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Finite Element Solution of Diffusion Problems with Irregular Data

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Summary. Diffusion problems occuring in practice often involve irregularities in the initial or boundary data resulting in a local break-down of the solution's regularity. This may drastically reduce the accuracy of discretization schemes over the whole interval of integration, unless certain precautions are taken. The diagonal Padé schemes of order 2μ, combined with a standard finite element discretization, usually require an unnatural step size restriction in order to achieve even locally optimal accuracy. It is shown here that this restriction can be avoided by means of a sample damping procedure which preserves the order of the discretization and, in the case $\mu=1$, does not increase the costs.

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1. General Discussion

We consider the (linear) convection-diffusion equation

$$\begin{aligned} &\partial_t u + Au = f \quad \text{in } \Omega \times (0,\infty), \\ &A = -\operatorname{div}(\alpha \operatorname{grad}) + \vec{\beta} \cdot \operatorname{grad} + \gamma \end{aligned} \tag{1.1}$$

subject to the initial condition

$$u|_{t=0} = u^0 \quad \text{in } \Omega, \tag{1.2}$$

and to the boundary condition

$$u|_\Gamma = d, \quad \alpha \partial_n u + \delta u|_{\partial\Omega - \Gamma} = g \quad \text{on } (0,\infty). \tag{1.3}$$

Here, Ω is a bounded domain in R^N, $N=1,2$ or 3, with sufficiently regular boundary $\partial\Omega$ consisting of two separated components Γ and $\partial\Omega - \Gamma$. The coefficients α, γ, δ and $\vec{\beta} = (\beta_1, \dots, \beta_N)$ as well as the data f, g and d are smooth functions of $x \in \bar{\Omega}$ and $t \geqq 0$, up to a finite number of "jump times" at which they are discontinuous in time. We assume that $\alpha>0$ on $\bar{\Omega}$ and, for simplicity, that $\alpha, \vec{\beta}, \gamma$ and δ are constant in time between each two consecutive jump times. The initial data u^0 may be "rough", e.g., a discontinuous function of $x\in\Omega$ (or even a sum of Dirac-measures). In practice, the coefficients $\alpha, \vec{\beta}$ and γ may also depend on t, or even on the solution u itself; also (1.1) may be a system of differential equations. We shall comment on these more general cases below.

Under the foregoing assumptions, the initial-boundary value problem (1.1)-(1.3) has a unique solution u which is smooth for all times $t>0$ other than the jump times. At time $t=0$ and at a jump time t_* it exhibits a certain singular behavior as $t\downarrow 0$ and $t\downarrow t_*$, respectively, depending on how irregular the data are. Because of this local break down of the solution's regularity one has to expect at least a local loss of accuracy when one of the usual discretization methods is applied to the problem. However, in practice one often finds a dramatic reduction in accuracy over the whole interval of integration, i.e., the schemes do not always have an automatic "smoothing property". In the following we shall study this phenomenon for a family of discretizations of problem (1.1)–(1.3) by A-stable single-step schemes (Padé schemes), combined with various finite element Galerkin discretizations of the spatial variable. In particular, we shall propose a simple damping device for the diagonal Padé schemes which guarantees that the full order of accuracy is achieved away from the critical times.

Suppose that problem (1.1)–(1.3) has been discretized by using a finite element Galerkin method of order $r\geqq 2$. This results in a finite dimensional problem of the form

$$\partial_t u_h + A_h u_h = F_h, \quad t\in(0,\infty), \qquad u_h(0)=u_h^0, \tag{1.4}$$

where $u_h(t)$ is sought in a finite element space S_h (h characterizing the mesh widths). A_h is a discrete analogue of the differential operator A, and the force term F_h also contains the nonhomogeneous boundary data which has been built into the equation. Problem (1.4) may be written as an initial value problem for a linear system of ODE's which is usually highly stiff (stiffness ratio $\sim h^{-2}$). This restricts the practical choice of time discretization methods to socalled "A-stable" schemes which are numerically stable for any choice of the time step k independent of h.

Let the discrete times $t_n = nk$, $n\geqq 0$, be chosen such that all the jump times belong to this set. Among the A-stable schemes we consider the diagonal and subdiagonal Padé methods based on rational approximations of the exponential function. For solving a system of ODE's, $y'(t)=f(t,y(t))$, one may use implicit difference formulas of the form

$$y_n = y_{n-1} + k\sum_{i=1}^{m} k^{i-1}[\alpha_i f_{n-1}^{(i-1)} - \beta_i f_n^{(i-1)}], \tag{1.5}$$

where $f_n^{(j)}=(d/dt)^j f(t_n, y_n)$, and α_i, β_i are determined as coefficients of the numerator and the denominator of a Padé approximation of e^z with index (ν,μ), $0\leqq \nu,\mu\leqq m$:

$$R_{\nu\mu}(z)=\frac{P_{\nu\mu}(z)}{Q_{\nu\mu}(z)} = e^z + O(|z|^{\nu+\mu+1}), \quad \text{for } z\leqq 0, \tag{1.6}$$

($\alpha_i=0$ if $i>\nu$, $\beta_i=0$ if $i>\mu$); see [4] and [5]. The global discretization error of the difference formula (1.5) has the order $s=\nu+\mu$. For a fixed amount of computational work an optimum in order is achieved by the diagonal Padé formulas with $\nu=\mu$. However, the latter schemes are only A-stable, whereas those with $\nu<\mu$ are strongly A-stable. Since A-stable schemes do not always damp local errors in the computation (strongly A-stable schemes do), one has to expect that the diagonal Padé schemes propagate the high-frequency errors caused by the local irregularities of the data, unless the step size is appropriately restricted, $k\sim h^2$; see [14] and [11].

For practical purposes the following Padé approximations are of particular interest:

$R_{01}(z)=(1-z)^{-1}$: backward Euler scheme ($s=1$),
$R_{11}(z)=(1-\frac{1}{2}z)^{-1}(1+\frac{1}{2}z)$: Crank-Nicolson scheme ($s=2$),
$R_{12}(z)=(1-\frac{2}{3}z+\frac{1}{6}z^2)^{-1}(1+\frac{1}{3}z)$; ($s=3$),
$R_{22}(z)=(1-\frac{1}{2}z+\frac{1}{12}z^2)^{-1}(1+\frac{1}{2}z+\frac{1}{12}z^2)$: ($s=4$).

