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GENERALIZED PREDICTOR-CORRECTOR METHODS OF HIGH ORDER FOR THE TIME INTEGRATION OF PARABOLIC DIFFERENTIAL EQUATIONS

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A general class of predictor-corrector methods is presented and explicit expressions for the local truncation error and the stability polynomial are derived. Examples of methods of orders up to 6 are given which are suitable for the integration of semi-discrete parabolic differential equations. By a large numbers of numerical experiments we show that the higher order methods are generally more efficient than the lower order methods. As a further illustration we compare the generalized predictor-corrector methods with the familiar ADI method confirming our general believe that for smooth parabolic problems high order time integrators are superiour to lower order integrators.

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1. INTRODUCTION

In the "Zweiten Seminar über Nümerische Behandlung von Differentialgleichungen" at Halle an outline of the so-called generalized predictor-corrector methods has been presented. In this paper we present the underlying theory for this class of methods. In particular, we will study the maximization of the real interval of stability and the construction of high order methods. The theory will be illustrated by applications to parabolic equations in several spatial dimensions. Special families of stabilized parabolic time integrators proposed in a few earlier papers [1,2,3,4] will be surveyed and are recognized as special cases of generalized predictor-corrector methods.

Starting with a semi-discrete form of the initial-boundary value problem, that is a system of ordinary differential equations (ODEs)

$$(1.1) \qquad \frac{dy(t)}{dt} = f(t,y), \quad y(t_0) = y_0,$$

with $f(t,y)$ and y_0 given, we will develop methods which can be regarded as an iteration process with a fixed number of iterations for solving the implicit linear multistep method

$$(1.2) \qquad \sum_{\ell=0}^{k} a_\ell y_{n+1-\ell} = \Delta t \sum_{\ell=0}^{k} b_\ell f(t_{n+1-\ell}, y_{n+1-\ell}), \quad a_0 = 1.$$

It will be convenient to write (1.2) in the more compact form

$$(1.3) \qquad Ly_{n+1} = \Sigma_n,$$

where L is the operator $y \to y - b_0 \Delta t f(t_{n+1}, y)$ and Σ_n is a sum of backvalues. Let $y^{(j)}$ denote the successive iteration results in the iterative solution process of (1.3). Then the iteration process discussed in this paper will be of the form

$$(1.4) \qquad \hat{L}\left(\sum_{\ell=0}^{j} \lambda_{j\ell} y^{(\ell)}, y^{(j-1)}\right) = \Sigma_n, \quad \sum_{\ell=0}^{j} \lambda_{j\ell} = 1, \quad j = 1,2,\ldots,m,$$

where $\hat{L}$ is an operator $(u,v) \to w$ satisfying the condition that if the $y^{(j)}$ converge to a vector y_{n+1} then y_{n+1} is the solution of (1.3), i.e.

$$(1.5) \qquad \hat{L}(y,y) = Ly.$$

The iterates $y^{(i)}$ can be computed by solving the successive relations (1.4) with respect to their first argument. Thus, we should look for operators $\hat{L}$ such that these relations can be solved without too much computational effort. The choice of $\hat{L}$ depends largely on the number of spatial dimensions of the original parabolic problem. In *three* space-dimensional problems it seems recommendable to choos $\hat{L}$ such that the solution of (1.4) only requires evaluations of the right-hand side function f: the operator $\hat{L}$ will be called *explicit* in its first argument. In *one* space-dimension *fully implicit* operators usually offer no problems. In *two* space dimensions, both *explicit* and *partially implicit* operators may be considered. Examples of these various types of operators will be discussed in the subsequent sections.

The proposed integration methods take into account that the spectral radius S of the Jacobian matrix of f(t,y), i.e.

$$(1.6) \qquad S := S(\frac{\partial f}{\partial y}),$$

is usually very large. Furthermore, they use only a limited number of arrays for storing y_n-vectors which enables us to integrate very large systems even on a small scale computer. Furthermore, the number of iterations m is automatically tuned to the integration step Δt desired or the step dictated by an error estimator. Thus, the integration method is in fact, a *family of methods* and the integration step prescribed picks out a suitable member of this family. The family may be considered as a generalization of the familiar predictor-corrector method and will be called a *generalized predictor-corrector method* (GPC method).

In a large number of experiments, both with explicit and partially implicit operators, using several linear and nonlinear parabolic equations in two dimensions as test problems, we will show that generally the higher order methods are the more efficient ones. The theory presented in the following sections also applies to higher order differential equations of the special form

$$(1.1') \qquad \frac{d^{\nu}y(t)}{dt^{\nu}} = f(t,y), \quad \frac{d^{i}y}{dt^{i}}(t_0) = y_0^{(i)}, \quad i = 0,1,\ldots,\nu-1,$$

where ν is a positive integer. Therefore, in all formulas we give the expressions for general ν.

2. FAMILIES OF INTEGRATION METHODS

In general, *explicit* methods have the disadvantage that a stability condition of the form

$$(2.1) \qquad (\Delta t)^{\nu} \leq \frac{\beta}{S},$$

has to be satisfied. Here, β is the *stability boundary* of the method. Since S is often extremely large, this condition may prescribe a considerably smaller integration step than accuracy would prescribe.

In the case of *partially implicit* methods, the lower order methods are usually not required to satisfy a stability condition. However, if one tries to increase the order of accuracy one is often again faced with a condition for the integration step Δt.

In order to avoid the undesirable situation that Δt is prescribed by stability instead of by accuracy, *families of methods* (of fixed order p) with stability boundaries varying from small until arbitrarily large have been proposed [2,3,4]. Let us denote such a family by $\{METH(m)\}_{m=1}^{\infty}$ and the corresponding stability boundaries by $\beta = \beta(m)$. The function $\beta(m)$ increases monotonically as m increases, hence for given values of Δt and S, the method METH(m) is stable if we choose m such that

$$(2.1') \qquad m \geq \gamma((\Delta t)^{\nu} S),$$

where $\gamma = \gamma(x)$ denotes the inverse function of $\beta = \beta(m)$. As might be expected, the larger m the larger the computational effort per step. In the references quoted above, m is sort of "stage-parameter" counting the right-hand side evaluations or the number of iterations per step.
In this paper, we will try to construct families of methods of the form (1.4) for which $\gamma(x)$ assumes values as small as possible. Since m is proportional to the computational effort per step the amount of work is bounded below by

$$C(\Delta t) := c\frac{m}{\Delta t} \approx c\,\frac{\gamma((\Delta t)^{\nu}S)}{\Delta t}, \quad c = \text{constant}.$$

Evidently, a suitable family of methods should at least satisfy the condition $C'(\Delta t) < 0$, i.e.

$$(2.2) \qquad \nu \times \gamma'(x) < \gamma(x).$$

3. GENERALIZED PREDICTOR-CORRECTOR METHODS

The framework of generalized predictor-corrector methods we want to propose in this paper, consists of four components: a *predictor equation*, a *corrector equation*, an *iteration operator* and an *iteration scheme*.

The predictor equation is defined by an explicit, linear $\tilde{k}$-step method $\{\tilde{\rho},\tilde{\sigma}\}$ providing an initial approximation $y^{(0)}$ to the numerical solution y_{n+1} at t_{n+1}.

The corrector equation is defined by an implicit, linear k-step method $\{\rho,\sigma\}$.

Let the corrector equation be written in the form (cf. (1.3))

$$(3.1) \qquad Ly := y - b_0(\Delta t)^{\nu} f(t_{n+1},y) = \Sigma_n.$$

We start with the classical predictor-corrector scheme in $P(EC)^mE$ mode. This scheme can be presented in the form

$$(3.2) \qquad y^{(j)} - b_0(\Delta t)^{\nu} f(t_{n+1},y^{(j-1)}) = \Sigma_n, \quad j = 1,2,\ldots,m,$$

where $y^{(m)}$ is adopted as the numerical solution y_{n+1}. More compactly we write

$$(3.3) \qquad \hat{L}(y^{(j)},y^{(j-1)}) = \Sigma_n, \quad j = 1,2,\ldots,m,$$

where $\hat{L}$ is the *iteration* operator

$$(3.4) \qquad \hat{L}\colon (u,v) \to u - b_0(\Delta t)^{\nu} f(t_{n+1},v).$$

Notice that $\hat{L}$ satisfies the consistency condition (1.5). Instead of the completely explicit operator (3.4) one may define the partially implicit iteration operator

$$(3.5) \qquad \hat{L}\colon (u,v) \to u - b_0(\Delta t)^{\nu} F(t_{n+1},u,v),$$

where $F(t,u,v)$ is a so-called *splitting function* satisfying the condition $F(t,y,y) \equiv f(t,y)$. This function should be chosen such that the relation (3.3) can "conveniently" be solved for $y^{(j)}$. Again, this iteration operator satisfies the condition (1.5).

