Error Structures and Extrapolation in Time for Parabolic Problems

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Abstract

We study asymptotic expansions of the time discretization error for some time stepping schemes applied to (semi-discretizations of) linear parabolic initial/boundary value problems. For this type of problems, the 'classical' theory of asymptotic error expansions (cf. [12]) cannot be applied directly; a more careful analysis is necessary to understand the structure of the time discretization error. We recall and discuss our respective results of [1] and [2] for the smooth case and present numerical experiments with extrapolation confirming these results. In the final section we discuss the case of nonsmooth solutions caused by inconsistent initial/boundary data.

1 Introduction

Within the context of discretization methods, acceleration techniques like *extrapolation* or *defect correction* can often be successfully applied to construct highly accurate solutions in a very efficient way (i.e., at low computational cost, combining low order 'basic' approximations in a systematic manner). In particular, there is a vast variety of literature dealing with acceleration techniques for the numerical solution of ordinary and partial differential equations (cf. for instance the monograph [9]).

Whether, in a given situation, such an accelerated algorithm displays its full potential efficiency strongly depends on certain *structural properties* of the discretization scheme which is used as the basis for acceleration. For extrapolation algorithms, for instance, the crucial point is that the global error of the basic scheme should behave in a sufficiently systematic way when the grid is refined systematically. The theoretical prerequisite which enables us to study this behavior are *asymptotic expansions* of the global discretization error in powers of the stepsize parameter (cf. for instance [12]).

The present paper, which is not too technical but of an expository nature, is devoted to extrapolation techniques applied to parabolic initial/boundary value problems. We

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focus our attention on the time discretization aspect, assuming that some reasonable spatially discrete semi-discretization of the underlying parabolic PDE is given (method of lines). Our first and most important concern is to make clear that a very careful analysis is necessary to predict and understand the performance of an accelerated algorithm like extrapolation for this class of problems. The point is that, due to the inherent *stiffness* of the given problem, the existence of a reasonable asymptotic error expansion is by no means a priori obvious, not even for simple linear parabolic PDEs with smooth solutions. This fundamental difficulty, which has not been analyzed in the existing literature, will be made clear in section 2 below; we will then recall and discuss the results of our analysis from [1] and [2], where the structure of the global time discretization error is studied for some simple, practically important time stepping schemes. In particular, the backward Euler and trapezoidal methods are considered in detail and rigorous, quantitative error expansions are presented. It turns out that these expansions are similar to 'conventional' asymptotic error expansions - a nontrivial result - but they also contain certain 'irregular' terms which may, to some extent, impair the full efficiency of extrapolation. Some numerical tests confirming these theoretical results are presented in section 3.

The considerations of [1] and [2] were restricted to linear constant coefficient problems with *smooth* solutions (consistent initial/boundary data). As already mentioned above, the typical difficulties and drawbacks caused by the stiffness are already visible here, such that the smooth case is nontrivial and indeed highly interesting from the theoretical point of view. In practice, however, *nonsmooth problems* (with inconsistent initial/boundary data) are more realistic and important. This general case, which is not covered by the results of [1] and [2], is considered in section 4.

2 Analysis of Global Error Structures (smooth case)

In this section we recall and discuss our theoretical results from [1] and [2] about error structures in the case of smooth solutions (consistent initial/boundary data).

We consider a class of linear, inhomogeneous constant coefficient parabolic initial/boundary value problems[1]

$$\frac{\partial u}{\partial t} = L\,u + g, \qquad (t,x) \in [0,T]\times\Omega \tag{2.1a}$$

$$u(0,x) = u_0(x), \qquad x \in \Omega \tag{2.1b}$$

$$u(t,x) = b(t,x), \qquad t \in [0,T], \quad x \in \partial\Omega \tag{2.1c}$$

with a second order elliptic (not necessarily selfadjoint) differential operator L. Let the problem data be given such that (2.1) admits a (sufficiently) smooth solution $u =$

[1] Ω is a bounded domain in $\mathbb{R}^d$ with a sufficiently smooth boundary $\partial\Omega$.

$u(t,x)$, with a certain number of moderate-sized derivatives. (See, however, section 4 below).

Assume that (2.1) is discretized in space, e.g. by a finite difference or finite element scheme, on a certain mesh or triangulation Ω_h of Ω, with 'meshwidth' h. The precise form of this semi-discretization is not so essential here; in any case we end up with a spatially discrete initial/boundary value problem, i.e., a system of ordinary differential equations[2]

$$\frac{du_h}{dt} = L_h\, u_h + f_h \tag{2.2}$$

with the corresponding initial condition. Typically, L_h in (2.2) is unbounded for decreasing h: $\|L_h\| \approx h^{-2}$.

By Δ_h we denote a suitable projection operator mapping functions $v(x)$ into their semi-discrete analoga $\Delta_h v$. The *spatial truncation error* $\sigma_h(t)$ is defined as the residual of $\Delta_h u$ (solution of original problem (2.1) restricted to spatial mesh Ω_h) w.r.t. to the semi-discretization (2.2).