In using the difference formulas (1.5) for the linear system (1.4) one has to take $f(t,u_h(t))=F_h(t)-A_h u_h(t)$. For the cases $\nu=\mu=1$ or 2, the fully discrete approximations $U^n_{h,k}$ are determined in S_h by the following recurrences

$$\left(I+\frac{k}{2}A_h\right)U^n_{h,k}=\left(I-\frac{k}{2}A_h\right)U^{n-1}_{h,k}+\frac{k}{2}(F^n_h+F^{n-1}_h), \tag{1.7}$$

$$\left(I+\frac{k}{2}A_h+\frac{k^2}{12}A_h^2\right)U^n_{h,k}=\left(I-\frac{k}{2}A_h+\frac{k^2}{12}A_h^2\right)U^{n-1}_{h,k}+\frac{k}{2}(F^n_h+F^{n-1}_h)$$
$$+\frac{k^2}{12}(A_hF^n_h-F^n_{ht}-A_hF^{n-1}_h+F^{n-1}_{ht}), \tag{1.8}$$

where $F^n_h=F_n(t_n)$ and $F^n_{ht}=\partial_t F_h(t_n)$. These schemes are of order $s=2$ and $s=4$, respectively.

If all the data of problem (1.1)–(1.3) are regular, i.e. smooth and compatible to sufficiently high order, and if the spatial discretization is appropriate, then one may expect optimal order convergence of $U^n_{h,k}$ to $u(t_n)$ as $h,k\to 0$, uniformly on bounded intervals of time (see [2] and [9]),

$$\max_{0\leqq t_n\leqq T}\|u(t_n)-U^n_{h,k}\|=O(h^r+k^s), \tag{1.9}$$

where $r\geqq 2$ and $s\geqq 1$ are the orders of the spatial and the time discretization, respectively, and $\|\cdot\|=(\int_\Omega|\cdot|^2\,dx)^{1/2}$.

For rough data the global order of convergence may reduce even to $o(1)$, in the extreme case. The main results of this paper are summarized in the following smoothing device:

Suppose that the discrete initial value $U^0_{h,k}$ is chosen as the L^2-projection of u^0 onto the trial space S_h, and further, that at t_0 and at each of the jump times 2μ of the diagonal (μ,μ)-Padé steps are replaced by subdiagonal $(\mu-1,\mu)$-Padé steps.

Then the approximation $U^n_{h,k}$ is accurate to optimal order,

$$\|u(t_n)-U^n_{h,k}\|=O(h^r+k^s), \tag{1.10}$$

at all times t_n uniformly bounded away from t_0 and from the jump times.

The strongly A-stable $(\mu-1,\mu)$-Padé steps provide the necessary damping of high-frequency error components which would normally be propagated by the only A-stable (μ,μ)-Padé scheme. The global order $s=2\mu$ of the discretization is not affected, since only a fixed finite number of lower order steps needs to be carried out. We emphasize that in this case no restriction on the step size k in terms of the spatial mesh size h is needed.

For the autonomous problem (1.1)–(1.3) one usually carries out the time stepping procedure by computing once an $L-U$-decomposition of the matrix corresponding to the operator $Q_{\mu\mu}(-kA_h)$ which reduces the work in each time step to solving twice a triangular algebraic system by back-substitution. Generally the damping procedure proposed above will increase the total amount of work. However, in the case $\mu=1$ (Crank-Nicolson scheme) one may apply the damping steps (backward Euler steps) with step size $k/2$ resulting in the operator to be decomposed

$$Q_{01}\left(-\frac{k}{2}A_h\right)=I+\frac{k}{2}A_h=Q_{11}(-kA_h).$$

Consequently, in this case the damping procedure does not necessarily increase the computational costs; indeed it is equivalent to once computing the average

$$\bar{U}^1_{h,k}=\tfrac{1}{4}(U^0_{h,k}+2U^1_{h,k}+U^2_{k,h})$$

for the Crank-Nicolson solution. The latter smoothing procedure has already been proposed by Lindberg [7] in connection with extrapolation of the trapezoidal rule when applied to stiff ODE-systems.

Difference formulas similar to (1.7) and (1.8) may also be obtained by approximating the force term $F_h(t)$ by numerical integration formulas; see Brenner, Crouzeix and Thomée [2].

To date, a rigorous justification of the above damping advice has only been given in the case of a linear autonomous system represented by problem (1.1)–(1.3); see the analysis of the following section. In the linear non-autonomous case, $A=A(t)$, we have been able to prove a corresponding result for at least the Crank-Nicolson scheme ($\mu=1$) in [9]. The question whether this analysis can be extended to higher order Padé schemes may have a negative answer, since there are examples of third order one-step schemes which smooth only up to order two when applied to problem (1.1)–(1.3), with $\alpha=\alpha(t)$; see Sammon [12]. However, if the time dependence only occurs in lower terms, $\vec{\beta}=\vec{\beta}(t)$ or $\gamma=\gamma(t)$, one may also prove smoothing of higher order. In the nonlinear case the situation is even less satisfactory. Strongly nonlinear problems with $\alpha=\alpha(u)$ cannot be rigorously analyzed yet, particularly since it is not even sufficiently clear how the solution u behaves at times when the data are irregular. Only in the weakly nonlinear case, with $\vec{\beta}=\vec{\beta}(u)$, are there partial results: For the

Navier-Stokes problem we can show that the Crank-Nicolson scheme combined with two backward Euler steps is second order accurate even when the initial flow is not fully compatible with the given boundary condition; see [6; Part IV].