A still more complicated iteration operator $\hat{L}\colon (u,v) \to w$ is defined by the implicit relations

$$(3.6) \qquad \begin{cases} \omega y^* + (1-\omega)v - b_0(\Delta t)^{\nu} F(t_{n+1},v,y^*) = w, \\ \omega u + (1-\omega)y^* - b_0(\Delta t)^{\nu} F(t_{n+1},u,y^*) = w, \end{cases}$$

where ω is a relaxation parameter and F is a splitting function such that the realtions in (3.6) can "conveniently" be solved for y^* and u. The multistep splitting methods analysed in [1] can be interpreted as the iteration scheme (3.3) employing the operator $\hat{L}$ defined by (3.6) with $\omega = 1$.

In principle, any iteration operator $\hat{L}\colon (u,v) \to w$ satisfying (1.5) together with the iteration scheme (3.3) can be used by solving the corrector equation (3.1). However, as we will show in the following sections, the performance of the iteration scheme can be greatly improved by replacing (3.3) by the scheme (1.4), where the iteration parameters $\lambda_{j\ell}$ serve to accelerate the convergence. The predictor-corrector method employing this iteration scheme will be called a *generalized predictor-corrector method*, briefly GPC method.

The special GPC methods generated by the explicit iteration operator (3.4) has been studied in [4]. The partially implicit GPC methods based on (3.6) were investigated in [2,3]. In this paper we present a general analysis of the iteration scheme (1.4).

4. THE LOCAL ERROR

In the analysis of the GPC method it is convenient to introduce the iteration polynomials

$$
\begin{aligned}
&R_0(x) = 1 \\
&R_j(x) = -\frac{1}{\lambda_{jj}}\{(\lambda_{jj-1}-1+x)R_{j-1}(x) + \sum_{\ell=0}^{j-2} \lambda_{j\ell}R_\ell(x)\}, \quad j = 1,2,\ldots,m.
\end{aligned} \tag{4.1}
$$

These polynomials characterize the iteration scheme (1.4). We observe that the coefficients $\lambda_{j\ell}$ are uniquely defined if we prescribe a sequence of polynomials $\{R_j(x)\}_{j=0}^{m}$ satisfying $R_j(0) = 1$.

The following theorem governs the accuracy of the GPC method. The proof of this result follows the proof of a similar theorem given in [4] and can be found in Appendix A to this paper.

THEOREM 4.1. *Let the GPC method converge to the solution of the corrector equation (3.1) as* $\Delta t \to 0$, *let* p *and* $\tilde{p}$ *be the respective orders of the corrector* $\{\rho,\sigma\}$ *and the predictor* $\{\tilde{\rho},\tilde{\sigma}\}$ *and let* $\hat{L}$ *satisfy the condition*

$$
\hat{L}(\eta+\varepsilon_1,\eta+\varepsilon_2) - \hat{L}(\eta,\eta) = J_1\varepsilon_1 + J_2\varepsilon_2 + (\Delta t)^\nu O(\|\varepsilon_1\|^2 + \|\varepsilon_1\|.\|\varepsilon_2\| + \|\varepsilon_2\|^2), \tag{4.2}
$$

where J_1 *and* J_2 *are non-singular matrices only depending on* η, Δt *and* ν. *Then*

$$
\begin{aligned}
y_{n+1} - y(t_{n+1}) &= R_m(A)[y^{(0)} - y(t_{n+1})] + [I-R_m(A)][\eta - y(t_{n+1})] \\
&\quad + O((\Delta t)^s), \quad s \geq 3\nu + 2\min\{p,\tilde{p}\},
\end{aligned} \tag{4.3}
$$

where the iteration matrix $A := J_1^{-1}J_2 + I$. □

EXAMPLE 4.1. In the case of the operator $\hat{L}(u,v) = u - b_0(\Delta t)^\nu f(t_{n+1},v)$ we have

$$
\hat{L}(\eta+\varepsilon_1,\eta+\varepsilon_2) - \hat{L}(\eta,\eta) = \varepsilon_1 - b_0(\Delta t)^\nu(\frac{\partial f}{\partial y}\varepsilon_2 + O(\|\varepsilon_2\|^2)).
$$

Hence, $J_1 = I$ and $J_2 = -b_0(\Delta t)^\nu \frac{\partial f}{\partial y}(t_{n+1},\eta)$.

EXAMPLE 4.2. For the iteration operator defined in (3.6) we derived

$$\hat{L}(\eta+\varepsilon_1,\eta+\varepsilon_2) - \hat{L}(\eta,\eta) = J_1\varepsilon_1 + J_2\varepsilon_2 + (\Delta t)^{\nu} O(\|\varepsilon_1\|^2 + \|\varepsilon_2\|^2 + \|\varepsilon_1\|\|\varepsilon_2\|),$$

with

$$J_1 = \frac{1}{2\omega-1}(\omega I - b_0 Z_2)(\omega I - b_0 Z_1),$$

(4.4)

$$J_2 = -\frac{1}{2\omega-1}[(1-\omega)I - b_0 Z_2][(1-\omega)I - b_0 Z_1],$$

where

$$Z_1 := (\Delta t)^{\nu}\frac{\partial F}{\partial u}(t_{n+1},\eta,\eta), \quad Z_2 := (\Delta t)^{\nu}\frac{\partial F}{\partial v}(t_{n+1},\eta,\eta).$$

Hence, the iteration matrix $A = J_1^{-1}J_2 + I$ assumes the form

$$A = (2\omega-1)(\omega I - b_0 Z_1)^{-1}(\omega I - b_0 Z_2)^{-1}(I - b_0 Z_1 - b_0 Z_2). \tag{4.5}$$

5. LINEAR STABILITY ANALYSIS

Suppose that the initial approximation $y^{(0)}$ is perturbed by an amount $\Delta y^{(0)}$ and the back-values $y_{n+1-\ell}$ are perturbed by $\Delta y_{n+1-\ell}$. Then, after m applications of (1.4), the resulting perturbation $\Delta y_{n+1} = \Delta y_{n+1}^{(m)}$ satisfies, in first approximation, the linear recurrence relation [4,5]

$$\pi(E;Z,R_m(A))\Delta y_{n+1-k} = 0, \quad n+1 \geq k, \tag{5.1}$$

where the characteristic polynomial $\pi(\zeta;Z,R)$ is defined by

$$\pi(\zeta;Z,R) := [I-R][I-b_0 Z]^{-1}[\rho(\zeta)-Z\sigma(\zeta)] + R[\tilde{\rho}(\zeta)-Z\tilde{\sigma}(\zeta)]\zeta^{k-\tilde{k}}. \tag{5.2}$$

Here, the matrices A and Z are defined by

$$Z := (\Delta t)^{\nu}\frac{\partial f}{\partial y}(t_{n+1},\eta), \quad A = J_1^{-1}J_2 + I, \tag{5.3}$$

$R_m(A)$ denotes the iteration polynomial defined in (4.1), and $\{\tilde{\rho},\tilde{\sigma}\}$ and $\{\rho,\sigma\}$ are the $\tilde{k}$-step predictor and k-step corrector, respectively.

Adopting the usual definition of stability we shall call the GPC method *stable* if the solution of (5.1) tends to zero as $n \to \infty$. If the matrices A and Z do not depend on n and if the matrix $\pi(\zeta;Z,R_m(A))$ can be reduced to diagonal form, then the necessary and sufficient condition for stability requires that $\det[\pi(\zeta;Z,R_m(A))]$ has its zeros inside the unit circle (cf. [7]). Thus we have proved

THEOREM 5.1. *Let the condition (4.2) be satisfied and let the matrices* A *and* Z *(defined in (5.3)) be independent of* t_{n+1}. *Then the* GPC *method is stable if the characteristic equation* $\det[\pi(\zeta;Z,R_m(A))] = 0$ *has its roots inside the unit circle.* □

In practice, the following corollary of this theorem is important.

COROLLARY 5.1. *Let the condition of Theorem 5.1 be satisfied. In addition, let* A *and* Z *have a common eigensystem* $\{e^{(i)}\}$ *with eigenvalues* $\alpha^{(i)}$ *and* $z^{(i)}$, *respectively. Then the* GPC *method is stable if the polynomials* $\{\pi(\zeta;z^{(i)},R_m(\alpha^{(i)}))\}$ *have their zeros within the unit circle for all* i. □

In the following, it will be assumed that the conditions of Corollary 5.1 are satisfied. It is convenient in our further analysis to define the *stability domain* $\mathcal{D}$ by the set of points in the (z,r)-plane where the polynomial $\pi(\zeta;z,r)$ has its roots on the unit disk. Suppose that we can prove that the region determined by

$$(5.4) \qquad -D_1 \le r \le D_2, \quad -D_3 \le z \le 0,$$

is contained in $\mathcal{D}$. Furthermore, Let Z have eigenvalues in the negative interval $[-(\Delta t)^{\nu}S,0]$ and let A have its eigenvalues in $[a,b]$. Then it follows from Corollary 5.1 that the GPC scheme is stable if

$$(5.5) \qquad -D_1 \le R_m(x) \le D_2 \quad \text{for} \quad a \le x \le b$$

$$(5.6) \qquad (\Delta t)^{\nu} \le \frac{D_3}{S}.$$

The condition (5.6) is a direct condition on the integration step. However, by choosing a suitable predictor-corrector pair $\{\tilde{\rho},\tilde{\sigma}\}$-$\{\rho,\sigma\}$ we can obtain stability domains $\mathcal{D}$ for which D_3 is sufficiently large so that in practice no restriction on the integration step holds. Condition (5.5) can be satisfied by choosing an appropriate iteration polynomial $R_m(x)$. We recall that the iteration polynomials $R_j(x)$ are more or less free except for the condition $R_j(0) = 1$ and the requirement that they should satisfy a two-step, inhomogeneous recurrence relation. In practice, (5.5) means that m should be sufficiently large and will lead to a condition of the form (2.1'). In the following section, the function $\gamma(x)$ in (2.1') will be derived in terms of the stability domain parameters D_1 and D_2. First, however, we give an example illustrating the magnitude of these parameters.