Remarks:

- The solution u_h of the 'intermediate' ODE system (2.2) will not be considered further. In fact, it is well known (cf. e.g. [11]) that the smoothness of u_h is not directly related to the smoothness of the original PDE solution u. In our analysis for smooth u, it is more natural to study the error $U_{h,\nu} - \Delta_h u(t_\nu)$ directly, without reference to u_h.

- In this paper we restrict our considerations to *time* discretization effects; we are not considering asymptotic error expansions w.r.t. h. In the rest of the present section this is reflected by the fact that $\sigma_h(t)$ appears as a fixed quantity which limitates the overall accuracy achievable on a given spatial mesh Ω_h.

Implicit Euler scheme.

Let us now consider the implicit (or backward) Euler scheme, with stepsize τ, applied to the semi-discretization (2.2) of (2.1):

$$\frac{1}{\tau}\Big(U_{h,\nu} - U_{h,\nu-1}\Big) = L_h\, U_{h,\nu} + f_h(t_\nu), \qquad \nu = 1,2,\ldots \tag{2.3}$$

with $U_{h,0} := \Delta_h u_0$. The vectors $U_{h,\nu}$ are the fully-discrete approximations for $u(t_\nu, x)$ ($t_\nu := \nu\tau$) at the spatial meshpoints $x \in \Omega_h$.

[2]We assume that the boundary condition (2.1c) is directly incorporated into (2.2). Thus, f_h in (2.2) depends on $g(t,x)$ and $b(t,x)$ in (2.1) and $\|f_h\|$ is proportional to a negative power of h (unless $b(t,x) \equiv 0$).

We shall now describe the structure of the global error $U_{h,\nu} - \Delta_h u(t_\nu)$ by means of an asymptotic expansion in powers of the stepsize τ. Let us consider an ansatz with three terms:

$$U_{h,\nu} - \Delta_h u(t_\nu) = \tau\, e_{h,1}(t_\nu) + \tau^2 e_{h,2}(t_\nu) + R_{h,\nu}. \tag{2.4}$$

The goal is to derive τ-independent functions $e_{h,1}(t)$ and $e_{h,2}(t)$ (which we choose spatially discrete) such that (2.4) holds with a remainder term $R_{h,\nu}$ that is (hopefully) small (of third order in τ) compared to the leading terms in (2.4). To this end we insert (2.4) into the numerical scheme (2.3), use Taylor expansions of u and of the $e_{h,i}$ about $t = t_\nu$ and equate coefficients of powers of τ. Together with the requirement that the $e_{h,i}$ should not depend on τ this leads to the following ODE systems for the $e_{h,i}$:

$$\frac{de_{h,1}}{dt} = L_h\, e_{h,1} + \frac{1}{2}\,\frac{d^2 \Delta_h u}{dt^2} \tag{2.5a}$$

$$\frac{de_{h,2}}{dt} = L_h\, e_{h,2} + \frac{1}{2}\,\frac{d^2 e_{h,1}}{dt^2} - \frac{1}{6}\,\frac{d^3 \Delta_h u}{dt^3} \tag{2.5b}$$

(note the recursive dependence of (2.5b) on (2.5a)). Furthermore, it turns out that the remainder term $R_{h,\nu}$ must satisfy a difference equation of the type (2.3):

$$\frac{1}{\tau}\Big(R_{h,\nu} - R_{h,\nu-1}\Big) = L_h\, R_{h,\nu} + \gamma_{h,\nu} + \sigma_h(t_\nu) \tag{2.6}$$

where $\gamma_{h,\nu}$ contains a factor τ^3 and is a certain collection of Taylor remainder terms of $\Delta_h u$ and the $e_{h,i}$. σ_h is the spatial truncation error. The initial values for $e_{h,i}$ and $R_{h,\nu}$ remain to be fixed; since $U_{h,0} = \Delta_h u_0$, it is natural to choose $e_{h,1}(0) = e_{h,2}(0) = R_{h,0} := 0$.

In order to show that the above expansion makes sense, one has to study the behavior of its coefficient functions $e_{h,i}$ and estimate its remainder term $R_{h,\nu}$. Recall that we have assumed that the problem data are given such that $u(t,x)$ is a smooth solution of (2.1) (more precisely: we assume existence and moderateness of those derivatives of u which influence our analysis). One might expect that, in this case, the solution $e_{h,1}$ of (2.5a) with the 'natural' initial value $e_{h,1}(0) = 0$ will also be smooth (possibly one degree less), similarly for $e_{h,2}$. This conjecture is, however, *false*: Indeed, $e_{h,1}$ and $e_{h,2}$ are well-defined τ-independent, moderate-sized functions, *but* it turns out (cf. [1]) that the higher derivatives of $e_{h,1}(t)$ at $t=0$ are affected by higher and higher powers of L_h and are therefore very large (unbounded for $h \to 0$) near $t=0$. The derivatives of $e_{h,2}$ (which recursively depends on $e_{h,1}$) behave even more critically. As a consequence, the inhomogeneous term $\gamma_{h,\nu}$ in (2.6), which depends on $d^3 e_{h,1}/dt^3$ and $d^2 e_{h,2}/dt^2$ (cf. [1]), is also very large in size (affected by some negative power of the spatial meshsize h) near $t = 0$. Thus, a straightforward estimate for $R_{h,\nu}$ (based on a stability argument for (2.6)) leads only to an estimate