Suppose now that the discretization scheme for solving problem (1.1)-(1.3) has been set up accordingly to our smoothing device. The first step in analyzing its smoothing behavior is to reduce the question to the case of rough initial data combined with homogeneous force and boundary values. To this end, let t_m be any of the critical times at which the data are irregular, and let v^m be the (unique) solution of the boundary value problem

$$A v^m = f|_{t=t_m} \quad \text{in } \Omega, \tag{1.11}$$

$$v^m|_\Gamma = d|_{t=t_m}, \quad \alpha \partial_n v^m + \delta v^m|_{\partial\Omega-\Gamma} = g|_{t=t_m}. \tag{1.12}$$

Here, we assume without loss of generality that the operator A combined with the boundary conditions (1.12) is regular. By construction, the problem

$$\partial_t v + A v = f \quad \text{in } \Omega \times (t_m, t_*], \tag{1.13}$$

$$v|_{t=t_m} = v^m \quad \text{in } \Omega, \tag{1.14}$$

$$v|_\Gamma = d, \quad \alpha \partial_n v + \delta v|_{\partial\Omega-\Gamma} = g \quad \text{on } (t_m, t_*], \tag{1.15}$$

has smooth and to second order compatible data on $[t_m, t_*]$, where $t_* \in (t_m, \infty)$ is the jump time next to t_m, or $t_* = \infty$. Using in an analogous way higher powers of A one may construct initial values v^m such that the corresponding problem (1.13)-(1.15) has compatible data to any fixed order. Then, the difference $\tilde{u} = u - v$ satisfies the homogeneous equations

$$\partial_t \tilde{u} + A\tilde{u} = 0 \quad \text{in } \Omega \times (t_m, t_*], \tag{1.16}$$

$$\tilde{u}|_\Gamma = 0, \quad \alpha \partial_n \tilde{u} + \delta \tilde{u}|_{\delta\Omega-\Gamma} = 0 \quad \text{on } (t_m, t_*], \tag{1.17}$$

and the initial condition

$$\tilde{u}|_{t=t_m} = \tilde{u}^m \equiv u|_{t=t_m} - v^m \quad \text{in } \Omega. \tag{1.18}$$

In general, the initial value $\tilde{u}^m$ is not compatible with the other data.

Suppose that, in the case $t_m > 0$, the smoothing error estimate (1.10) is already known to hold on $(0, t_m]$, e.g., in particular, there holds

$$\|u(t_m) - U^m_{h,k}\| = O(h^r + k^s). \tag{1.19}$$

Let $V^n_{h,k} \in S_h$ be the discrete solution of problem (1.13)-(1.15) corresponding to the initial value $V^m_{h,k} = P_h v^m \in S_h$ (P_h being the L^2-projection onto S_h). Then, there holds the "smooth data" error estimate (see [10] and [2])

$$\sup_{t_m \leqq t_n \leqq t_*} \|v(t_n) - V^n_{h,k}\| = O(h^r + k^s). \tag{1.20}$$

The difference $\tilde{U}^n_{h,k} \equiv U^n_{h,k} - V^n_{h,k}$ satisfies initially $\tilde{U}^0_{h,k} = P_h \tilde{u}^0$ if $t_m = 0$, and

$$\|\tilde{u}(t_m) - \tilde{U}^m_{h,k}\| = O(h^r + k^s), \tag{1.21}$$

if $t_m > 0$. Hence, in order to justify our smoothing device, it remains to show that there holds

$$\|\tilde{u}(t_n) - \tilde{U}_{h,k}^n\| = O(h^r + k^s), \tag{1.22}$$

for times $t_n \in (t_m, t_*]$ uniformly bounded away from t_m. Clearly, without loss of generality we may take $t_m = 0$.

2. Error Analysis for the Homogeneous Problem

In the following we shall prove the smoothing error estimate (1.22) for the homogeneous problem

$$\partial_t u + Au = 0 \quad \text{in } \Omega \times (0, \infty), \tag{2.1}$$

$$u|_{t=0} = u^0 \quad \text{in } \Omega, \tag{2.2}$$

$$u|_\Gamma = 0, \quad \alpha \partial_n u + \delta u|_{\partial\Omega - \Gamma} = 0 \quad \text{on } (0, \infty), \tag{2.3}$$

where the operator A is as in (1.1), the assumptions on the coefficients being the same as in the previous section.

We shall use the standard notation $L^2(\Omega)$ for the space of all square-integrable functions on Ω with inner product $(v, w) = \int_\Omega vw\,dx$ and norm $\|v\| = (v, v)^{1/2}$. $H^m(\Omega)$, $m \in N$, is the m-th-order Sobolev space on Ω of all L^2-functions possessing generalized derivatives up to order m in $L^2(\Omega)$, provided with its natural norm

$$\|v\|_m \equiv \Big(\sum_{0 \le l \le m} \|\nabla^l v\|^2 \Big)^{1/2};$$

$H_\Gamma^1(\Omega)$ is the subspace of those functions in $H^1(\Omega)$ which vanish on Γ in the generalized sense. Since $\partial\Omega$ is smooth by assumption, the domain of definition of A,

$$D(A) = \{v \in H_\Gamma^1(\Omega),\ Av \in L^2(\Omega),\ \alpha \partial_n v + \delta v|_{\partial\Omega - \Gamma} = 0\}$$

is contained in $H^2(\Omega)$. Without loss of generality it is assumed that A is coercive. Then, for $p \in N$, the powers $A^{p/2}$ are well defined with domains of definition $D(A^{p/2}) \subset H^p(\Omega)$.

For functions $v, w \in H_\Gamma^1(\Omega)$ we introduce the bilinear form

$$a(v, w) = (\alpha \operatorname{grad} v, \operatorname{grad} w) + (\vec{\beta} \operatorname{grad} v, w) + (\gamma v, w) + [\delta v, w],$$

where $[\phi, \psi] = \int_{\partial\Omega - \Gamma} \phi\psi\,d\sigma$. Clearly, there holds

$$(Av, \phi) = a(v, \phi), \qquad v \in D(A),\ \phi \in H_\Gamma^1(\Omega). \tag{2.5}$$

Below, we shall use the symbol "c" for a generic positive constant which may vary with the context but is always independent of the solution u and of the discretization parameters h and k.

