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Wolfgang Hackbusch
Kristian Witsch (Eds.)

Numerical Techniques in Continuum Mechanics

Vieweg

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Notes on Numerical Fluid Mechanics
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Foreword

The GAMM Committee for Efficient Numerical Methods for Partial Differential Equations (GAMM-Fachausschuß "Effiziente numerische Verfahren für partielle Differenzialgleichungen") organizes conferences and seminars on subjects concerning the algorithmic treatment of partial differential equation problems.

The first seminar "Efficient Solution of Elliptic Systems" was followed by a second one held at the University of Kiel from January 17th to January 19th, 1986. The title was

"Efficient Numerical Methods in Continuum Mechanics".

The equations arising in continuum mechanics have many connections to those of fluid mechanics, but are usually more complex. Therefore, much attention has to be paid to the efficient discretization, postprocessing and extrapolation.

The seminar was attended by 66 scientists from 10 countries. Most of the 21 lectures presented at the seminar treated the discretization of equations in continuum mechanics by finite elements, methods for improving the accuracy of these approximations and the use of boundary elements. Other contributions presented efficient methods for investigating bifurcations which play an essential role in practical applications. These proceedings contain 11 contributions in alphabetical order.

The editors and organizers of the seminar would like to thank the land Schleswig-Holstein and the DFG (Deutsche Forschungsgemeinschaft) for their support.

Kiel, November 1986

W. Hackbusch
K. Witsch

Contents

OPTIMAL ERROR ESTIMATES AND ADAPTIVE TIME AND SPACE STEP CONTROL FOR LINEAR PARABOLIC PROBLEMS

by

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0. Introduction

In this note we present recent developments in the program for constructing adaptive algorithms for numerical methods for parabolic type problems or stiff initial value prolems that was initiated in Johnson [6] and was continued in Eriksson, Johnson [3] and Johnson, Nie, Thomée [7].

Solutions of parabolic problems typically are nonsmooth in initial transients but become smoother as time increases. To minimize the work required to compute an approximate solution of a parabolic problem to a certain accuracy one therefore would like to use a numerical method which automatically adapts the mesh size (in time and space) according to the smoothness of the exact solution and automatically chooses a fine mesh in a transient and increases the mesh size as the exact solution becomes smoother. Our objective is to construct such adaptive algorithms that in particular satisfy the following criteria:

The error in the approximate solution is controlled globally in time to a given tolerance. (0.1)
The algorithm is efficient in the sense that the mesh size is not chosen unnecessarily small. (0.2)
The extra work required for the mesh control is small. (0.3)
The algorithm can be theoretically justified. (0.4)
No, or only very rough, a priori information of the exact solution is required. (0.5)

To be able to satisfy (0.5), the necessary information concerning the smoothness of the exact solution (of course) must be obtained from the computed approximate solution as the computation proceeds.

In [7] this program was carried out in detail in the particular case of a backward Euler semi-discretization in time of a linear parabolic problem with error control in the L_2-norm in space. We shall in this paper present extensions of these results to a fully discrete linear parabolic problem with now discretization also in space and with a higher order (third order) accurate method for the time discretization. The presented algorithm is easy to implement, satisfies (0.1) - (0.5) and seems according to our numerical tests to perform very satisfactory in practice. We believe that this type of algorithm may be very useful in applications. Extensions to non-linear parabolic problems will be presented in subsequent work.

Our discretization method is obtained by using a standard finite element method in space and the discontinuous Galerkin method in time. We consider in this paper the case of a piecewise linear approximation in time resulting in a third order accurate implicit Runge-Kutta type time-stepping scheme. Note that the backward Euler method considered in [3] corresponds to the discontinuous Galerkin method with piecewise constants. Our adaptive method is based on an a posteriori error estimate involving only the computed approximate solution. This estimate is obtained through an optimal a priori error estimate involving the unknown exact solution together with a result showing that under reasonable assumptions the quantities depending on the exact solution may be estimated using the computed approximate solution. In this note the adaptivity in space is restricted so that we only allow space meshes that become coarser as time increases. As indicated this covers the standard situation where the exact solution becomes smoother with increasing time. However, with given heat production terms or boundary conditions varying rapidly in time, reverse situations may occur. Such cases may be handled by the present technique through restart but would otherwise require a (non-obvious) extension of the argument.