$$\|R_{h,\nu}\| \le C h^{-k} \tau^3 \tag{2.7}$$

with some constant C and a certain positive integer k. But such an estimate is worthless: It is not uniformly valid for $h \to 0$; with decreasing h, the right hand side of (2.7) tends to infinity. But also for fixed, small h the quantity $Ch^{-k}\tau^3$ will usually be so large that $R_{h,\nu}$ would be expected to be a dominant - but not a neglible - term in our expansion (2.4). Such a result would be useless for practical purposes like e.g. an analysis of extrapolation.

In other words: An asymptotic error expansion (2.4) makes sense only if its coefficient functions and, in particular, its remainder term do not depend in a critical way on $\|L_h\| \approx h^{-2} \gg 0$. Generally speaking, *our goal must be to derive quantitative estimates which depend in a natural way on the smoothness of the given problem but remain unaffected by critical problem parameters.* Such a quantitative theory has been presented in [1, 2]; it is based on a careful study of $\gamma_{h,\nu}$ in (2.6) and on certain strengthened stability estimates for the implicit Euler scheme (cf. the second remark after Theorem 1). Refraining from a discussion of all the technical details, we quote

Theorem 1. *For (sufficiently) smooth u, the full global error $U_{h,\nu} - \Delta_h u(t_\nu)$ of the implicit Euler scheme admits an asymptotic expansion* (2.4), *where $e_{h,1}(t)$ and $e_{h,2}(t)$ are moderate-sized, τ-independent solutions of* (2.5a),(2.5b) *and where the remainder term $R_{h,\nu}$ can be estimated by*

$$\|R_{h,\nu}\|_2 \le \Big(C_0 + \frac{C_1}{t_\nu}\Big)\tau^3 + \bar{C} \max_{0 \le t \le t_\nu} \|\sigma_h(t)\|_2 \tag{2.8}$$

with certain τ- and h-independent, moderate-sized bounds C_0, C_1 and $\bar{C}$.

Remarks:

- The estimate (2.8) says that (besides the influence of the spatial truncation error) the remainder term $R_{h,\nu}$ shows a *reduced order*, namely $O(\tau^2)$, at the first grid points after $t=0$; but these order reductions are *algebraically damped* (damped like $1/\nu = \tau/t_\nu$) with increasing ν. The full, quantitative, h-independent order $O(\tau^3)$ reappears 'away from' $t=0$.

- In the proof of the above result it turns out that so-called *smoothing property* of the implicit Euler scheme, i.e.[3]

$$\Big\| (I-\tau L_h)^{-\nu} - e^{t_\nu L_h} \Big\|_2 \le \frac{C}{\nu}, \quad \nu \ge 1 \tag{2.9}$$

plays an essential role. (2.9) is well known and has been used to derive convergence results in nonsmooth situations. As we see now, it is also of essential importance for a sound understanding of global error structures, even for smooth problems.

[3] (2.9) is valid under natural assumptions: If L_h is selfadjoint we assume negative definiteness; for non-selfadjoint L_h case we assume that a sectorial condition is satisfied (see [2],[7]). Note further that another 'smoothing estimate' of a more complicated type than (2.9) is also required (cf. [1]).

- The theoretical considerations in [1] suggest that Theorem 1 can be generalized to longer expansions, with a remainder term which is $O(\tau^2)$ near $t = 0$ and is damped down like ν^{2-p}, attaining its full conventional, quantitative order $O(\tau^p)$ away from $t=0$.

Theorem 1 allows obvious predictions about the performance of τ-extrapolation based on the implicit Euler scheme. The numerical examples given in section 3 below show that Theorem 1 indeed describes the error structure in a precise way.

Implicit trapezoidal rule.

The implicit trapezoidal rule applied to (2.2),

$$\frac{1}{\tau}\Big(U_{h,\nu} - U_{h,\nu-1}\Big) = \frac{1}{2}\Big(L_h U_{h,\nu-1} + L_h U_{h,\nu}\Big) + \frac{1}{2}\Big(f_h(t_{\nu-1}) + f_h(t_\nu)\Big) \tag{2.10}$$

is second order convergent[4] and is a candidate for τ^2-extrapolation; we expect an asymptotic error expansion in even powers of τ. However, the existence and precise form of a reasonable asymptotic expansion, valid uniformly in h, is again not obvious here. Similarly as for the implicit Euler scheme, a careful quantitative analysis is necessary. In [2] we have studied a short expansion

$$U_{h,\nu} - \Delta_h u(t_\nu) = \tau^2 e_{h,2}(t_\nu) + R_{h,\nu} \tag{2.11}$$

where $e_{h,2}$ is a solution of

$$\frac{de_{h,2}}{dt} = L_h\, e_{h,2} + \frac{1}{12}\,\frac{d^3 \Delta_h u}{dt^3} \tag{2.12}$$

and $R_{h,\nu}$ satisfies the certain 'trapezoidal type' difference equation. From [2] we quote the following result:

Theorem 2. *For (sufficiently) smooth u, the full global error $U_{h,\nu} - \Delta_h u(t_\nu)$ of the implicit trapezoidal rule admits an asymptotic expansion* (2.11)*, where $e_{h,2}(t)$ is a moderate-sized, τ-independent solution of* (2.12) *and where the remainder term $R_{h,\nu}$ can be estimated by*

$$\|R_{h,\nu}\|_2 \le \Big(C_0 + \frac{C_1}{t_\nu}\Big)\tau^4 + \bar{C} \max_{0\le t\le t_\nu} \|\sigma_h(t)\|_2 \tag{2.13}$$

with certain τ- and h-independent, moderate-sized bounds C_0, C_1 and $\bar{C}$.

[4] This is true for constant coefficient problems with smooth solutions, as considered in this section; for such problems the trapezoidal rule is indeed a very accurate integration method. However, instabilities may arise for more difficult problem classes (cf. also section 4).

Remarks:

- Theorem 2 says that the expansion (2.11) is 'almost perfect': the remainder term shows a reduced order ($O(\tau^3)$ instead of $O(\tau^4)$ near $t=0$) but is again $O(\tau^4)$ away from $t=0$. Thus we expect that (at least) one step of τ^2-extrapolation will perform satisfactorily.

- The proof of Theorem 2 requires certain strengthened stability estimates for the trapezoidal rule (for details cf. [2], section 3).

- In contrast to Theorem 1, Theorem 2 cannot be generalized to longer expansions, because at the τ^4-level, the global error behaves in an irregular way (oscillations occur which are not damped out sufficiently fast because, except for the case where τ is very small compared to h, the trapezoidal rule does not satisfy a smoothing estimate analogous to (2.9)).

For numerical evidence we again refer to section 3.

Supplementary remarks.

- It is well known that the implicit midpoint (or Crank-Nicolson) scheme,

$$\frac{1}{\tau}\Big(U_{h,\nu} - U_{h,\nu-1}\Big) = L_h\,\frac{1}{2}\Big(U_{h,\nu-1} + U_{h,\nu}\Big) + f_h\Big(\tfrac{1}{2}(t_{\nu-1} + t_\nu)\Big) \qquad (2.14)$$

  is more robust than the trapezoidal rule in the sense that it remains stable also for non-constant coefficient problems. However, its local accuracy (consistency) properties are worse than for the trapezoidal rule. As a consequence, it can be shown that a result like Theorem 2 does not hold for the Crank-Nicolson scheme; in general, the unavoidable oscillations occur already at the τ^2-level.

- In our analysis of global error structures, the essential difficulty was caused by the fact that the $e_{h,i}(t)$ with initial values $e_{h,i}(0) = 0$ are not sufficiently smooth functions (cf. the discussion preceding Theorem 1). This suggests the idea to try an alternative way of prescribing the initial values in our expansion, with appropriately chosen $e_{h,i}(0) \neq 0$ and $R_{h,0} \neq 0$ such that in the case of (2.4), for instance, $e_{h,1}(0) + e_{h,2}(0) + R_{h,0} = U_{h,0} - \Delta_h u_0 = 0$ is again satisfied. But then, $R_{h,0} = O(\tau)$ (and not $O(\tau^3)$), and again a nontrivial analysis of $R_{h,\nu}$ would be necessary. This approach may be worth considering if one aims at analysis of defect correction algorithms, where the smoothness of the $e_{h,i}(t)$ w.r.t. t plays an important role.

- Our paper [2] also contains a model problem analysis and numerical examples for a locally one-dimensional (Euler-type) splitting method.

- Of course, many questions remain unsolved. First of all, the problem class considered in this paper is relatively simple; an analysis for problems with a time-dependent or nonlinear spatial differential operator L has not been done so far.

  Furthermore, one would like to relax the smoothness assumptions w.r.t. u, at least for schemes like implicit Euler which are well known to perform satisfactorily in nonsmooth cases. This latter point is discussed in section 4 below.

3 Extrapolation: Numerical Examples (smooth case)

The following numerical examples[5] have been selected among the experiments presented in [2]; their main purpose is to illustrate that, for problems with smooth solutions, Theorems 1 and 2 of section 2 describe the respective global error structures in a realistic way. Since we are interested in the effects of time discretization, we directly refer to a spatially discrete stiff system here, suppressing spatial discretization errors:

$$\begin{aligned} \frac{du_h}{dt} &= L_h\left(u_h - \varphi_h\right) + \frac{d\varphi_h}{dt} \\ u_h(0) &= \varphi_h(0) \end{aligned} \tag{3.1}$$

with the smooth solution $u_h(t) \equiv \varphi_h(t)$.[6] L_h is taken as the standard finite difference discretization (based on 2nd order central difference quotients) of the 1D Laplace operator $\partial^2 u/\partial x^2$ on a uniform mesh $\Omega_h \subset \Omega = (0,1)$ with $h = 1/64$.