EXAMPLE 5.1. Consider the predictor-corrector pair defined by extrapolation of preceding y_n-values and by backward differentiation formulas (*EP-BD methods*). For ODEs of first order, such methods were considered in [3,4] where (D_1,D_2,D_3)-values has been computed. For future reference these values are listed below. In all cases $D_3 = \infty$. Larger D_1 and D_2 values can be obtained for finite values of D_3 (see the discussion in [4]). □

Table 5.1. (D_1,D_2)-values applying to EP-BD methods

p	$\tilde{p}$=0	$\tilde{p}$=1	$\tilde{p}$=2	$\tilde{p}$=3	$\tilde{p}$=4	$\tilde{p}$=5	$\tilde{p}$=6
2	(1,1)	(1/3,1)	(1/7,1/2)				
3	(1,1)	(1/3,1)	(1/7,1/2)	(1/15,1/5)			
4	(.75,1)	(1/3,1)	(1/7,.495)	(1/15,.1999)	(1/31,.0827)		
5	(.44,1)	(.33,1)	(1/7,.47)	(1/15,.1704)	(1/31,.0751)	(1/63,1/28)	
6	(.13,1)	(.07,1)			(1/31,.0289)	(1/63,.0147)	(1/127,.01128)

6. COMPUTATION OF THE MINIMAL NUMBER OF ITERATIONS IN GPC METHODS

We consider the family of GPC methods defined in Section 3 for $m = 1,2,3,\ldots$ and we assume that the stability domain $\mathcal{D}$ has a sufficiently large D_3-value and non-zero D_1 and D_2 values ≤ 1. Furthermore, we assume that $A = \alpha_0 I + O((\Delta t)^\nu)$ as $\Delta t \to 0$ where α_0 is a constant lying in the positive eigenvalue interval $[a,b]$. The general theorems will be illustrated by applying them to the explicit operator (3.4) and the partially implicit operator (3.6), and by deriving the function $\gamma(x)$ occurring in (2.1'). First, we will consider the convential iteration scheme (3.3).

6.1. The conventional iteration scheme

The conventional iteration scheme (3.3) gives rise to iteration polynomials of the form

$$(6.1) \qquad R_j(x) = (1 - \frac{x}{\alpha_0})^j, \quad j = 0,1,\ldots,m.$$

The following theorem is immediate from condition (5.5):

THEOREM 6.1. *The iteration polynomials (6.1) generate a stable method of order* $p^* = \min\{p, \tilde{p}+\nu m\}$ *if*

$$m \geq \max\left\{\frac{\ell n D_2}{\ell n(1 - \frac{a}{\alpha_0})}, \frac{\ell n D_i}{\ell n(\frac{b}{\alpha_0} - 1)}\right\}; \quad b \leq 2\alpha_0,$$

where $i = 1$ *for* m *odd and* $i = 2$ *for* m *even.* □

EXAMPLE 6.1. In the explicit case (3.4) we have $a = \alpha_0 = 1$ and $b = 1 + b_0(\Delta t)^\nu S$. Theorem 6.1 yields

$$m \geq \frac{\ell n D_i}{\ell n[b_0(\Delta t)^\nu S]}, \quad i = 1,2; \quad b_0(\Delta t)^\nu S \leq 1,$$

from which we derive

$$\gamma(x) = \begin{cases} \dfrac{\text{const}}{\ell n(b_0 x)} & \text{for} \quad x \leq 1/b_0 \\ \infty & \text{for} \quad x > 1/b_0. \end{cases}$$

Evidently, this function indicates that the iteration polynomials (6.1) combined with the explicit operators (3.4) are not suitable for the integration of equations with large values of $(\Delta t)^\nu S$. □

EXAMPLE 6.2. Next consider the partially implicit operators (3.6). From (4.5) we find

$$(6.2)\qquad a = (2\omega-1)\frac{1+b_0(\Delta t)^\nu S}{(\omega+\frac{1}{2}b_0(\Delta t)^\nu S)^2},\quad b = \frac{2\omega-1}{\omega}\,\frac{1+b_0(\Delta t)^\nu S}{\omega+b_0(\Delta t)^\nu S},\quad \alpha_0 = \frac{2\omega-1}{\omega^2}.$$

Theorem 6.1 leads to the stability conditions

$$m \geq \gamma((\Delta t)^\nu S),\quad (\omega-2)b_0(\Delta t)^\nu S \leq \omega,$$

where

$$\gamma(x) = \max\left\{\frac{\ell nD_2}{\ell n\left(1-\frac{1+b_0x}{(1+b_0x/2\omega)^2}\right)},\ \frac{\ell nD_i}{\ell n\left(\frac{(\omega-1)b_0x}{\omega+b_0x}\right)}\right\},$$

with $i = 1$ for m odd and $i = 2$ for m even. Assuming $\omega < 2$ and $(\Delta t)^\nu S$ large these conditions reduce to

$$(6.3)\qquad m \geq \gamma((\Delta t)^\nu S),\quad \gamma(x) \approx \max\left\{-\frac{\ell nD_2}{4\omega^2}\,b_0x,\ \frac{\ell nD_i}{\ell n(\omega-1)}\right\}.$$

This family of methods is only of practical interest if either $D_2 = 1$ *and* m *even* or $D_2 = 1$, m *odd and* $1 + D_1^{1/m} < \omega < 2$.

The methods investigated in [1] are of the type indicated in this example. Choosing the EP-BD predictor-corrector pair mentioned in Example 5.1, we conclude from Table 5.1 that for first order ODEs the stability conditions can be satisfied by using a predictor of order $\tilde{p} = 0$ or $\tilde{p} = 1$ and a corrector of order $p = 2(1)6$. Using even values of m, *unconditionally stable time integrators of order* $p^* = \min\{p, \tilde{p}+m\}$ *are obtained.* □

6.2. Optimal predictor-corrector methods

Let us have a closer look at the local error of GPC methods as given in Theorem 4.1. Choosing a corrector equation of sufficiently high order, the local error (4.3) is mainly determined by the term

$$R_m(A)[y^{(0)} - y(t_{n+1})].$$

This suggests choosing either a *high order predictor* or iteration polynomials such that $R_m(A)$ *damps the dominant components* in the predictor error sufficiently strongly. If neither of these conditions is satisfied an inaccurate method is obtained. For instance, in view of this observation we should not expect that the methods discussed in Example 6.2 are very accurate because the stability conditions require a low order predictor while the matrix

$$R_m(A) = (1 - \frac{\omega^2}{2\omega-1}A)^m,$$

only damps eigenvectors with eigenvalues close to $(2\omega-1)/\omega^2$ (unless m is rather large). Assuming that the eigenvectors of low frequency are the dominant ones and that in an actual computation $(\Delta t)^\nu S$ is large, it can be shown [2] that the eigenvalues corresponding to high frequencies are concentrated in the neighbourhood of the origin and the lower frequencies are located in the interval, say, $[(2\omega-1)/2\omega, (2\omega-1)/\omega]$. Thus, the methods of Example 6.2, although being unconditionally stable if $D_2 = 1$ and m even, have the disadvantage of a rather large local error.

We will first discuss the case of *high order predictors*.

6.2.1. Higher order predictors

In view of the stability condition (5.5) we are led to iteration polynomials of the form (cf. [4])

$$(6.4a) \qquad R_m(x) = \tfrac{1}{2}[D_2 - D_1 + (D_2+D_1)T_m(w_0 - w_1 x)].$$

Here, T_m denotes the Chebyshev polynomial of degree m and w_0, w_1 are free parameters which are used to satisfy the conditions $R_m(0) = 1$ and $R_m(b) = D_2$ for m even and $R_m(b) = -D_1$ for m odd (see Figure 6.1). By a standard argument from minimax theory it can be shown that these iteration polynomials are optimal with regard to maximizing the stability boundary.