We assume in this paper that the space discretization is quasi-uniform on each time level and thus the local element size in space only depends on time. It is conceivable to allow also a dependence on the space variable and thus work with space meshes refined locally in space. The control of such local refinements will however require local error estimates the proof of which will involve additional technical complications. A first step towards adaptive local refinements for elliptic problems based on local error estimates was taken in [5]. We hope to be able to extend this type of results to parabolic problems in future work.

An outline of this note is as follows. In Section 1 we introduce the fully discrete numerical method and state the optimal a priori error estimate. In Section 2 we formulate the associated adaptive algorithm, and finally, in Section 3 we present the results of some numerical experiments. For a proof of the a priori error estimate, we refer to [4]. The proof of the a posteriori error estimate, which is analogous to a corresponding proof in [7], will be given in a future publication.

For a more detailed comparison (as concerns the time discretization) of adaptive methods of the type considered in this note with earlier methods presented in the literature for numerical methods for stiff systems of ordinary differential equations, we refer to the discussion in [6]. Let us here just remark that with the earlier approach to adaptivity for stiff problems it seems as if one faces serious difficulties with respect to all the conditions (0.1)-(0.4).

1. Discretization and a priori estimates

As a model problem we shall consider the following parabolic problem: Find $u:(0,\infty) \to H^2(\Omega) \cap H_0^1(\Omega)$ such that

$$\begin{aligned} u_t - \Delta u &= f \quad \text{in} \quad \Omega,\ t > 0, \\ u(0) &= u_0 \quad \text{in} \quad \Omega, \end{aligned} \tag{1.1}$$

where Ω is a bounded domain in R^d with smooth boundary Γ, u_0 and f are given data and $u_t = \frac{\partial u}{\partial t}$. Here and below

$H^s(\Omega)$ denotes for $s \geq 0$ the usual Sobolev space (of functions with derivatives of order s square integrable over Ω) with norm $\|\cdot\|_s$ and corresponding semi-norm $|\cdot|_s$ and $H_0^1(\Omega) = \{v \in H^1(\Omega): v = 0 \text{ on } \Gamma\}$. As is well-known, (1.1) may be given the following variational formulation: Find $u:(0,\infty) \to H_0^1(\Omega)$ such that

$$(u_t,v) + (\nabla u, \nabla v) = (f,v) \quad \forall\, v \in H_0^1(\Omega),\ t > 0 \qquad (1.2)$$

and $u(0) = u_0$, where $(.,.)$ denotes the $L_2(\Omega)$-inner product.

To discretize (1.2) let $0 = t_0 < t_1 < \ldots < t_n < \ldots$, be a subdivision of $(0,\infty)$ into time intervals $I_n = (t_{n-1}, t_n]$ of length $k_n = t_n - t_{n-1}$ and let $S_n \subset H_0^1(\Omega)$, $n = 1,2,\ldots,$ be finite dimensional spaces satisfying for some $r \geq 2$ and constant $\bar{C}$,

$$\inf_{\psi \in S_n} \|\varphi - \psi\|_j \leq \bar{C} h_n^{r-j} |\varphi|_r, \quad j = 0,1,\ \forall \varphi \in H^r(\Omega). \qquad (1.3)$$

Here the S_n are typically finite element spaces based on continous piecewise polynomial functions of degree at most $r - 1$ on quasi-uniform triangulations of Ω with mesh size h_n. For a given non-negative integer q we introduce for $n = 1,2,\ldots,$ the finite dimensional space V_n consisting of functions on I_n with values in S_n that vary as polynomials of degree at most q in time:

$$V_n = \{v: I_n \to S_n : v(t) = \sum_{j=0}^{q} t^j a_j,\ a_j \in S_n\}.$$

We shall seek an approximate solution U in the space V defined by

$$V = \{v:(0,\infty) \to H_0^1(\Omega): v|_{I_n} \in V_n,\ n = 1,2,\ldots,\}.$$

To account for the fact that the functions in V may be discontinuous in time at the discrete time levels t_n, we introduce the notation