For any initial value $u^0 \in L^2(\Omega)$, problem (2.1)-(2.3) has a unique solution $u(t) \in H^1_\Gamma(\Omega)$ which is characterized by

$$(\partial_t u, \phi) + a(u, \phi) = 0 \qquad \forall \phi \in H^1_\Gamma(\Omega), \tag{2.6}$$

for $t>0$, and $\|u(t)-u^0\| \to 0$ as $t \downarrow 0$. This "weak" solution is smooth for all times $t>0$, $u(t) \in D(A^{p/2})$ for $p \in N$, and satisfies the a priori estimate

$$\|u(t)\|_{2p} + \|\partial_t^p u(t)\| \leqq c t^{q/2-p} \|u^0\|_q, \tag{2.7}$$

for $t>0$ and $0 \leqq q/2 \leqq p$, provided that $u^0 \in D(A^q)$; for a proof based on energy method see [8].

For discretizing problem (2.1)-(2.3) with respect to the spatial variable, we consider a finite element Galerkin method of order $r \geqq 2$; the trial spaces S_h are merely required to be (finite dimensional) subspaces of $L^2(\Omega)$, in order to allow for non-standard types of approximation. The orthogonal projection of $L^2(\Omega)$ onto S_h is denoted by P_h. The semidiscrete approximation $u_h(t) \in S_h$ to $u(t)$ is determined by the equation

$$(\partial_t u_h, \phi_h) + a_h(u_h, \phi_h) = 0 \qquad \forall \phi_h \in S_h, \ t>0, \tag{2.8}$$

where $a_h(\cdot,\cdot)$ is a proper extension of the bilinear form $a(\cdot,\cdot)$ to $S_h \times S_h$. The initial value $u_h(0) = u_h^0 \in S_h$ is an approximation to u^0 of order r, which will be specified below. The bilinear form $a_h(\cdot,\cdot)$ is assumed to be coercive on $S_h \times S_h$, i.e., $a_h(\phi_h, \phi_h) > 0$ for $\phi_h \in S_h - \{0\}$. Hence, the linear operator $A_h: S_h \to S_h$ determined by

$$a_h(v_h, \phi_h) = (A_h v_h, \phi_h), \qquad v_h, \phi_h \in S_h,$$

is regular. We assume that there holds

$$\|(A^{-1} - A_h^{-1} P_h) f\| \leqq c h^p \|f\|_{p-2}, \tag{2.9}$$

for $f \in H^{p-2}(\Omega)$, $2 \leqq p \leqq r$. This approximability condition is satisfied by the usual finite element schemes for solving elliptic boundary value problems; for examples see [3] and [13]. We further assume that the semidiscrete solution satisfies the a priori estimate

$$\|\partial_t^p u_h(t)\| \leqq c t^{-p} \|u_h^0\|, \qquad t>0, \tag{2.10}$$

for $0 \leqq p \leqq \max(r/2, s)$; this may be shown by arguments analogous to those used for proving the a priori estimate (2.7).

If, for instance, $u_h^0 = P_h u^0$, we have the "smooth data" convergence result

$$\sup_{t \geqq 0} \|(u-u_h)(t)\| \leqq c h^p \|u^0\|_p, \tag{2.11}$$

for $u^0 \in D(A^{p/2})$, $0 \leqq p \leqq r$; see [13] and [3].

For rough data, $u^0 \in L^2(\Omega)$, we shall prove the following smoothing result:

Theorem 1. *If $u^0 \in L^2(\Omega)$, then there holds*

$$\|(u-u_h)(t)\| \leqq c t^{-r/2} \{h^r \|u_h^0\| + \|u^0 - u_h^0\|_{-r}\}, \tag{2.12}$$

for $t>0$, *where*

$$\|v\|_{-r}=\sup\{(v,\phi),\ \phi\in D(A^{r/2}),\ \|\phi\|_r=1\}.$$

Proof. We employ the parabolic duality argument introduced in [8]. Let $T>0$ be arbitrarily fixed. For any $\phi\in L^2(\Omega)$, $\|\phi\|=1$, let $v(t)\in H^1_\Gamma(\Omega)$ and $v_h(t)\in S_h$ be the solutions of the "backward" equations

$$\partial_t v - A^* v = 0, \qquad T>t\geqq 0, \tag{2.13}$$

and

$$\partial_t v_h - A_h^* v_h = 0, \qquad T>t\geqq 0, \tag{2.14}$$

corresponding to the initial values $v(T)=\phi$ and $v_h(T)=P_h\phi$, respectively. Clearly, these problems are well-posed. A^* and A_h^* are the L^2-adjoints of A and A_h, respectively. Then, by construction there holds

$$\frac{d}{dt}(u,v)=(\partial_t u,v)+(u,\partial_t v)=-(Au,v)+(u,A^*v)=0, \tag{2.15}$$

and, correspondingly,

$$\frac{d}{dt}(u_h,v_h)=0, \quad \text{on } [0,T]. \tag{2.16}$$

Hence, setting $e\equiv u-u_h$ and $\eta\equiv v-v_h$, we find that

$$\begin{aligned}(e(T),\phi)&=(u(T),v(T))-(u_h(T),v_h(T))\\ &=\left(u\left(\frac{T}{2}\right),v\left(\frac{T}{2}\right)\right)-\left(u_h\left(\frac{T}{2}\right),v_h\left(\frac{T}{2}\right)\right)\\ &=\left(e\left(\frac{T}{2}\right),v\left(\frac{T}{2}\right)\right)-\left(e\left(\frac{T}{2}\right),\eta\left(\frac{T}{2}\right)\right)+\left(u\left(\frac{T}{2}\right),\eta\left(\frac{T}{2}\right)\right).\end{aligned} \tag{2.17}$$

We shall estimate the three terms on the right separately.