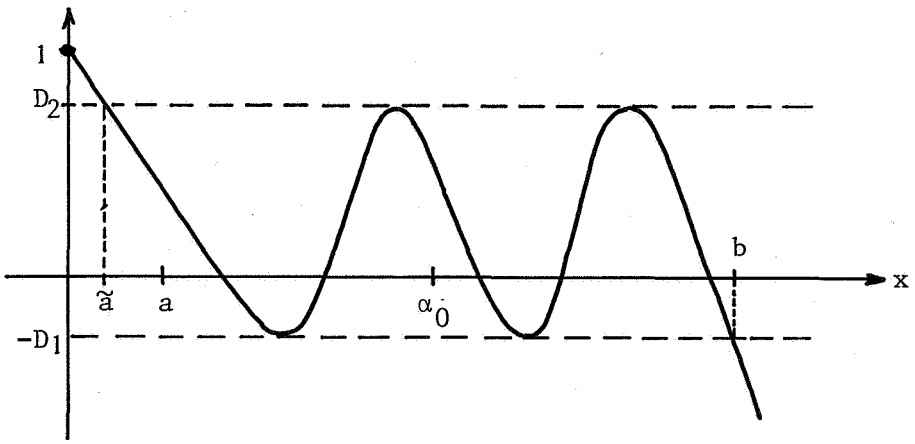

Figure 6.1. The polynomial $R_m(x)$

A straightforward calculation reveals that the parameters w_0 and w_1 are given by

$$(6.4b) \qquad w_0 = \cosh\frac{d_0}{m}, \quad d_0 := \operatorname{arccosh}\left(\frac{2+D_1-D_2}{D_1+D_2}\right),$$

$$(6.4c) \qquad w_1 = \frac{w_0+1}{b}.$$

Let $\tilde{a}$ be the point where $R_m(x)$ equals D_2 "for the first time" (see Figure 6.1). Then the stability condition (5.5) is satisfied if $a \geq \tilde{a}$. This leads us to the following theorem.

THEOREM 6.2. *Let the iteration polynomials be choosen such that* $R_m(x)$ *is of the form (6.4). Then the method is stable if*

$$(6.5) \qquad m \geq \frac{d_0}{\operatorname{arccosh}\left(\frac{b+a}{b-a}\right)}. \qquad \square$$

We observe that no condition on m is obtained if $D_2 = 1$. Unfortunately, only the lower order predictors give rise to $D_2 = 1$ (see e.g. Table 5.1). This case will be considered in more detail in Section 6.2.2.

Furthermore, it follows from (6.2) that for $\Delta t \to 0$ the lower bound on

m tends to zero (because $b-a \to 0$). Thus, for Δt sufficiently small we obtain a one-stage method (m=1) with the iteration polynomial

$$(6.6) \qquad R_1(x) = \tfrac{1}{2}[D_2-D_1+(D_2+D_1)(w_0-w_1x)] = 1 - \frac{1+D_1}{b}x.$$

When Δt decreases further it is allowed to decrease D_1 too (provided that $R_1(a) \le D_2$) which will improve the accuracy of the method. Let us choose

$$(6.7) \qquad D_1 = O(\Delta t) \quad \text{as} \quad \Delta t \to 0,$$

then the following theorem holds:

THEOREM 6.3. *Let* $R_m(x)$ *be defined by (6.4) and (6.7), and let* m *be the smallest integer satisfying (6.5). Then the family of resulting methods is of order* $p^* = \min\{\tilde{p}+\nu, p\}$. □

In actual computation where relatively large integration steps are used, one should not expect that the asymptotic order p^* given by this theorem is actually obtained. Therefore, although the theorem suggests choosing $\tilde{p} + \nu = p$, it is often recommendable to choose $\tilde{p} + \nu > p$ because the predictor error generally dominates the truncation error.

EXAMPLE 6.3. Let us again consider the explicit case (3.4) considered in Example 6.1. Substitution of $a = 1$ and $b = 1 + b_0(\Delta t)^\nu S$ in (6.5) leads to the stability condition

$$(6.8) \qquad m \ge \gamma((\Delta t)^\nu S), \quad \gamma(x) := \frac{d_0}{\operatorname{arccosh}(1+\frac{2}{b_0 x})}.$$

It is of interest to see how $\gamma(x)$ behaves for large values of x. In first approximation we have

$$\gamma(x) \approx \tfrac{1}{2}d_0\sqrt{b_0 x},$$

which satisfies condition (2.2) for $\nu = 1$. In Table 6.1 the function $\gamma(x >> 1)$ is given for the EP-BD methods specified in Example 5.1. The EP-BD methods using a zero- or first-order predictor are unconditionally

stable (i.e. $\gamma(x) \equiv 0$) and are omitted.

Table 6.1. Constant c in $\gamma(x) \approx c\sqrt{x}$ for $\nu = 1$

p	$\tilde{p}=2$	$\tilde{p}=3$	$\tilde{p}=4$	$\tilde{p}=5$	$\tilde{p}=6$
2	.65				
3	.59	.97			
4	.56	.91	1.22		
5	.55	.92	1.19	1.44	
6			1.34	1.56	1.71

REMARK. In this example, the value of a is set to 1. However, if one has available an estimate of the (in modulus) smallest eigenvalue δ of the Jacobian matrix $\partial f/\partial y$, it may be advantageous to use the explicit operator with $a = 1 + b_0(\Delta t)^\nu \delta$. From (6.5) we find

$$m \geq \frac{d_0}{\operatorname{arccosh}(1+\frac{2a}{b-a})} \simeq \tfrac{1}{2} d_0 \sqrt{b}\, \frac{1}{\sqrt{a}} \quad (b \gg a) .$$

Hence, for not too small values of $b_0(\Delta t)^\nu \delta$, this results in a considerable reduction of the number of iterations.

EXAMPLE 6.4. In the partially implicit case (3.6) we derive from (6.2) and (6.5)

$$(6.9a) \qquad m \geq \gamma((\Delta t)^\nu S), \quad \gamma(x) := \frac{d_0}{\operatorname{arccosh}\left[1 + 8\omega \frac{\omega + b_0 x}{b_0^2 x^2}\right]}.$$

In order to minimize $\gamma(x)$ we choose $\omega = \omega(x)$ such that the expression in square brackets is maximal, i.e. ω as large as possible. Since we should satisfy $a \leq \alpha_0 \leq b$, it follows from (6.2) that

$$1 \leq \omega \leq \tfrac{1}{2}[1 + \sqrt{1+b_0(\Delta t)^\nu S}].$$

Hence, the optimal value of ω is apparently given by

$$(6.9b) \qquad \omega = \tfrac{1}{2}[1 + \sqrt{1+b_0(\Delta t)^\nu S}].$$

For large values of x we derive from (6.9a) and (6.9b)

(6.9') $\quad m \geq \gamma((\Delta t)^{\nu}S), \quad \gamma(x) \approx \frac{1}{4}\sqrt{2}\, d_0 \sqrt[4]{b_0 x}$

which satisfies (2.2) for $\nu = 1,2$ and 3. The analogue of Table 6.1 is given by Table 6.2.

Table 6.2. Constants c in $\gamma(x) \approx c\sqrt[4]{x}$ for $\nu = 1$

p	$\tilde{p}=2$	$\tilde{p}=3$	$\tilde{p}=4$	$\tilde{p}=5$	$\tilde{p}=6$
2	.51				
3	.48	.80			
4	.47	.78	1.04		
5	.48	.80	1.03	1.25	
6			1.18	1.38	1.51

6.2.2. Lower order predictors

Assuming that the dominant frequencies correspond to eigenvectors of Z with eigenvalues in the interval $[-(\Delta t)^{\nu}S^*,0]$ we are led to consider polynomials $R_m(x)$ which are small in magnitude on the interval $[a^*,b^*]$, where $[a^*,b^*]$ is the interval of eigenvalues α of A that correspond to the eigenvalues of Z in $[-(\Delta t)^{\nu}S^*,0]$.

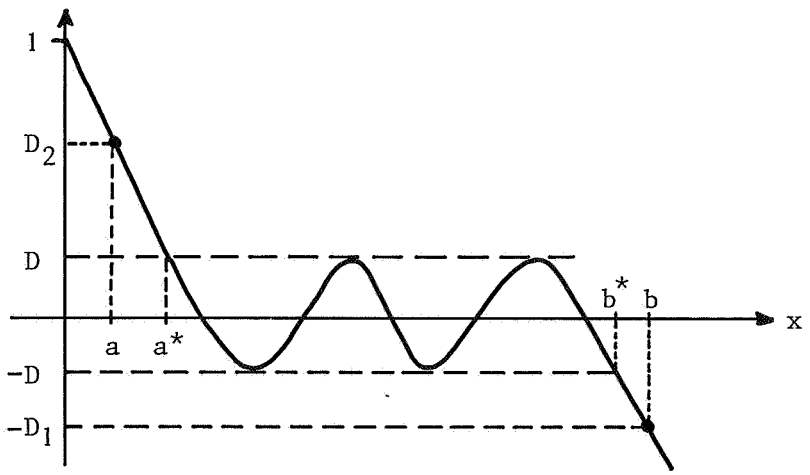

Figure 6.2. The polynomial $R_m(x)$

Requiring that $R_m(x)$ is bounded by D in the interval $[a^*,b^*]$ (see Figure 6.2), and recalling that $R_m(0) = 1$, we arrive at the iteration polynomial

$$(6.10) \qquad R_m(x) = DT_m\left(\frac{b^*+a^*-2x}{b^*-a^*}\right), \quad D := T_m^{-1}\left(\frac{b^*+a^*}{b^*-a^*}\right),$$

where it is assumed that $D \le D_1$ and $D \le D_2$.
The stability requirements read:

$$(6.11) \qquad \begin{cases} R_m(b) \begin{cases} \le D_2 & \text{for m even} \\ \ge -D_1 & \text{for m odd} \end{cases} \\ R_m(a) \le D_2 \end{cases}.$$

THEOREM 6.4. *Let the iteration polynomials be such that* $R_m(x)$ *is of the form (6.10) and let*

$$c_0 = \operatorname{arccosh}\left(\frac{b^*+a^*}{b^*-a^*}\right), \quad c_1 = \operatorname{arccosh}\left(\frac{b^*+a^*-2a}{b^*-a^*}\right), \quad c_2 = \operatorname{arccosh}\left(\frac{2b-a^*-b^*}{b^*-a^*}\right).$$

Then the method is stable if m *satisfies the inequality*

$$(6.12) \qquad m \le \min\left\{\frac{\operatorname{arccosh}[D_2\cosh(mc_0)]}{c_1}, \frac{\operatorname{arccosh}[D_i\cosh(mc_0)]}{c_2}\right\}$$

where $i = 1$ *for* m *odd and* $i = 2$ *for* m *even.* □

The proof of this theorem straightforwardly follows from (6.11). Unlike the result of Theorem 6.2, the lower bound on m is here implicitly defined. However, in a few special cases more explicit results can be derived from this theorem.