Let us first consider the backward Euler scheme (2.3). It is well known and indeed straightforward to predict the convergence order of the various steps of τ-extrapolation on the basis of a conventional asymptotic error expansion. Here, as trivial consequence of Theorem 1, the global error $U_{h,\nu} - \Delta_h u(t_\nu)$ (or rather, in our present experimental setting, $U_{h,\nu} - u_h(t_\nu)$) admits an expansion $\tau e_{h,1}(t_\nu) + O(\tau^2)$ where the O-constant is moderate-sized (independently of h), and therefore it is easy to conclude that the first extrapolation step will yield $O(\tau^2)$-accuracy. Concerning the second extrapolation step, however, Theorem 1 does not imply third order accuracy w.r.t. τ because, near $t=0$, the estimate (2.8) does not imply the existence of an expansion $\tau e_{h,1}(t_\nu)+\tau^2 e_{h,2}(t_\nu)+O(\tau^3)$ with a moderate-sized, h-independent O-constant.

Table 3.1 illustrates the situation by means of numerical experiment. It displays the L_2-norm of the global error $U_{h,\nu} - u_h(t_\nu)$, at $t_\nu = 0.1$, for τ-extrapolation based on the backward Euler scheme.[7] The first extrapolation step shows a significant increase in accuracy compared to the basic approximation, but the higher extrapolation steps indeed 'slow down'.

[5] ANSI double precision arithmetic was used.

[6] $\varphi_h(t)$ was chosen as the spatial restriction of $\varphi(t,x) = e^{-t}\cos(x)$.

[7] On the coarsest grid shown in Table 3.1, two backward Euler steps were performed prior to extrapolation.

||global error|| at t=0.1   h=1/64   Table 3.1

tau	Euler	1st EX	2nd EX	3rd EX
1/20	1.024E-03			
1/40	5.450E-04	6.629E-05		
1/80	2.820E-04	1.895E-05	3.192E-06	
1/160	1.435E-04	5.097E-06	4.807E-07	9.459E-08

observed order

	0.91		
	0.95	1.81	
	0.97	1.89	2.73

Table 3.2 shows the corresponding results at $t = 2$ for *global extrapolation* (i.e., the Euler approximations on the various grids were computed independently of each other over the whole integration interval before extrapolation was performed). Now we see that, in contrast to Table 3.1, also the second (and even the third) extrapolation step works very satisfactorily, and the full conventional order is observed. This can be explained by Theorem 1: (2.8) shows that, sufficiently away from the start, the full conventional order $O(\tau^3)$ reappears due to a damping effect.

||global error|| at t=2.0   h=1/64   Table 3.2

GLOBAL EXTRAPOLATION

tau	Euler	1st EX	2nd EX	3rd EX
1/20	3.028E-04			
1/40	1.499E-04	2.963E-06		
1/80	7.460E-05	7.318E-07	1.176E-08	
1/160	3.721E-05	1.819E-07	1.455E-09	1.774E-11

observed order

	1.01		
	1.01	2.02	
	1.00	2.01	3.02

Local extrapolation, where the integration is 'restarted' after each extrapolation interval, obviously cannot not profit by this damping phenomenon and, indeed, numerical experience shows that it yields significantly less accurate results away from the start, such that global extrapolation will usually be more efficient at high tolerances. (In our example, the difference amounts up to three orders of magnitude, see [2].) For an illustration consider Fig. 1, which displays the errors obtained after 3 steps of global and