First, let $\tilde v_h(t)\in S_h$ be the solution of the backward equation (2.14) corresponding to initial time $\frac{T}{2}$ and initial value $\tilde v_h\left(\frac{T}{2}\right)=P_h v\left(\frac{T}{2}\right)$. Then, in view of (2.15) and (2.16) there holds

$$\begin{aligned}\left(e\left(\frac{T}{2}\right),v\left(\frac{T}{2}\right)\right)&=\left(u\left(\frac{T}{2}\right),v\left(\frac{T}{2}\right)\right)-\left(u_h\left(\frac{T}{2}\right),\tilde v_h\left(\frac{T}{2}\right)\right)\\ &=(u^0-u_h^0,v(0))+(u_h^0,v(0)-\tilde v_h(0)).\end{aligned}$$

Using the smoothing a priori estimate (2.7) for v and the smooth data error estimate (2.11) for $v-\tilde v_h$ (both with time reversed), we find that

$$\begin{aligned}\left|\left(e\left(\frac{T}{2}\right),v\left(\frac{T}{2}\right)\right)\right|&\leqq ct^{-r/2}\|\phi\|\,\|u^0-u_h^0\|_{-r}+h^r\|u_h^0\|\left\|v\left(\frac{T}{2}\right)\right\|\\ &\leqq ct^{-r/2}\{h^r\|u_h^0\|+\|u^0-u_h^0\|_{-r}\},\end{aligned} \tag{2.18}$$

and, if $u_h^0 = P_h u^0$,

$$\left|\left(e\left(\frac{T}{2}\right), v\left(\frac{T}{2}\right)\right)\right| \leqq c t^{-r/2} h^r \|u^0\|. \tag{2.19}$$

By an analogous argument we conclude also that

$$\left|\left(u\left(\frac{T}{2}\right), \eta\left(\frac{T}{2}\right)\right)\right| \leqq c t^{-r/2} h^r \|u^0\|. \tag{2.20}$$

Next, we take $\chi \in D(A)$ to be the solution of the equation $A\chi = A_h u_h\left(\frac{T}{2}\right)$ in Ω. In view of (2.9) and (2.10) there holds

$$\|\chi\|_2 \leqq c \left\|A_h u_h\left(\frac{T}{2}\right)\right\| \leqq c t^{-1} \|u_h^0\|, \tag{2.21}$$

and

$$\left\|\chi - u_h\left(\frac{T}{2}\right)\right\| = \left\|(A^{-1} - A_h^{-1} P_h) A_h u_h\left(\frac{T}{2}\right)\right\| \leqq c h^2 t^{-1} \|u_h^0\|. \tag{2.22}$$

Further, let $\tilde{u}(t) \in H_\Gamma^1(\Omega)$ and $\tilde{u}_h(t) \in S_h$ be the solutions of the problems (2.1) and (2.8) corresponding to initial time $\frac{T}{2}$ and initial values $\tilde{u}\left(\frac{T}{2}\right) = \chi$ and $\tilde{u}_h\left(\frac{T}{2}\right) = P_h \chi$, respectively. Again, from (2.15) and (2.16), it follows that

$$\begin{aligned}\left(u_h\left(\frac{T}{2}\right), \eta\left(\frac{T}{2}\right)\right) &= \left(u_h\left(\frac{T}{2}\right) - \chi, \eta\left(\frac{T}{2}\right)\right) + \left(\tilde{u}\left(\frac{T}{2}\right), v\left(\frac{T}{2}\right)\right) - \left(\tilde{u}_h\left(\frac{T}{2}\right), v_h\left(\frac{T}{2}\right)\right) \\ &= \left(u_h\left(\frac{T}{2}\right) - \chi, \eta\left(\frac{T}{2}\right)\right) + ((\tilde{u} - \tilde{u}_h)(T), \phi).\end{aligned} \tag{2.23}$$

This implies, in view of (2.21), (2.22), the smooth data error estimate (2.11) and the discrete a priori estimate (2.10), that

$$\begin{aligned}\left|\left(u_h\left(\frac{T}{2}\right), \eta\left(\frac{T}{2}\right)\right)\right| &\leqq \left\|\chi - u_h\left(\frac{T}{2}\right)\right\| \left\|\eta\left(\frac{T}{2}\right)\right\| + \|(\tilde{u} - \tilde{u}_h)(T)\| \\ &\leqq c h^2 \left\|A_h u_h\left(\frac{T}{2}\right)\right\| \\ &\leqq c t^{-1} h^2 \|u_h^0\|.\end{aligned} \tag{2.24}$$

Inserting the estimates (2.24), (2.18) and (2.19) into (2.17), we find that

$$\|e(T)\| \leqq c t^{-r/2} \|u^0 - u_h^0\|_{-r} + c t^{-1} h^2 \|u_h^0\|, \tag{2.25}$$

and, if $u_h^0 = P_h u^0$, that

$$\|e(T)\| \leqq c t^{-1} h^2 \|u^0\|. \tag{2.26}$$

This provides us with the starting point for an induction argument for proving the full order smoothing result (2.12).

Using the estimates (2.18) and (2.20) in (2.17), we obtain

$$\|e(T)\| \leqq \left\| e\left(\frac{T}{2}\right)\right\| \left\| \eta\left(\frac{T}{2}\right)\right\| \|v(T)\|^{-1} + ct^{-r/2}h^r\|u_h^0\| + \|u^0 - u_h^0\|_{-r}, \tag{2.27}$$

and, if $u_h^0 = P_h u^0$,

$$\|e(T)\| \leqq \left\| e\left(\frac{T}{2}\right)\right\| \left\| \eta\left(\frac{T}{2}\right)\right\| \|v(T)\|^{-1} + ct^{-r/2}h^r\|u^0\|. \tag{2.28}$$

Clearly, starting with the basic results (2.25) and (2.26) we can use (2.27) and (2.28) to prove the desired result (2.12) by a finite number of induction steps. This completes the proof.

We note that the L^2-projection $P_h u^0$ automatically satisfies

$$\|u^0 - P_h u^0\|_{-r} + h^r\|P_h u^0\| \leqq ch^r\|u^0\|. \tag{2.29}$$

Next, we consider the discretization of the semidiscrete problem (2.9) with respect to time. The fully discrete approximation $U_{h,k}^n \in S_h$ to $u(t_n)$ is determined by a diagonal (μ, μ)-Padé scheme of order $s = 2\mu$,

$$U_{h,k}^n = R_{\mu\mu}(-kA_h)\, U_{h,k}^{n-1}, \qquad n \geqq 2\mu + 1. \tag{2.30}$$

According to our smoothing device, the first 2μ values $U_{h,k}^n$, $n = 1, \dots, 2\mu$, are computed by $(\mu-1, \mu)$-Padé steps

$$U_{h,k}^n = R_{\mu-1,\mu}(-kA_h)\, U_{h,k}^{n-1}, \qquad U_{h,k}^0 = u_h^0. \tag{2.31}$$

Then, we have the following result.