$$v_n^{\pm} = \lim_{s \to 0^{\pm}} v(t_n + s).$$

We shall consider the following numerical method for (1.2): Find $U \in V$ such that for $n = 1,2,\ldots,$ $U \equiv U|_{I_n}$ satisfies

$$\int_{I_n} \{(U_t,v) + (\nabla U,\nabla v)\}dt + (U_{n-1}^+ - U_{n-1}^-, v_{n-1}^+) =$$
$$\int_{I_n} (f,v)dt \quad \forall\, v \in V_n, \tag{1.4}$$

where $U_0^- = u_0$. Note that with $q = 0$, (1.4) reduces to the following method: For $n = 1,2,\ldots,$ find $U_n \equiv U_n^- \quad S_n$ such that

$$(U_n - U_{n-1},v)+k_n(\nabla U_n,\nabla v) = (\int_{I_n} f(t)dt,v) \quad \forall v \in S_n, \tag{1.5}$$

which is a variant of the well-known backward Euler method where the average over I_n of the right hand side f is used instead of the usual value $f(t_n)$. Further, for $q = 1$ we get the following method

$$(\Psi_n,v) + k_n(\nabla\phi_n, v) + \frac{k_n}{2}(\nabla\Psi_n,\nabla v) + (\phi_n,v)$$
$$= (\phi_{n-1} + \Psi_{n-1},v) + (\int_{I_n} fdt,v) \tag{1.6}$$
$$\frac{1}{2}(\Psi_n,w) + \frac{k_n}{2}(\nabla\phi_n,\nabla w) + \frac{k_n}{3}(\nabla\Psi_n,\nabla w)$$
$$= (\frac{1}{k_n}\int_{I_n} (t-t_{n-1})fdt,w)$$
$$\forall v,w \in S_n$$

where

$$U|_{I_n} = \phi_n + \frac{t-t_{n-1}}{k_n}\Psi_n, \quad \phi_n,\ \Psi_n \in S_n.$$

If $f = 0$, then this method for the time discretization corresponds to the subdiagonal Padé method of order 3, see [2].

In this paper we shall consider (1.4) with $q = 1$, that is, the method (1.6). The a priori estimate on which the adaptive algorithm for (1.6) is based reads as follows. We use the notation

$$\|v\|_{s,I_n} = \max_{t\in I_n} \|v(t)\|_s, \quad \|v\|_{I_n} \equiv \|v\|_{0,I_n}, \quad \|v\| \equiv \|v\|_0,$$

and

$$L_N = (\log \frac{t_N}{k_N} + 1)^{1/2}.$$

By C and C_i, $i = 0,\dots,3$, we denote positive constants only depending on the parameter γ and the constant $\bar{C}$ in (1.3).

Theorem 1. Let u be the solution of (1.1) and U that of (1.4) with $q = 1$. Suppose that $S_n \subseteq S_{n-1}$ for $n = 2,3,\dots$, and that for some constant $\gamma > 1$ the time steps satisfy $\gamma k_n \le t_N - t_{n-1}$ for $1 \le n < N$, $N = 1,2,\dots$. Then we have for $N = 1,2,\dots$,

$$\|u-U\|_{I_N} \le L_N \max(C_0 h_n^r |u|_{r,I_n} + \min(C_1 k_n \|u_t\|_{I_n},$$
$$C_2 k_n^2 \|u_{tt}\|_{I_n})). \tag{1.7}$$

Theorem 2. Under the assumptions of Theorem 1 one has for $N = 1,2,\dots$,

$$\|u(t_N) - U_N^-\| \le L_N \max_{n\le N}(C_0 h_n^r \|u\|_{r,I_n} \tag{1.8}$$
$$+ \min(C_1 k_n \|\Delta u\|_{I_n},\ C_2 k_n^2 \|\Delta u_t\|_{I_n},\ C_3 k_n^3 \|\Delta u_{tt}\|_{I_n})).$$

It follows that the method (1.4) with $q = 1$ is second order accurate globally in time and third order accurate at the discrete time levels t_N. We also note that (1.7) is, disregarding the logarithmic factor, optimal in the sense that for some positive constant c

$$\inf_{v\in V} \|u-v\|_{(0,t_N)} \ge c \max_{n\le N} (h_n^r |u|_{r,I_n} + k_n^2 \|u_{tt}\|_{I_n}).$$

Clearly also (1.8) is optimal in the sense that we cannot increase the exponents of the factors h_n^r and k_n^3, neither can we use weaker norms on u while keeping the exponents of h_n and k_n. The adaptive algorithm to be introduced will be based on (1.8). The optimality of (1.8) will guarantee that condition (0.2) will be satisfied.