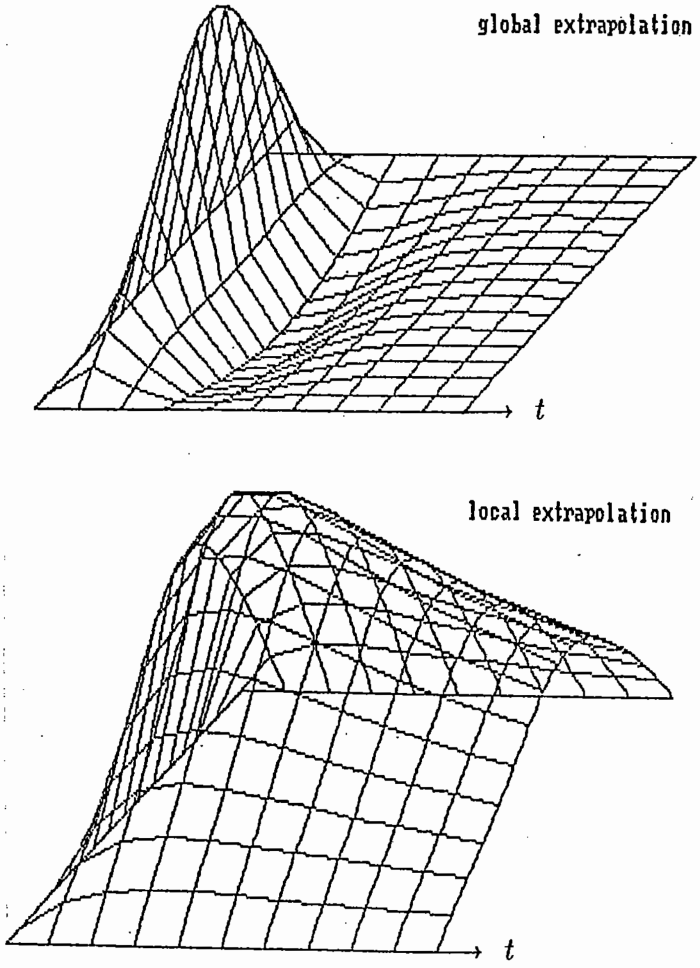

Figure 1: Errors in extrapolation for example (3.1), $t \in [0,1]$

local extrapolation, resp., for $t \in [0,1]$, with $h = 1/64$ and coarsest stepsize $\tau = 1/20$.[8] The different behavior is clearly visible.

These examples demonstrate that Theorem 1 is in very good accordance with numerical reality. It should, however, be mentioned that the difference between global and local extrapolation may be less relevant in practical situations where the tolerance requirements are usually not very high, and where the effects of spatial discretization errors are also present.

Table 3.3 displays a result (situation as in Table 3.1) for τ^2-extrapolation based on the implicit trapezoidal rule (2.10). Again, the numbers are in good accordance with our theory (Theorem 2): The first extrapolation step features its full potential efficiency, yielding a $O(\tau^4)$-approximation. (The estimate (2.13) seems to be slightly

[8] In Fig. 1, the results are displayed on a coarser grid. The maximal error (near $t=0$) is about 10^{-7} (cf. Table 3.1).

too pessimistic here; cf. [2] for an explanation.) The higher extrapolation steps yield no further increase in accuracy, which is in accordance with our remark of section 2 concerning the fact that Theorem 2 cannot be extended to the case of longer expansions.

||global error|| at t=0.1 h=1/64 Table 3.3

tau	ITR	1st EX	2nd EX	3rd EX
1/20	9.880E-06			
1/40	2.445E-06	4.858E-08		
1/80	6.097E-07	2.592E-09	2.134E-09	
1/160	1.523E-07	1.466E-10	9.098E-11	1.012E-10

observed order

	2.01		
	2.00	4.23	
	2.00	4.14	4.55

For a comparison of local and global extrapolation based on the trapezoidal rule, see [1] (the difference is much less significant as for the backward Euler scheme).

Remark: Extrapolation w.r.t. the spatial mesh parameter h has intentionally not been considered here; it is a subject of interest on its own. In practice one will of course aim at a suitable combination of extrapolation in time and space.

4 The Nonsmooth Case

Let us now drop the assumption that the initial and boundary data in (2.1) are such that the solution $u(t,x)$ is smooth up to $t=0$. The nonsmooth case (inconsistent initial/boundary data) is not covered by the results of [1] and [2]; however, the ideas of these papers turn out to be valuable also for the treatment of nonsmooth situations.

We restrict our considerations to the case where the given problem (2.1) is homogeneous (i.e., $g(t,x)\equiv 0$ and $b(t,x)\equiv 0$). The initial function $u_0(x)$ is only assumed to be in $L_2(\Omega)$. Numerical illustration will be given for the model problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad (t,x)\in[0,1]\times\Omega, \qquad \Omega=(0,2) \tag{4.1a}$$

$$u(0,x) \equiv 1, \tag{4.1b}$$

$$u(t,0) \equiv u(t,2)\equiv 0 \tag{4.1c}$$

which has the theoretical solution

$$u(t,x)=\sum_{n=1}^{\infty}\Big[1-(-1)^n\Big]\frac{2}{n\pi}\sin\Big(\frac{n\pi x}{2}\Big)\exp\Big(-\frac{n^2\pi^2 t}{4}\Big). \tag{4.2}$$

Theoretical considerations.

In the case of inconsistent initial/boundary data, derivatives of the solution u (for test problem (4.1) already u itself) are not well-defined on $\partial\Omega$ for $t = 0$; however, $u(t, x)$ typically smoothes down rapidly and belongs to $C^\infty(\bar{\Omega})$ for positive t. Under natural assumptions, a spatial discretization

$$\frac{du_h}{dt} = L_h\, u_h \tag{4.3a}$$

$$u_h(0) = \Delta_h u_0 \tag{4.3b}$$

of our problem has analogous smoothing properties, and a typical global error estimate reads

$$\|u_h(t) - \Delta_h u(t)\|_2 \leq \bar{C} h^2 t^{-1} \|u_0\|_2, \qquad t > 0 \tag{4.4}$$

(cf. for instance [4], [6], [3] for the precise details).

