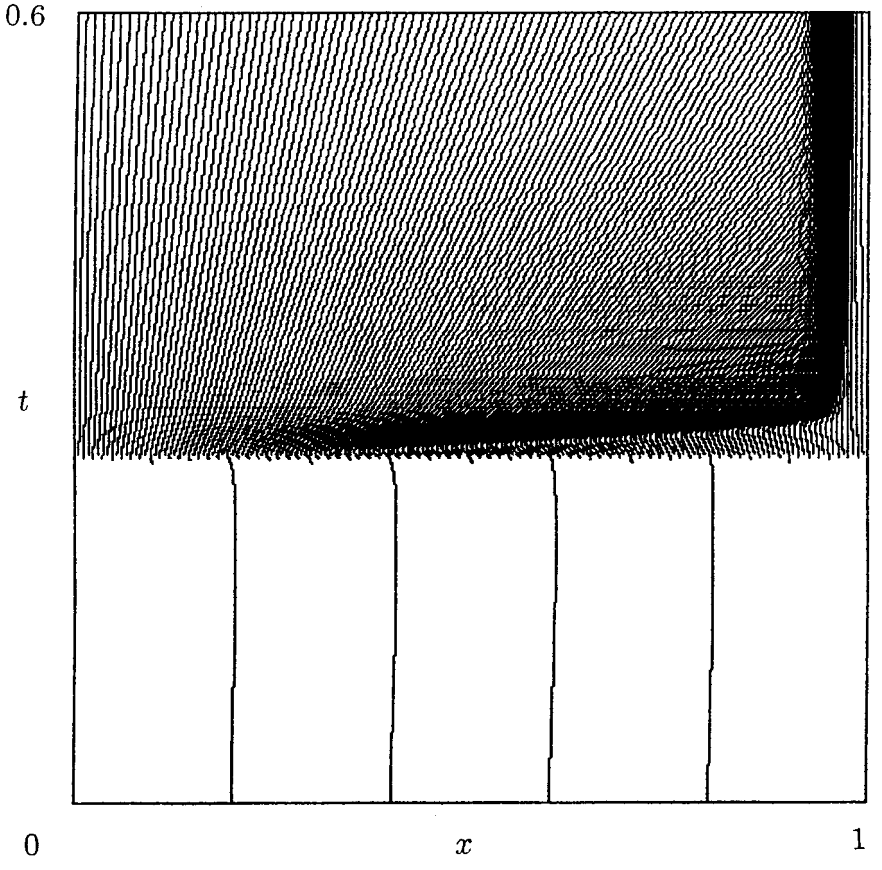

Fig. 1. Trajectories of nodes constructed by the procedure of [1]

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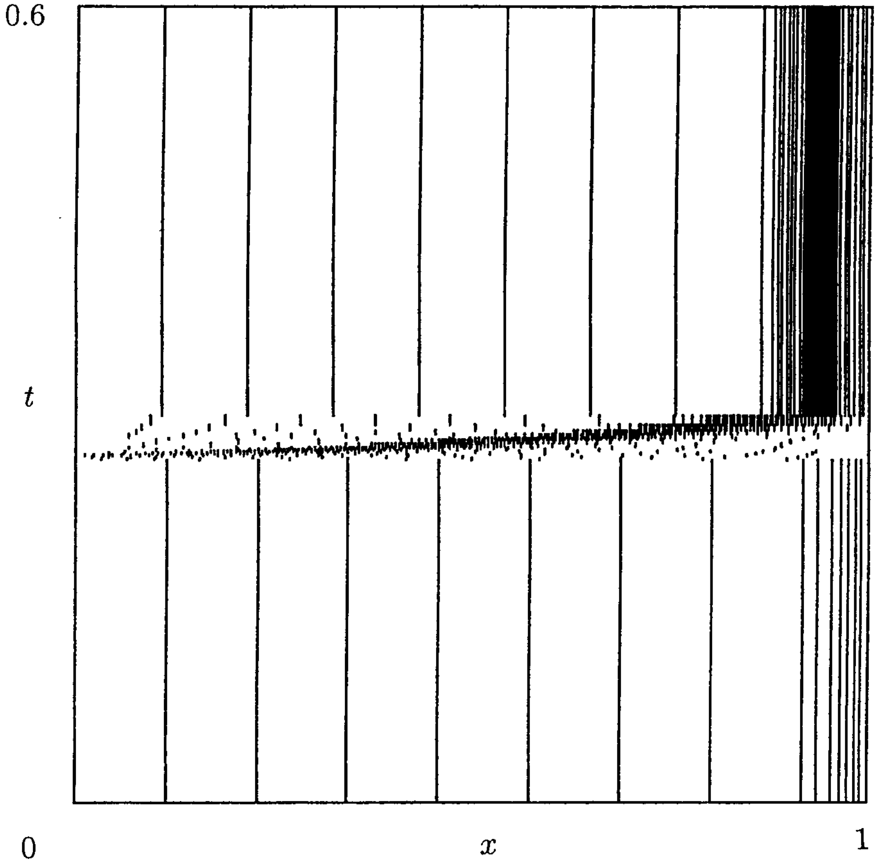

Fig. 2. Trajectories of nodes constructed by the procedure of [3]