Remark 1.1. In general the minimum on the right hand side of (1.8) will be given by the third order tem $C_3 k_n^3 \|\Delta u_{tt}\|_{I_n}$. However, for the very few first steps instead the first order term $C_1 k_n \|\Delta u\|_{I_n}$ may give the minimum. Note that in the case $f \equiv 0$ this term may be replaced by

$$C_1 \int_{I_n} \|u_t(s)\| ds,$$

which is useful on the first interval where u_t may be unbounded. □

Remark 1.2. Note that the only constant in (1.7) and (1.8) depending on t_N is the logarithmic constant L_N. This means that it is possible to integrate over long time-intervals essentially without accumulation of errors. This reflects the parabolic nature of our problem. □

2. The adaptive algorithm

Suppose $\delta > 0$ is a given tolerance and that we want the error $e = u-U$ in the approximate solution given by (1.4) with $q = 1$ to satisfy

$$\|e_n\| \leq \delta, \; n = 1,2,\ldots \tag{2.1}$$

Relying on the a priori error estimate (1.8) we are then led to try to choose the time steps k_n and the space steps h_n so that for $n = 1,2,\ldots,$

$$L_n \max(C_0 h_n^r |u|_{r,I_n}, \min(C_1 k_n \|\Delta u\|_{I_n}, C_2 k_n^2 \|\Delta u_t\|_{I_n}, C_3 k_n^3 \|\Delta u_{tt}\|_{I_n})) \sim \frac{\delta}{2}. \tag{2.2}$$

Of course, here the quantities $|u|_{r,I_n}$, $\|\Delta u\|_{I_n}$, etc. are not known in advance. However, it is possible to estimate these quantities through the computed solution U and this leads to the adaptive algorithm which we shall now describe. Let us first introduce the discrete counterparts $\Delta_n: H_0^1(\Omega) \to S_n$ of the Laplace operator Δ defined as follows:

$$(-\Delta_n \varphi, \psi) = (\nabla\varphi, \nabla\psi), \quad \forall \psi \in S_n. \tag{2.3}$$

Let us now for simplicity assume that $r = 2$ and let us recall that by elliptic regularity

$$|\varphi|_2 \leq C\|\Delta\varphi\|$$

if $\varphi = 0$ on Γ. This means that in (2.2) the quantity $|u|_{2,I_n}$ may be replaced by $C\|\Delta u\|_{I_n}$. Replacing now in (2.2) Δ by Δ_n, u by U and time derivatives by simple difference quotients, we are led to the following criterion for choosing the local time and space steps:

$$L_n \max(C_0 h_n^2 d_{1n}, \min(C_1 k_n d_{1n}, C_2 k_n^2 d_{2n}, C_3 k_n^3 d_{3n})) \sim \frac{\delta}{2}, \quad (2.4)$$

where

$$d_{1n} = \| \Delta_n U_n^- \|, \quad (2.5a)$$

$$d_{2n} = \| \frac{\Delta_n U_n^- - \Delta_{n-1} U_{n-1}^-}{k_n} \|, \qquad n > 1, \quad (2.5b)$$

$$d_{3n} = \frac{1}{k_n} \| \frac{\Delta_n U_n^- - \Delta_{n-1} U_{n-1}^-}{k_n} - \frac{\Delta_{n-1} U_{n-1}^- - \Delta_{n-2} U_{n-2}^-}{k_{n-1}} \|, \quad n > 2, \quad (2.5c)$$

and where we set $d_{21} = d_{31} = d_{32} = \infty$. To determine h_n and k_n from (2.4) we would in principle have to (approximately) solve nonlinear equations since the d_{in} depend on h_n and k_n. In our implementation however we have simply used the predicted values of h_n and k_n resulting from replacing in (2.4) the d_{in} by the quantities $d_{i,n-1}$ available if U has been computed up to time t_{n-1}. We have also replaced the logarithmic factor L_n by 1. Thus our algorithm for automatic choice of space and time step in (1.4) with $q = 1$ is as follows: For $n = 1,2,\ldots,$ choose