Let us now consider the *implicit Euler scheme* (2.3) applied to (4.3); for the following it is useful (but not necessary) that the reader is familiar with [1]. For a study of the full global error $U_{h,\nu} - \Delta_h u(t_\nu)$, it is reasonable here to consider the error $U_{h,\nu} - u_h(t_\nu)$ of the time discretization and the spatial discretization error $u_h(t_\nu) - \Delta_h u(t_\nu)$ separately. The estimate (4.4) shows that $u_h(t_\nu) - \Delta_h u(t_\nu)$ is only $O(h^2\tau^{-1})$ at the first time steps after the start but is damped down away from $t = 0$. Furthermore, the time discretization error of the implicit Euler scheme features a similar damping behavior: The estimate (2.9), which is nothing but a nonsmooth global error estimate for the Euler scheme applied to the homogeneous problem, shows that the order of convergence p must be expected to break down to $p = 0$, but only at the first time steps after the start.

The question is whether an asymptotic error expansion makes sense in this situation. It does, if we are able to identify a leading component in the time discretization error which is independent of τ. Of course, our expansion must suffer from the order reduction near $t = 0$; but again we may hope for damping, such that τ-extrapolation (i.e., elimination of the leading component) may again be successfully applicable away from $t = 0$.

Let us thus study a short expansion for the discretization error in time:

$$U_{h,\nu} - u_h(t_\nu) = \tau\, e_{h,1}(t_\nu) + \tilde{R}_{h,\nu}. \tag{4.5}$$

Analogously as in section 2, $e_{h,1}(t)$ ($e_{h,1}(0) = 0$) is a solution of

$$\frac{de_{h,1}}{dt} = L_h\, e_{h,1} + \frac{1}{2}\frac{d^2 u_h}{dt^2} = L_h\, e_{h,1} + \frac{1}{2} L_h^2 e^{tL_h} \Delta_h u_0 \tag{4.6}$$

hence,

$$e_{h,1}(t) = \frac{1}{2} t^{-1} (tL_h)^2 e^{tL_h} \Delta_h u_0 \tag{4.7}$$

(note that $(tL_h)^2 e^{tL_h}$ is uniformly bounded in t and h). Furthermore, $\tilde{R}_{h,\nu}$ ($\tilde{R}_{h,0} = 0$) is a solution of

$$\frac{1}{\tau}\left(\tilde{R}_{h,\nu} - \tilde{R}_{h,\nu-1}\right) = L_h \tilde{R}_{h,\nu} + \gamma_{h,\nu} \tag{4.8}$$

where the inhomogeneity $\gamma_{h,\nu}$ contains a factor τ^2 and depends on d^3u_h/dt^3 and $d^2e_{h,1}/dt^2$ (cf. [1]). Refraining from working out all the technical details here, we consider one typical term appearing in $\gamma_{h,\nu}$ which reads

$$\tau^2 L_h^3 e^{t_{\nu-1}L_h} I_{h,1} \Delta_h u_0 \tag{4.9}$$

where $I_{h,1} := (\tau L_h)^{-2}[I - (I - \tau L_h) e^{\tau L_h}]$ is bounded in norm independently of h. The component in $\tilde{R}_{h,\nu}$ corresponding to (4.9) reads $\tau^2 S_{h,\nu} \Delta_h u_0$ where

$$S_{h,\nu} := \tau \sum_{\ell=1}^{\nu} (I - \tau L_h)^{\ell-\nu-1} e^{t_{\ell-1}L_h} I_{h,1} L_h^3 \Delta_h u_0. \tag{4.10}$$

The linear operator $S_{h,\nu}$ is very similar to that one estimated in ([1], Lemma 4.2, eq. (4.25)), but with an additional factor $L_h = \tau^{-1}(\tau L_h)$. In fact, a look at the proof of Lemma 4.2 in [1] shows

$$S_{h,\nu} = \tau^{-2} \tau L_h \Big[(I - \tau L_h)^{-\nu} - e^{t_\nu L_h}\Big] \tag{4.11}$$

(cf. (2.9)), and the estimate presented there can easily be adapted, yielding

$$\|S_{h,\nu}\|_2 \le \frac{C}{t_\nu^2}, \qquad \nu \ge 1 \tag{4.12}$$

with a moderate-sized, h-independent constant C. This leads us to the desired bound for the component in $\tilde{R}_{h,\nu}$ corresponding to (4.9); the various other contributions can be estimated in an similar way on the basis of Lemma 4.2 in [1].[9]

As a result of all these considerations (cf. (4.4), (4.7), (4.12 ...)) we may formulate the following Theorem, which is valid under natural assumptions on the problem and its semi-discretization:

Theorem 3. *For $u_0 \in L_2(\Omega)$, the full global error of the implicit Euler scheme applied to the homogeneous problem admits an asymptotic expansion*

$$U_{h,\nu} - \Delta_h u(t_\nu) = \tau\, e_{h,1}(t_\nu) + R_{h,\nu} \tag{4.13}$$

where the function $e_{h,1}(t)$ is independent of τ and bounded in norm by

$$\|e_{h,1}(t)\|_2 \le \frac{C_1}{t} \|u_0\|_2, \qquad t > 0 \tag{4.14}$$

and where $R_{h,\nu}$ can be estimated by

$$\|R_{h,\nu}\|_2 \le \left(\frac{C_2}{t_\nu^2}\tau^2 + \frac{\bar{C}}{t_\nu} h^2\right) \|u_0\|_2, \qquad \nu \ge 1 \tag{4.15}$$

with certain τ- and h-independent, moderate-sized bounds C_1, C_2 and $\bar{C}$.