THEOREM 6.5. *Let* $R_m(x)$ *be of the form (6.10), and let*

$$D_2 = 1, \quad b^* + a^* \ge b.$$

Then the method is stable for all even values of m. *If in addition* $b^* = b$, *then the method is also stable for all odd values of* m. □

It has already been observed that only low order predictors give rise to $D_2 = 1$. Hence, the corresponding GPC methods will have relatively large truncation errors unless m is large (in order to obtain small D-values). Since the only reason for applying an unconditionally stable GPC method is to save computing time we should choose m small. Consequently, the unconditionally stable GPC methods indicated in Theorem 6.5 should only be applied if one does not want accurate results.

EXAMPLE 6.5. Let us consider the interval $[a^*,b^*]$ that corresponds to the interval $[-S^*,0]$ in the case of the partially implicit operator (3.6). A straightforward calculation yields (cf. (6.2))

$$(6.13)\qquad a^* = (2\omega-1)\frac{1+b_0(\Delta t)^\nu S^*}{(\omega+\frac{1}{2}b_0(\Delta t)^\nu S^*)^2},\quad b^* = \frac{2\omega-1}{\omega}\cdot\frac{1+b_0(\Delta t)^\nu S^*}{\omega+b_0(\Delta t)^\nu S^*}.$$

Since we expect the parameter S^* should be chosen sufficiently large, say $S/10 \le S^* \le S/3$, we have $b^* \approx (2\omega-1)/\omega \approx b$. Chosing a predictor-corrector pair with $D_2 = 1$ (e.g. a BD-corrector with an EP-predictor of order $\tilde{p} = 0$ or $\tilde{p} = 1$ (see Table 5.1)) we conclude from Theorem 6.5 that the generated GPC method is unconditionally stable. The damping factor D is given by

$$D = T_m^{-1}\left(\frac{(\omega+\frac{1}{2}b_0(\Delta t)^\nu S^*)^2 + \omega(\omega+b_0(\Delta t)^\nu S^*)}{(\omega+\frac{1}{2}b_0(\Delta t)^\nu S^*)^2 - \omega(\omega+b_0(\Delta t)^\nu S^*)}\right).$$

It is easily verified that for given $b_0(\Delta t)^\nu S^*$ within the admissible range of ω-values specified by $a^* \le \alpha_0 \le b^*$ the value of D is minimized if

$$(6.14)\qquad \omega = \omega^* := [1 + \sqrt{1+b_0(\Delta t)^\nu S^*}],$$

to obtain approximately

$$(6.15)\qquad D = T_m^{-1}\left(\frac{\omega^*+1}{\omega^*-1}\right).$$

In actual computation it is convenient to prescribe the damping factor D and to derive the appropriate number of iterations from D. Thus, requiring a damping factor $D(\le D_1)$, we find from (6.15) for $S^* >> 1$

(6.16) $\quad m \approx \gamma((\Delta t)^{\nu} S), \quad \gamma(x) = \frac{1}{4}\sqrt{2}\, d_1 \sqrt[4]{b_0 x S^*/S}$

where we have written $d_1 := \operatorname{arccosh}(1/D)$. This condition is of the same basic form as condition (6.9'). □

7. NUMERICAL EXAMPLES

In this section we present results obtained by $EP_p - BD_p$ pairs employing the explicit iteration operator (3.4) and the (partially) implicit operator (3.6). The iteration scheme (1.4), that is the parameter matrix $(\lambda_{j\ell})$, is chosen such that either the iteration polynomial (6.4) or (6.10) is generated. For a discussion of this aspect and a detailed treatment of the implementation of this type of methods we refer to [4].

The aim of our experiments is to show that high order time integration of parabolic problems is more efficient than first or second order time integration as is usual in solving parabolic problems. For the sake of comparison we also give results obtained by the familiar and popular ADI method of Peaceman and Rachford [6]. All experiments deal with semi-discrete parabolic problems of the form (1.1), i.e. $\nu = 1$. The spatial discretization is achieved by standard 5-point discretization on a uniform grid with mesh size $\Delta x = 1/20$. The solutions of our test examples are chosen in such a way that this semi-discretization does not introduce an error, i.e. the solution of the system of ODEs equals the solution of the PDE, restricted to the grid points.

In order to compare the efficiencies of the various methods we compute the relation between the maximal error ε at the end point of the integration interval and the total number of iterations N needed to perform the integration. Assuming that $\varepsilon = O((\Delta t)^{p^*})$ as $\Delta t \to 0$ where p^* is the order of the method, and observing that the number of iterations per step of the GPC method is given by $m \approx c(p^*,q)[\Delta t S]^q$ where $q = \frac{1}{2}$ for the explicit iteration operator, and $q = \frac{1}{4}$ for the partially implicit operator, we arrive at the relation

(7.1) $\quad \log 1/\varepsilon \approx -C + \frac{p^*}{1-q} \log N \text{ as } \Delta t \to 0.$

For a given problem (i.e. S (and S^*) prescribed) the quantity C only depends on p^* and q.

For the ADI method of Peaceman & Rachford a similar relation holds with $p^* = 2$ and $q = 0$.

This asymptotic relation suggests presenting the numerical results using the linear regression model

$$\log 1/\varepsilon = -\bar{C} + \frac{\bar{p}^*}{1-q} \log N, \tag{7.2}$$

where $\bar{C}$ and $\bar{p}^*$ are the regression parameters and the data (i.e. ε and N) follow from the experiments. By means of the values of $\bar{C}$ and $\bar{p}^*$ we obtain an easy tool for comparing the various methods and at the same time we obtain by means of $\bar{p}^*$ the *effective order* of the method.

7.1 Specification of the methods

The *explicit* $EP_{\tilde{p}} - BD_p$ method is the method described in the Examples 5.1 and 6.3. The *implicit* $EP_{\tilde{p}}$-BD_p method is described in Example 6.4 if $\tilde{p} \geq 2$ and in Example 6.5 if $\tilde{p} < 2$. In the latter case the damping parameter D and the "low frequency" parameter S^* are defined by $D = 10^{-2}$ and $S^* = S/10$. The ADI method as well as the implicit $EP_{\tilde{p}}$-BD_p method require a splitting of the function f(t,y) in (1.1). We assume that f can be written as $f(t,y) = f_1(t,y) + f_2(t,y)$, where the splitting functions f_1 and f_2 correspond to the one-dimensional differential operators in x_1- and x_2-direction, respectively.

Now, the (nonlinear) ADI method (written in the so-called Varga form [8]) is defined by

$$\begin{aligned} y^* &= y_n + \tfrac{1}{2}\Delta t f_1(t_n+\tfrac{1}{2}\Delta t, y^*) + \tfrac{1}{2}\Delta t f_2(t_n,y_n) \\ y_{n+1} &= 2y^* - y_n + \tfrac{1}{2}\Delta t f_2(t_{n+1},y_{n+1}) - \tfrac{1}{2}\Delta t f_2(t_n,y_n). \end{aligned} \tag{7.3}$$

The inhomogeneous term, if any, is equally distributed over f_1 and f_2.

The splitting function $F(t_{n+1},u,v)$ used in the implicit $EP_{\tilde{p}}$-BD_p method (cf. (3.6)) is defined by

(7.4) $$F(t_{n+1},u,v) = f_1(t_{n+1},u) + f_2(t_{n+1},v).$$

The method used for solving the implicit relations in the implicit methods consists of just one Newton iteration employing Jacobian matrices evaluated at t_n in the case of ADI and at t_{n+1} (using extrapolated y-values) in the case of the implicit EP-BD methods.

The starting values were taken from the exact solution.