Theorem 2. *If the first 2μ of the (μ, μ)-Padé steps are replaced by subdiagonal $(\mu - 1, \mu)$-Padé steps, then there holds*

$$\|u_h(t_n) - U_{h,k}^n\| \leqq ct_n^{-2\mu}k^{2\mu}\|u_h^0\|, \qquad n > 0. \tag{2.32}$$

Proof. In order to better illustrate the role of the damping steps (2.31), we first consider the self-adjoint case, $A_h = A_h^*$, where a simple proof of (2.32) can be given by spectral arguments. (Usually, the discrete operator A_h is self-adjoint if equation (2.1) does not contain a convection term, $\vec{\beta} = 0$.)

Let $\{\lambda_i, i = 1, \dots, N\}$, $N = \dim S_h$, be the eigenvalues (real and positive) of the operator A_h, and let $\{w_i, i = 1, \dots, N\} \subset S_h$ be a corresponding L^2-orthonormal system of eigenvectors. For $n \geqq 2\mu$, we have the expansions

$$u_h(t_n) = e^{-t_n A_h} u_h^0 = \sum_{i=1}^N \alpha_i e^{-\lambda_i t_n} w_i,$$

and

$$U_{h,k}^n = \sum_{i=1}^N \alpha_i R_{\mu-1,\mu}(-k\lambda_i)^{2\mu} R_{\mu\mu}(-k\lambda_i)^{n-2\mu} w_i,$$

where $\alpha_i = (u_h^0, w_i)$ are the Fourier coefficients of u_h^0. Then, by Parseval's identity,

$$\|u_h(t_n) - U_{h,k}^n\|^2 = \sum_{i=1}^{N} \alpha_i^2 \sigma_{i,n}^2, \tag{2.33}$$

where

$$\sigma_{i,n} = |e^{-nk\lambda_i} - R_{\mu-1,\mu}(-k\lambda_i)^{2\mu} R_{\mu\mu}(-k\lambda_i)^{n-2\mu}|.$$

Setting $\tau = k\lambda_i$, we can write

$$\begin{aligned}\sigma_{i,n} = \Bigg| & R_{\mu-1,\mu}(-\tau)^{2\mu}\{e^{-\tau} - R_{\mu\mu}(-\tau)\} \sum_{j=0}^{n-2\mu-1} e^{-j\tau} R_{\mu\mu}(-\tau)^{n-2\mu-1-j} \\ & + e^{-(n-2\mu)\tau}\{e^{-\tau} - R_{\mu-1,\mu}(-\tau)\} \sum_{j=0}^{2\mu-1} e^{-j\tau} R_{\mu-1,\mu}(-\tau)^{2\mu-1-j}\Bigg|.\end{aligned}$$

To estimate $\sigma_{i,n}$, we note that, for $\tau > 0$,

$$|e^{-\tau} - R_{\mu\mu}(-\tau)| \leqq c\tau^{2\mu+1}, \qquad |e^{-\tau} - R_{\mu-1,\mu}(-\tau)| \leqq c\tau^{2\mu}.$$

Further, there holds

$$\begin{gathered}|R_{\mu-1,\mu}(-\tau)| \leqq c \max(1, \tau^{-1}), \qquad \tau > 0, \\ |R_{\mu\mu}(-\tau)| \leqq ce^{-\delta\tau}, \ 0 < \tau \leqq 1, \qquad |R_{\mu\mu}(-\tau)| \leqq ce^{-\delta/\tau}, \ 1 < \tau < \infty.\end{gathered}$$

with some constant $\delta > 0$; this may be verified by using the particular form of the Padé approximations of $e^{-\tau}$.

Using the foregoing estimates we conclude that, for $\tau \leqq 1$,

$$\begin{aligned}\sigma_{i,n} &\leqq c\left\{\tau^{2\mu+1} e^{-\delta n\tau} \frac{1 - e^{-\delta(n-2\mu)\tau}}{1 - e^{-\delta\tau}} + e^{-(n-2\mu)\tau}\tau^{2\mu}\right\} \\ &\leqq c\{n\tau^{2\mu+1} e^{-\delta n\tau} + e^{-n\tau}\tau^{2\mu}\} \leqq cn^{-2\mu}.\end{aligned} \tag{2.34}$$

(Notice that $(1 - e^{-mx})(1 - e^{-x})^{-1} \leqq cm$, for $x > 0$ and $m \in N$.)

For $\tau > 1$, it follows directly from the definition of $\sigma_{i,n}$ that

$$\sigma_{i,n} \leqq c\{e^{-n\tau} + \tau^{-2\mu} e^{-\delta(n-2\mu)/\tau}\} \leqq cn^{-2\mu}. \tag{2.35}$$

Using now (2.34) and (2.35) in (2.33), we obtain the desired result

$$\|u_h(t_n) - U_{h,k}^n\|^2 \leqq cn^{-4\mu} \sum_{i=1}^{N} \alpha_i^2 = c\left(\frac{k}{t_n}\right)^{4\mu} \|u_h^0\|^2.$$

If the operator A_h is not self-adjoint spectral arguments do not apply. For this case we use the energy method combined with a time discrete analogue of the parabolic duality argument already employed in the proof of Theorem 1. For brevity, we only sketch the main steps leading to the smoothing result (2.32).

First, we state the smooth data error estimate

$$\sup_{0 \leqq t_m < \infty} \|u_h(t_n) - U_{h,k}^n\| \leqq c k^{2\mu} B_{2\mu}^0, \tag{2.36}$$

where

$$B_{2\mu}^0 = \sum_{j=0}^{2\mu} \|\partial_t^j u_h(0)\|;$$

arguments for proving this may be found in [9] and in [8]. A crucial assumption in what follows is that we already know a low order smoothing error estimate of the form

$$\|u_h(t_n) - U_{h,k}^n\| \leqq c t_n^{-1} k \|u_h^0\|, \quad t_n > 0, \tag{2.37}$$

to hold, provided that at least one damping $(\mu-1, \mu)$-Padé step is carried out at time t_0. Such an estimate has been shown in [9] for the Crank-Nicolson scheme (applied to the general nonautonomous problem) under the stronger assumption that *two* damping steps are required; in the autonomous case, the sharp result may be proven by energy method following the line of argument used in the proofs of Lemmas 3.1 and 3.3 in [10].