[9] The analysis in [1] applies to selfadjoint problems; see [2] for the nonselfadjoint case.

Extrapolation: Numerical examples.

Similarly as in the smooth case (section 3), the relevance of our theoretical considerations can be demonstrated by means of numerical experiments. Tables 4.1 and 4.2 display the L_2-norm of the full global error $U_{h,\nu} - \Delta_h u(t_\nu)$, for the extrapolated Euler scheme applied to the standard finite difference approximation of (4.1), at $t=0.1$ and $t = 1$, respectively. In contrast to Table 4.1, where the 'stagnation' of our discrete approximation is clearly visible (totally reduced order), global extrapolation performs successfully at $t=1$ (Table 4.2). Note that, at $t=1$, the (fixed) spatial discretization error for $h = 1/128$ is about $5 * 10^{-6}$; this error level is efficiently achieved by two steps of τ-extrapolation with relatively large values of τ.

||global error|| at t=0.1 h=1/128 Table 4.1

tau	Euler	1st EX	2nd EX
1/20	3.394E-02		
1/40	4.738E-02	6.325E-02	
1/80	5.611E-02	6.512E-02	6.576E-02

observed order

	-0.48	
	-0.24	-0.04

||global error|| at t=1.0 h=1/128 Table 4.2

GLOBAL EXTRAPOLATION

tau	Euler	1st EX	2nd EX
1/20	1.159E-02		
1/40	5.819E-03	4.959E-05	
1/80	2.918E-03	1.569E-05	4.388E-06

observed order

	0.99	
	1.00	1.66

Local τ-extrapolation again yields less accurate results in situations where the spatial error is not dominant.

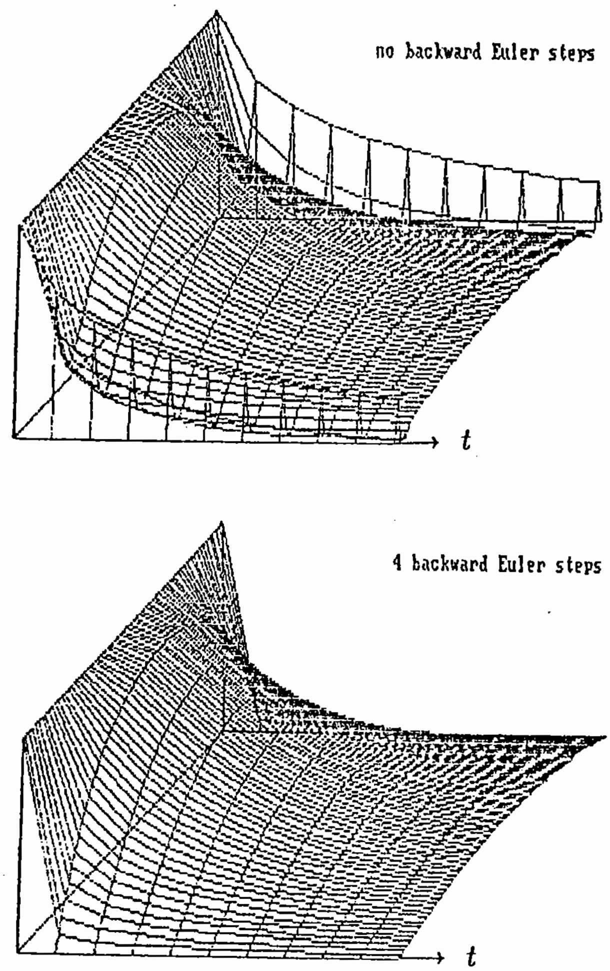

Figure 2: Crank-Nicolson approximations for example (4.1), $t \in [0, 1]$

Crank-Nicolson scheme and concluding remarks.

Due to its intrinsic lack of damping, the Crank-Nicolson (trapezoidal, midpoint) scheme applied to problem (4.1) suffers from stability drawbacks (Fig. 2, first part, displays a typical Crank-Nicolson approximation involving spurious modes near the boundary). Thus, also τ^2-extrapolation must be expected to be not very successful, and numerical experience shows that it does indeed not significantly improve the approximation quality.

A well-known remedy (cf. [10]) restoring satisfactory damping properties is to combine the Crank-Nicolson scheme with a certain number of backward Euler steps at the beginning (Fig. 2, second part, shows a Crank-Nicolson approximation based on four initial Euler steps). To our experience, however, such a modified scheme is neither suitable as a basis for extrapolation.

It is an open question whether the full conventional effiency of τ^2-extrapolation based on symmetric schemes can be achieved by appropriate algorithmic measures.

Rather, the extrapolated Euler scheme seems to be the superior method, especially in nonsmooth situations.

Further remarks and numerical examples concerning extrapolation applied to parabolic problems can e.g. be found in [8] and [5]. Note, however, that no satisfactory quantitative analysis is given in these papers (not even for the smooth case).

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