7.2 A linear problem

Our first problem originates from the linear equation

(7.5) $$\frac{\partial u}{\partial t} = \Delta u + g(t,x_1,x_2), \quad 0 \le t,x_1,x_2 \le 1,$$

where the source term g, the Dirichlet boundary conditions and the initial condition are taken from the exact solution

(7.6) $$u(t,x_1,x_2) = 1 + e^{-t}(x_1^2+x_2^2).$$

In Table 7.1 the values $\bar{C}$ and $\bar{p}^*$ are listed. These values were obtained by performing experiments with $\Delta t \in [1/10,1/40]$. For the spectral radius we used the approximation $S = 8/(\Delta x)^2 = 3200$. For a list of (log $1/\varepsilon$,N)-values we refer to Appendix B.

Table 7.1. $(\bar{C},\bar{p}^*)$-values

Method	p = 2	p = 4	p = 6
Expl. EP_p-BD_p	(9.44,3.06)	(14.98,4.46)	(17.47,5.24)
Impl. EP_p-BD_p	(3.83,3.80)	(4.67,4.75)	(6.76,6.23)
Impl. EP_1-BD_p	(2.09,2.32)	(2.18,2.42)	(2.36,2.53)
ADI	(-3.41,2.0)		

The explicit and implicit EP_p-BD_p methods show an effective order $\bar{p}^*$ which is acceptably close to the asymptotic order $p^* = p$. By virtue of this high effective order these methods are superior to the EP_1-BD_p methods which behave hardly better than a second order method. Finally, the classical ADI method shows its second order behaviour perfectly.

In Figure 7.1 the lines (7.2) are presented for the EP_p-BD_p and the ADI methods. The drawn part of these lines covers the range of ε- and N-values obtained from the experiments. Its continuation (only in the stable range) has been dotted. This figure clearly demonstrates the superiority of the

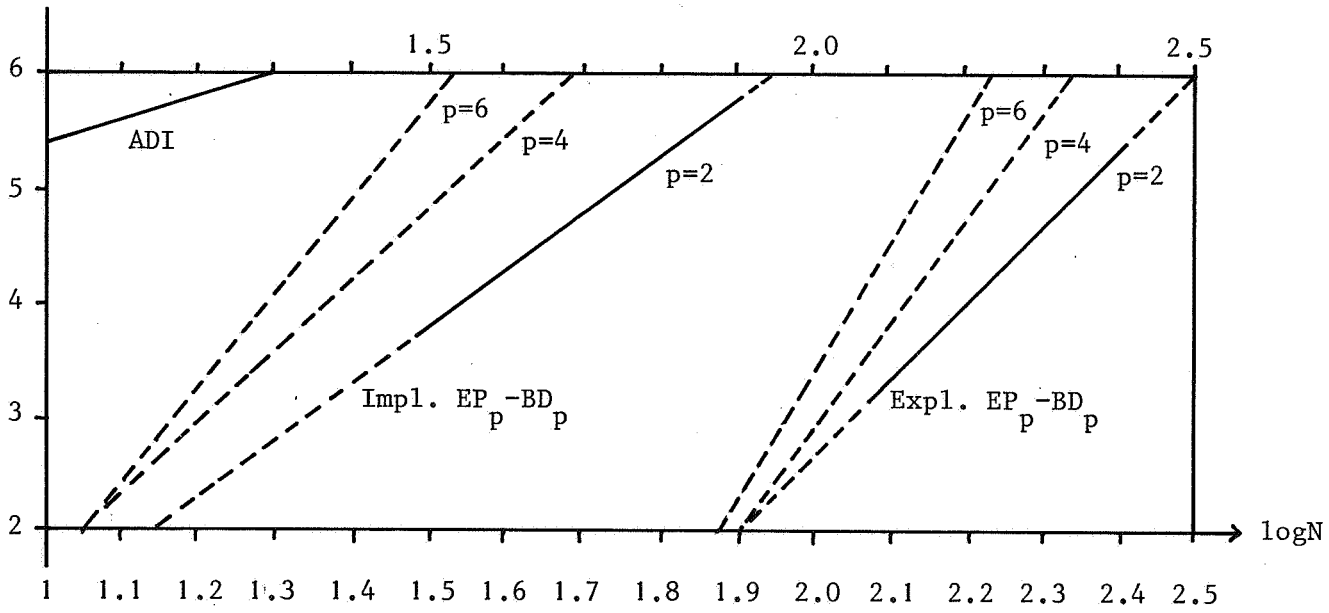

Figure 7.1. (logN,log1/ε)-values for problem (7.5)

higher order methods within the EP-BD class. The explicit and implicit EP-BD methods are difficult to compare because an explicit EP-BD iteration is so much cheaper than an implicit EP-BD iteration that the larger number of iterations does not necessarily imply more computing time. The ADI method requires roughly the same computational effort per iteration as the implicit EP-BD method. Therefore, for this example the ADI method is the most efficient of all.

7.3. A mildly nonlinear problem

Consider the problem [3]

$$(7.7) \qquad \frac{\partial u}{\partial t} = \frac{x_1+x_2}{2(1+t)}\,\Delta(u^3) + g(t,x_1,x_2), \quad 0 \le t,x_1,x_2 \le 1,$$

where the Dirichlet boundary conditions, the initial condition and the inhomogeneous term g follow from the exact solution

$$(7.8) \qquad u(t,x_1,x_2) = \tfrac{1}{2}(x_1+x_2)\sin(2\pi t).$$

Performing experiments with Δt from the interval [1/10,1/80] we arrive at Table 7.2. The spectral radius S was estimated by

$$S(\partial f/\partial y)\big|_{t=t_n} \simeq 1.1\,\frac{24}{(\Delta x)^2} \max_{t\in[t_n,t_n+\Delta t]} \left(\frac{\sin^2 2\pi t}{1+t}\right),$$

where the factor 1.1 is added to obtain a safe upper bound. In the experiments (a complete list of $(\log 1/\varepsilon,N)$-values can be found in Appendix B) the lower order implicit EP_p-BD_p methods were unstable

Table 7.2. $(\bar{C},\bar{p}^*)$-values

Method	p = 2	p = 4	p = 6
Expl. EP_p-BD_p	(13.92,3.36)	(23.14,5.16)	(40.06,8.20)
Impl. EP_p-BD_p	(4.02,2.66)	(8.34,4.42)	(13.84,6.54)
Impl. EP_1-BD_p	(2.69,1.88)	(2.42,1.93)	(-10.20,-2.45)
ADI	(2.13,2.16)		

for $\Delta t = 1/10$ and the ADI method as well as the EP_1-BD_p methods behaved unstably for $\Delta t \ge 1/30$. From Table 7.2 we may conclude that again the theoretical and effective orders of accuracy are in good agreement, except for the EP_1-BD_p methods which behave rather poor. Moreover, this example

illustrates the limited value of the EP_1-BD_p methods: their strength lies in situations where the problem is (almost) linear, with a large value of S and where only a modest accuracy is required.

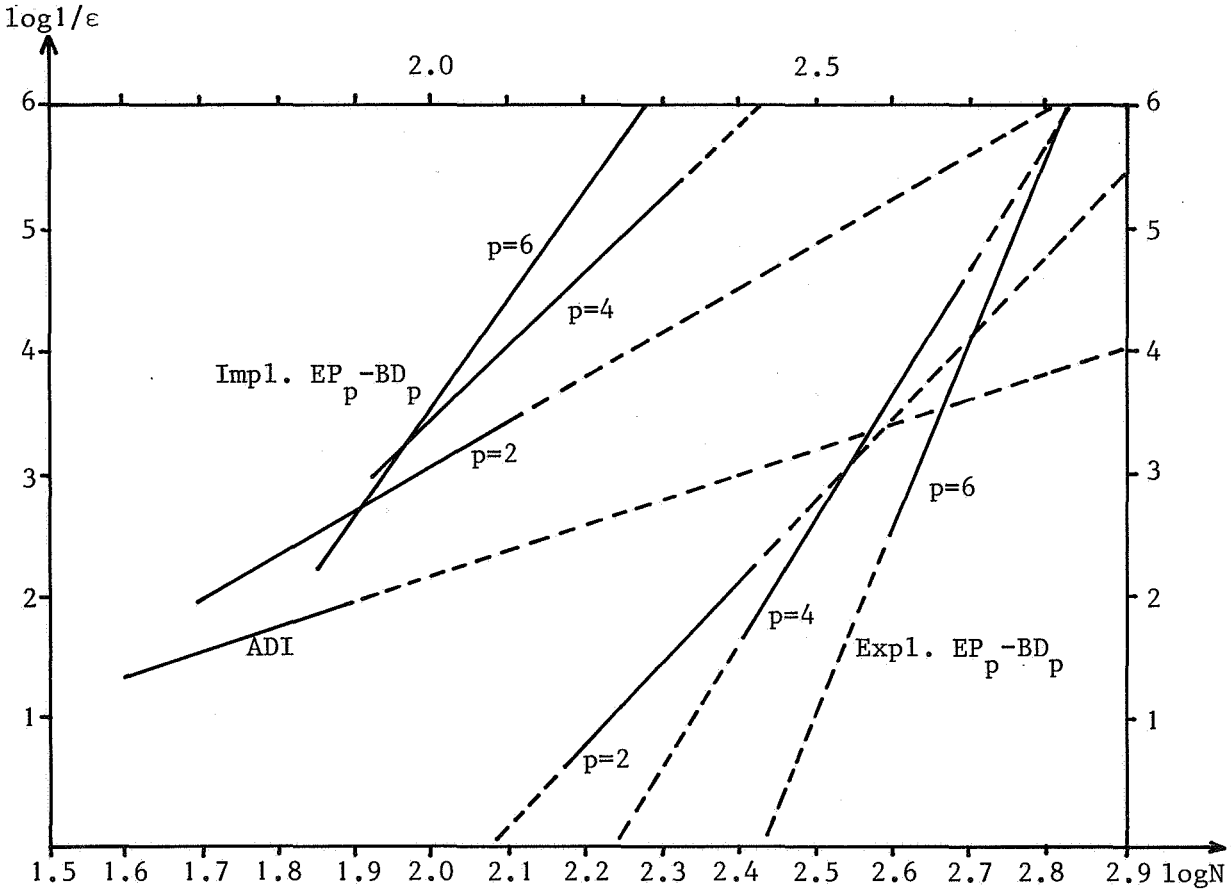

Figure 7.2. (logN,log1/ε)-values for problem (7.7)