$$h_n = \left(\frac{\delta}{2C_0 d_{1,n-1}}\right)^{1/2} \quad (2.6a)$$

$$k_n = \max\left(\frac{\delta}{2C_1 d_{1,n-1}}, \left(\frac{\delta}{2C_2 d_{2,n-1}}\right)^{1/2}, \left(\frac{\delta}{2C_3 d_{3,n-1}}\right)^{1/3}\right). \quad (2.6b)$$

If the predicted steps according to (2.6) and the corresponding solution U_n^- satisfy (2.4) the steps h_n and k_n are accepted and the computation proceeds, otherwise h_n and k_n are modified accordingly until (2.4) is met.

In our numerical tests with $f \equiv 0$ and $u|_\Gamma \equiv 0$ for $t > 0$, requiring (2.4) to be satisfied up to a factor two, the predictions (2.6) were always accepted.

The adaptive method for the backward Euler method (1.5) corresponding to (2.4) reads:

$$L_n \max(C_0 h_n^2 d_{1n},\ C_1 k_n d_{1n}) \sim \frac{\delta}{2} . \tag{2.7}$$

In [7] we proved under certain natural assumptions an a posteriori error estimate for the backward Euler method with discretization only in time of essentially the following form:

$$\|e_N^-\| \leq L_N \max_{n \leq N} C_1 k_n d_{1n} . \tag{2.8}$$

This estimate clearly justifies time step control for the backward Euler method according to (2.7) and we see that if the computational criterion (2.7) is satisfied, then by (2.8) the time discretization error is controlled globally in time to the given tolerance δ. Note that no previous result of this nature for stiff initial value problems seems to be available in the literature.

Now, it is possible to prove under similar assumptions an a posteriori error estimate for (1.4) with $q = 1$ corresponding to (2.7), that is an a posteriori estimate of essentially the form

$$\|e_N^-\| \leq L_N \max_{n \leq N} (C_0 h_n^2 d_{1n} + \min(C_1 k_n d_{1n}, C_2 k_n^2 d_{2n}, C_3 k_n^3 d_{3n})) . \tag{2.9}$$

By this estimate it follows that mesh control through (2.4) will guarantee that the error is controlled globally to the tolerance δ. The detailed proof of (2.9), which is analogous to the proof of (2.8) given in [7], will appear in a subsequent note.

Remark. Let $\{\chi_1, \dots, \chi_M\}$ be a finite element basis for S_n and let $A_n = (a_{ij}^n)$ and $B_n = (B_{ij}^n)$ be the corresponding stiffness and mass matrices with elements

$$a_{ij}^n = (\nabla\chi_i, \nabla\chi_j),$$

$$b_{ij}^n = (\chi_i, \chi_j).$$

For $\varphi \in S_n$ with

$$\varphi = \sum_{i=1}^{M} \xi_i \chi_i, \qquad \xi_i \in \mathbb{R},$$

we then have

$$\Delta_n \varphi = \sum_{i=1}^{M} \eta_i \chi_i, \quad \eta_i \in \mathbb{R},$$

where

$$\eta = M^{-1} A \xi, \qquad \eta = (\eta_i), \quad \xi = (\xi_i).$$ □

3. Numerical results

In this section we present the results of some numerical experiments using the method (1.6) with mesh control according to (2.6) in the case of the one-dimensional problem

$$\begin{aligned} u_t - u_{xx} &= 0, & 0 < x < 1, \quad t > 0, \\ u(0,t) = u(1,t) &= 0, & t > 0, \\ u(x,0) &= u_0(x), & 0 < x < 1, \end{aligned} \qquad (3.1)$$

with initial functions u_0 of varying degree of smoothness. The space meshes were restricted to be uniform subdivisions $\Omega_n = \{J\}$ of $\Omega = (0,1)$ into intervals J of length $h_n = 2^{-m}$, $m \in \mathbb{Z}^+$ with

$$S_n = \{v \in H_0^1(\Omega) : v|_J \text{ is linear } \forall J \in \Omega_n\}.$$