Let $t_n \geqq 2\mu$ be arbitrarily fixed. Since the operators $R_{\mu\mu}(-kA_h)$ and $R_{\mu-1,\mu}(-kA_h)$ commute, the fully discrete solution $U_{h,k}^n$ is invariant with respect to shifting the damping steps (2.31) within the discrete set of times $0 \leqq t_m < t_n$. Thus, we may assume that the 2μ damping steps are carried out at times $t_0, \ldots, t_{\mu-1}$ and $t_{n-\mu}, \ldots, t_{n-1}$. From the proof of Theorem 1 we recall the notation $v_h(t)$ for the solution of the "backward" semidiscrete problem (2.14), corresponding to an arbitrarily fixed initial value $\phi_h \in S_h$. Let $V_{h,k}^m \in S_h$ be the corresponding backward fully discrete solution defined by $V_{h,k}^n = \phi_h$ and

$$V_{h,k}^{m-1} = R_{\nu\mu}(-kA_h) V_{h,k}^m, \qquad n \geqq m \geqq 1, \tag{2.38}$$

where $\nu = \mu$ for $n - \mu \geqq m \geqq \mu + 1$, and $\nu = \mu - 1$ for $n \geqq m \geqq n - \mu + 1$ and $\mu \geqq m \geqq 1$. By construction, there holds

$$\begin{aligned}(U_{h,k}^m, V_{h,k}^m) &= (R_{\nu\mu}(-kA_h) U_{h,k}^{m-1}, V_{h,k}^m) \\ &= (U_{h,k}^{m-1}, R_{\nu\mu}(-kA_h^*) V_{h,k}^m) = (U_{h,k}^{m-1}, V_{h,k}^{m-1}),\end{aligned} \tag{2.39}$$

for $n \geqq m \geqq 1$. We set $u_h^m = u_h(t_m)$, $E^m = u_h^m - U_{h,k}^m$, and correspondingly, $v_h^m = v_h(t_m)$, $H^m = v_h^m - V_{h,k}^m$. Then, the relations (2.16) and (2.39) imply that

$$\begin{aligned}(E^n, \phi_h) &= (u_h^n, v_h^n) - (U_{h,k}^n, V_{h,k}^n) \\ &= (u_h^{[n/2]}, v_h^{[n/2]}) - (U_{h,k}^{[n/2]}, V_{h,k}^{[n/2]}) \\ &= (E^{[n/2]}, v_h^{[n/2]}) - (E^{[n/2]}, H^{[n/2]}) + (u_h^{[n/2]}, H^{[n/2]}),\end{aligned} \tag{2.40}$$

where for $p \in R_+$, $[p]$ denotes the largest integer less or equal p. Next, let $\tilde{U}_{h,k}^m \in S_h$ be determined by equation (2.38) starting at time $t_{[n/2]}$ with initial value $\tilde{U}_{h,k}^{[n/2]} = u_h^{[n/2]}$. In view of (2.16) and (2.39), there holds

$$\begin{aligned}(u_h^{[n/2]}, H^{[n/2]}) &= (u_h^{[n/2]}, v_h^{[n/2]}) - (\tilde{U}_{h,k}^{[n/2]}, V_{h,k}^{[n/2]}) \\ &= (u_h^n - \tilde{U}_{h,k}^n, \phi_h).\end{aligned}$$

Consequently, by the smooth data error estimate (2.36) and the smoothing a priori estimate (2.10),

$$(u_h^n, H^n) \leqq c t_n^{-2\mu} k^{2\mu} \|u_h^0\| \, \|\phi_h\|. \tag{2.41}$$

In an analogous way one concludes that

$$(E^n, v_h^n) \leqq c t_n^{-2\mu} k^{2\mu} \|u_h^0\| \, \|\phi_h\|. \tag{2.42}$$

Using (2.42) and (2.41) in (2.40) leads us to

$$(E^n, \phi_h) \leqq c t_n^{-2\mu} k^{2\mu} \|u_h^0\| \, \|\phi_h\| + \|E^{[n/2]}\| \, \|H^{[n/2]}\|. \tag{2.43}$$

We now apply the basic smoothing error estimate (2.37) to $E^{[n/2]}$ and $H^{[n/2]}$ (for the latter with time reversed) and set $\phi_h = E^n$ in (2.43), to obtain

$$\|E^n\| \leqq c t_n^{-2} k^2 \|u_h^0\|. \tag{2.44}$$

Clearly, using the same type of argument repeatedly for $E^{[n/2]}$ and $H^{[n/2]}$, we can successively improve the result (2.44) up to the desired order $O(t_n^{-2\mu} k^{2\mu})$. This requires exactly 2μ damping steps; the details are omitted.

3. Applications

We discuss three problems to which our smoothing device may be applied; for two of them we also present some numerical results.

1) Diffusion of Carbon Dioxide Through a Membrane

A solution of carbon dioxide in water is pumped through a membrane tube which is surrounded by a glass cylinder. There is a steady flow of nitrogen through the region between the membrane and the glass wall which takes up the carbon dioxide penetrating through the membrane. This permits us to consider the diffusion process as being stationary in time. Using cylinder coordinates (r, z), r being the radial distance from the cylinder axis and z the axial coordinate starting with $z=0$ at the inlet, the concentration of the carbon dioxide, $c = c(r, z)$, is described by the *diffusion equation*

$$w \partial_z c - \frac{1}{r} \partial_r (D r \partial_r c) = 0, \quad 0 < r < 1, \ z > 0, \tag{3.1}$$

subject to the initial condition

$$c(r, 0) = \begin{cases} 1, & 0 < r < R \\ 0, & R < r < 1, \end{cases} \tag{3.2}$$

where $R = .2$ is the radius of the membrane tube. The boundary conditions are of Neumann type,

$$\partial_r c(0, z) = \partial_r c(1, z) = 0, \qquad z > 0. \tag{3.3}$$

The quantity to be computed is the carbon dioxide concentration at the outlet, $c(r, 100)$.