In Figure 7.2 the lines (7.2) are shown for the EP_p-BD_p and ADI methods. This figure shows that, using an implicit EP-BD method, the higher order ones are superior if an accuracy is required for which $\log 1/\varepsilon > 3$, approximately. For the explicit EP-BD methods the fourth-order member seems to be the most efficient one in the practical accuracy range.

7.4 A strongly nonlinear problem

To construct a strongly nonlinear example we start with the porous

medium operator

$$\Delta(u^m), \quad m \geq 2.$$

For measuring the errors and for starting the multistep methods, it is convenient to have available an analytic solution, which is chosen to be

$$u(t,x_1,x_2) = (x_1+x_2)^{\frac{2}{5}} e^{-t^2}, \tag{7.9}$$

where t,x_1 and x_2 are defined on the unit iterval $[0,1]$. This solution is also used to prescribe the initial- and Dirichlet boundary conditions. Now, by setting $m = 5$ and introducing an inhomogeneous term we arrive at

$$\frac{\partial u}{\partial t} = \Delta(u^5) + g(t,x_1,x_2), \tag{7.10}$$

where g is determined by the solution (7.9). For a safe upper bound of the spectral radius S we used

$$S(\partial f/\partial y)\big|_{t=t_n} = 1.1 \frac{40}{(\Delta x)^2} 3e^{-t^2}.$$

In Table 7.3 we list the $(\bar{C},\bar{p}^*)$-values obtained from several experiments with $\Delta t \in [1/10, 1/100]$. The results of this

Table 7.3. $(\bar{C},\bar{p}^*)$-values

Method	p = 2	p = 4	p = 6
Expl. EP_p-BD_p	(9.63,2.22)	(25.46,5.09)	(36.90,6.89)
Impl. EP_p-BD_p	(3.39,2.50)	(7.20,4.31)	(13.82,6.73)
Impl. EP_1-BD_p	(3.42,2.30)	(0.10,1.52)	(-.61,1.20)
ADI	(.68,2.25)		

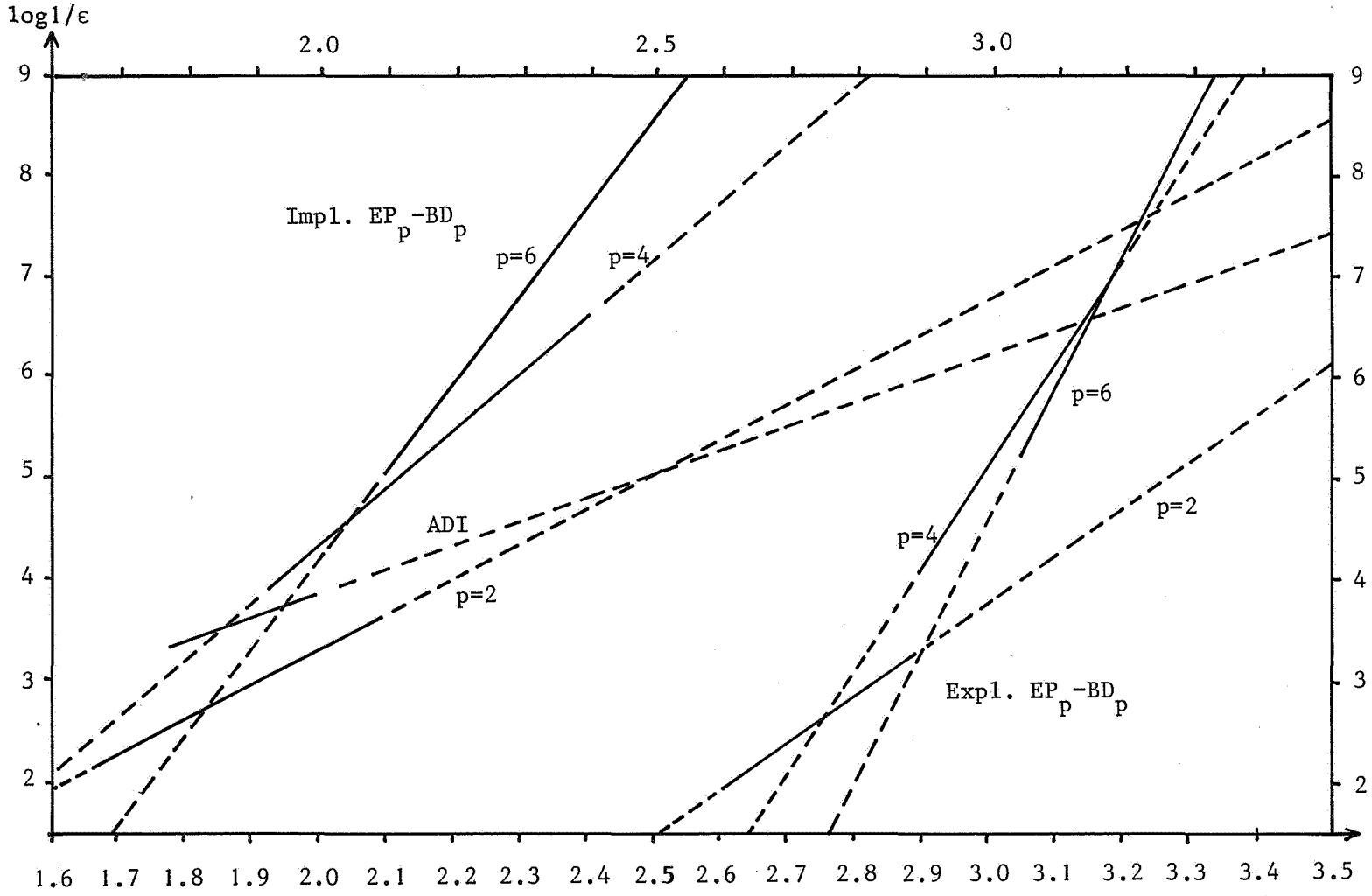

Figure 7.3. (logN,log1/ε)-values for problem (7.10)

example are similar to those of the previous problem. The ADI method behaved unstably for $\Delta t \geq 1/40$. From Figure 7.3 it is clear that the higher-order implicit EP_p-BD_p methods are preferable. The 6th order method is the most efficient one to obtain highly accurate results ($\log 1/\varepsilon \geq 4.5$), otherwise the 4th order method is recommended. For the explicit EP_p-BD_p methods, again the 4th order one is superior in the usual range of accuracies ($2.5 \leq \log 1/\varepsilon \leq 7$). For this example the EP-BD methods using a low order predictor behaved unsatisfactory and are not competitive with the other variants.

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Appendix A.

Proof of Theorem 4.1.

Let the iteration error be defined by

$$\text{(A1)} \qquad \varepsilon_j = y^{(j)} - \eta,$$

η being the exact solution of the corrector equation. Assuming that the integration process has been exact sofar (localizing assumption [5]), the local error of the scheme (1.4) is given by

$$\text{(A2)} \qquad y_{n+1} - y(t_{n+1}) = y_{n+1} - \eta + \eta - y(t_{n+1}) = \varepsilon_m + (\eta - y(t_{n+1})).$$

The term in parentheses is the local error of the corrector which is well-defined (see e.g. [5]). Here we consider the iteration error ε_m. Substitution of (A1) into the scheme (1.4) yields

$$\hat{L}\Big(\sum_{\ell=0}^{j} \lambda_{j\ell}(\varepsilon_\ell+\eta), \varepsilon_{j-1}+\eta\Big) = \Sigma_n = L\eta = \hat{L}(\eta,\eta).$$

Using $\Sigma_{\ell=0}^{j} \lambda_{j\ell} = 1$ (cf. (1.4)) we obtain

$$\hat{L}(\eta+\lambda_{jj}\varepsilon_j+\sum_{\ell=0}^{j-1}\lambda_{j\ell}\varepsilon_\ell, \eta+\varepsilon_{j-1}) - \hat{L}(\eta,\eta) = 0,$$

or, by virtue of condition (4.2),

$$\text{(A3)} \qquad \begin{aligned} \varepsilon_j = &-\frac{1}{\lambda_{jj}}\{(\lambda_{jj-1}+A-I)\varepsilon_{j-1} + \sum_{\ell=0}^{j-2}\lambda_{j\ell}\varepsilon_\ell\} + \\ &(\Delta t)^\nu O(\|\varepsilon_j\|^2 + \|\sum_{\ell=0}^{j-1}\lambda_{j\ell}\varepsilon_\ell\|^2 + \|\sum_{\ell=0}^{j-1}\lambda_{j\ell}\varepsilon_\ell\|.(\|\varepsilon_j\|+\|\varepsilon_{j-1}\|) + \\ &\|\varepsilon_j\|.\|\varepsilon_{j-1}\| + \|\varepsilon_{j-1}\|^2), \end{aligned}$$

where we have written $A - I$ for $J_1^{-1}J_2$. First, we observe that

$$\text{(A4)} \qquad \begin{aligned} \varepsilon_0 = y^{(0)} - \eta &= y^{(0)} - y(t_{n+1}) + y(t_{n+1}) - \eta \\ &= O((\Delta t)^{\tilde{p}+\nu}) + O((\Delta t)^{p+\nu}) =: O((\Delta t)^s), \quad s \geq \nu + \min(\tilde{p},p). \end{aligned}$$

Now, let us assume that

$$\text{(A5)} \qquad \varepsilon_j = R_j(A)\varepsilon_0 + 0((\Delta t)^{2s+\nu}), \quad j = 0,\ldots,i-1.$$

Then,

$$\varepsilon_i = -\frac{1}{\lambda_{ii}}\{(\lambda_{ii-1}+A-I)[R_{i-1}(A)\varepsilon_0+((\Delta t)^{2s+\nu})]+$$
$$\sum_{\ell=0}^{i-2}\lambda_{j\ell}\,[R_\ell(A)\varepsilon_0+0((\Delta t)^{2s+\nu})]\} +$$
$$(\Delta t)^{\nu}0(\|\varepsilon_i\|^2 + (\Delta t)^{2s} + \|\varepsilon_i\|(\Delta t)^s),$$

because of the induction assumption that $\|\varepsilon_j\| = 0((\Delta t)^s)$, $j = 0,\ldots,i-1$. Hence,

$$\text{(A6)} \qquad \varepsilon_i = R_i(A)\varepsilon_0 + 0((\Delta t)^{2s+\nu}) + (\Delta t)^{\nu}0(\|\varepsilon_i\|^2 + \|\varepsilon_i\|(\Delta t)^s).$$

Suppose $\varepsilon_i = 0((\Delta t)^q)$; then, according to (A6), q has to satisfy

$$\text{(A7)} \qquad 0((\Delta t)^q) = 0((\Delta t)^s) + 0((\Delta t)^{2s+\nu}) + 0((\Delta t)^{2q+\nu}) + 0((\Delta t)^{\nu+q+s}).$$

It is easily verified that the values $q = -\nu$ and $q = s$ are the only possibilities to satisfy (A7).

However, if ε_i behaves as $0((\Delta t)^{-\nu})$, we have no convergence of the iteration scheme as $\Delta t \to 0$ which contradicts the assumption of the Theorem. Consequently, $q = s$ and we have that (A5) also holds for $j = i$ and therefore for all j.

Now, the expression (4.3) follows trivially. □

Appendix B.

In this appendix we give a complete overview of all test results. For a specification of the methods and the definition of log $1/\varepsilon$, N, $\bar{p}^*$ and $\bar{C}$ we refer to Section 7. In the tables below, an unstable behaviour of a method is denoted by *.

B.1

For the linear problem (7.5) we obtained the following results:

Table B.1.1. Explicit EP_p-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/30	1/40	$\bar{p}^*$	$\bar{C}$
2	3.21/120	4.50/180	4.77/210	5.02/240	3.06	9.44
3	4.53/180	5.86/260	6.42/330	7.04/360	3.94	13.23
4	5.99/220	7.28/320	8.10/390	8.72/440	4.46	14.98
5	7.34/260	8.79/380	9.73/450	10.39/520	5.08	17.28
6	8.65/310	10.29/440	11.17/540	11.47/640	5.24	17.47

Table B.1.2. Implicit EP_p-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/30	1/40	$\bar{p}^*$	$\bar{C}$
2	3.22/30	4.83/40	5.30/60	5.55/80	3.80	3.83
3	4.67/40	5.97/60	6.56/90	6.92/120	3.47	2.54
4	6.09/50	7.34/80	8.12/120	8.86/120	4.75	4.67
5	7.65/60	8.86/100	9.74/120	10.38/160	4.91	4.04
6	8.63/70	10.37/120	11.37/150	12.40/200	6.23	6.76

Table B.1.3. Implicit EP_1-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/30	1/40	$\bar{p}^*$	$\bar{C}$
2	2.86/40	3.81/80	3.93/90	4.34/120	2.32	2.09
3	2.96/40	3.47/60	4.04/90	4.47/120	2.37	2.13
4	3.02/40	3.53/60	4.12/90	4.56/120	2.42	2.18
5	3.06/40	3.58/60	4.17/90	4.62/120	2.45	2.20
6	3.06/40	3.62/60	4.22/90	4.67/120	2.53	2.36

Table B.1.4. ADI method

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/30	1/40	$\bar{p}^*$	$\bar{C}$
2	5.42/10	6.02/20	6.37/30	6.63/40	2.0	-3.41

B.2

The results for the mildly nonlinear problem (7.7) are given in the following tables.

Table B.2.1. Explicit EP_p-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/30	1/40	$\bar{p}^*$	$\bar{C}$
2	.65/146	1.38/190	1.99/227	2.28/258	3.36	13.92
3	1.35/217	2.54/281	3.12/332	3.60/378	4.65	20.35
4	1.86/270	3.21/352	3.94/415	4.34/474	5.16	23.14
5	1.95/318	3.45/410	4.44/486	5.07/553	6.54	30.78
6	2.16/377	4.10/485	5.24/571	6.04/652	8.20	40.06

Table B.2.2. Implicit EP_p-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/30	1/40	1/80	$\bar{p}^*$	$\bar{C}$
2	*	1.92/48	2.25/59	2.69/73	3.53/136	2.66	4.02
3	*	2.40/66	3.05/88	3.40/104	4.29/185	3.11	5.07
4	*	2.94/85	3.76/109	4.24/135	5.42/220	4.42	8.34
5	1.96/60	3.40/97	4.30/126	4.96/160	6.51/258	4.91	9.40
6	2.15/73	4.04/116	5.14/151	6.01/185	7.82/304	6.54	13.84

Table B.2.3. Implicit EP_1-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/30	1/40	1/60	1/80	$\bar{p}^*$	$\bar{C}$
2	*	2.44/113	2.76/149	3.01/191	1.88	2.69
3	2.67/93	3.06/108		3.46/184	1.81	1.99
4	*	2.72/102	3.23/143	3.33/179	1.93	2.42
5	*	*		3.00/173		
6	*	*	3.19/137	2.88/169	-2.45	-10.20

Table B.2.4. ADI method

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/30	1/40	1/60	1/80	$\bar{p}^*$	$\bar{C}$
2	*	1.33/40	1.71/60	1.98/80	2.16	2.13

B.3

For the strongly nonlinear example (7.10) we found the results as given below

Table B.3.1. Explicit EP_p-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/40	$\bar{p}^*$	$\bar{C}$
2	1.97/418	2.68/589	3.30/834	2.22	9.63
3	3.55/625	4.66/874	5.53/1238	3.33	15.04
4	3.98/781	5.59/1093	7.01/1548	5.09	25.46
5	4.63/918	6.12/1287	7.63/1818	5.05	25.32
6	4.95/1090	6.99/1526	9.03/2155	6.89	36.90

Table B.3.2. Implicit EP_p-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/10	1/20	1/40	$\bar{p}^*$	$\bar{C}$
2	2.09/46	3.06/77	3.56/127	2.50	3.39
3	3.58/67	4.65/115	5.95/193	3.87	5.88
4	3.89/86	5.28/147	6.54/249	4.31	7.20
5	4.62/103	5.97/173	7.49/295	4.71	8.05
6	4.95/123	6.94/208	8.98/346	6.73	13.82

Table B.3.3. Implicit EP_1-BD_p methods

p \ Δt	$\log\frac{1}{\varepsilon}$ / N 1/30	1/40	1/60	$\bar{p}^*$	$\bar{C}$
2	*	3.75/224	4.26/292	2.30	3.42
3	4.40/170	4.62/215	4.67/284	0.89	-1.79
4	4.22/167	4.86/203	4.74/279	1.52	0.10
5	4.16/164	4.31/194	4.59/274	1.44	0.09
6	4.12/162	4.32/193	4.49/270	1.20	-0.61

Table B.3.4. ADI method

	$\log\frac{1}{\varepsilon}$ / N						
p \ Δt	1/20	1/40	1/60	1/80	1/100	$\bar{p}^*$	$\bar{C}$
2	*	*	3.33/60	3.61/80	3.83/100	2.25	.68