In this problem we are confronted with a discontinuity of the initial data and, hence, have to expect the gradient $\partial_r c$ to have a singularity at $z=0$. Further complications arise from the discontinuity of the diffusion coefficient,

$$D(r)=\begin{cases} 1.96\cdot 10^{-4}, & 0<r<R \\ 0.14, & R<r<1, \end{cases}$$

and from the fact that the coefficient $w(r)$ (determined by the velocity of the water and nitrogen flows) degenerates at the boundaries,

$$w(r)=\begin{cases} 2w_1\{1-(r/R)^2\}, & 0<r<R \\ 2w_2\{1-r-(1-R^2)\ln r/\ln R\}\{1+R^2+(1-R^2)/\ln R\}^{-1}, & R<r<1, \end{cases}$$

where $w_1=2.5/(\pi R^2)$, $w_2=2.77/(\pi(1-R^2))$.

The discontinuity of $D(r)$ does not affect the accuracy of the discretization as long as $r=R$ is taken as one of the spatial mesh points. Also, our numerical experiment has shown that the degeneration of the coefficient $w(r)$ at $r=R$ and $r=1$ has no significant influence on the global behavior of the scheme. Although, our error analysis of § 2 does not quite cover this complicated case, the damping advice proved to be of some value. For discretizing problem (3.1)–(3.3) we used the finite element Galerkin method, the trial functions being piecewise linear in r, combined with the Crank-Nicolson scheme. Following the damping advice, the discrete starting value $C^0_{h,k}$ has been taken as the L^2-projection of $c(\cdot, 0)$ onto the trial space and two backward Euler steps have been carried out at the beginning of the time stepping process. However, it turned out that in this problem due to the extrem change of the diffusion constant at $r=R$, only four backward Euler steps provided sufficient damping. The outflow concentration, $c(r, 100)$, has been calculated using the fixed spatial mesh size $h=1/300$ and the three time steps $k=10$, 5, 2.5. This allowed us in the usual way to detect the asymptotic rate of convergence for the time discretization.

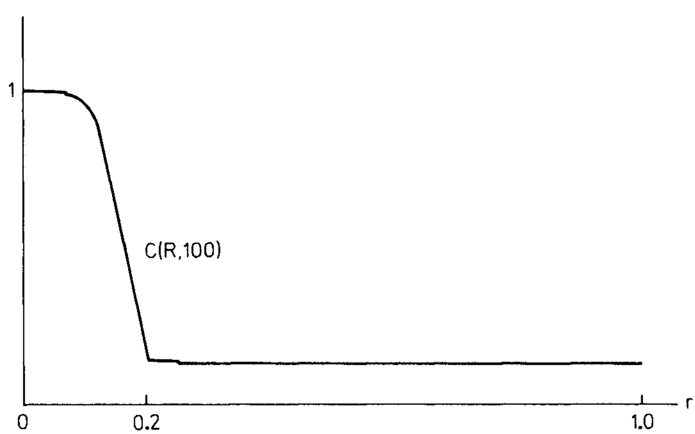

Fig. 1. Outflow concentration $c(r, 100)$

The figures show the concentration profile at the outlet as obtained by the C.-N. scheme with four b.E. damping steps (Fig. 1) and the asymptotic rates of convergence for the C.-N. scheme wothout damping, for the C.-N. scheme with four b.E. damping steps and for the b.E. scheme (Fig. 2).

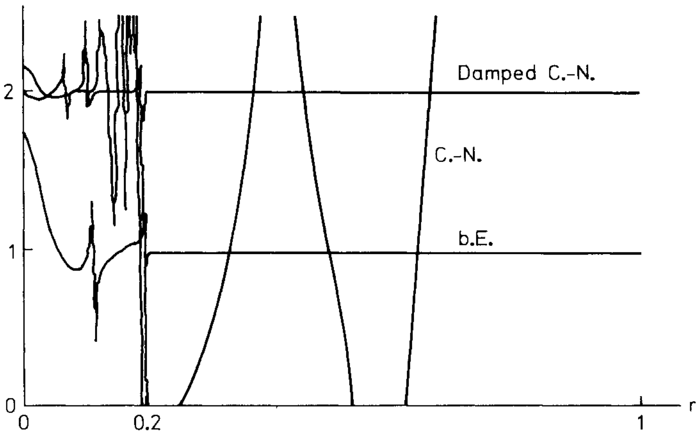

Fig. 2. Rates of convergence

2) Cooling of a Heated Glass Cylinder

A heated glass cylinder is subjected to cooling by an air blast where the intensity of the air stream is varied discontinuously in time. Using again cylinder coordinates (r, z), and assuming the cylinder to have infinite length in z-direction, the temperature distribution $T = T(r, t)$ is described by the *heat equation*

$$\partial_t T - \frac{a}{r}\, \partial_r (r \partial_r T) = 0, \quad 0 < r < R, \ t > 0, \tag{3.4}$$

subject to the initial condition

$$T(r, 0) = T_0, \quad 0 < r < R, \tag{3.5}$$

and to the boundary condition

$$\partial_r T(0, t) = 0, \quad a \partial_r T(R, t) = b \{T_\infty - T(R, t)\}, \quad t > 0. \tag{3.6}$$

We consider the case when the intensity of the cooling is piecewise constant in time,

$$b(t) = m b_0, \quad m \Delta t \leqq t < (m+1) \Delta t, \quad m \geqq 0.$$

The parameters are chosen as follows:

$$R = 1, \quad \Delta t = 5, \quad a = 4.3 \cdot 10^{-3}, \quad b_0 = 6.2 \cdot 10^{-3}, \quad T_0 = 850, \quad T_\infty = 20.$$

At each of the critical times, $t=0, 5, 10, \ldots$, we have to expect a singularity of $\partial_t T$ and $\partial_r^2 T$.

For discretizing problem (3.4)–(3.6) we used again the finite Element Galerkin method, the trial functions being piecewise linear in r, and the Crank-Nicolson scheme. The spatial mesh size was $h=1/100$, and the time steps were $k=1/2$, $1/4$, $1/8$. Following the damping advice, two backward Euler steps have been carried out after each of the critical times. The following pictures show the temperature distribution at time $t=20$, i.e., after three jumps of $b(t)$, (Fig. 3) and the asymptotic rates of convergence found for the C.-N. scheme without damping, for the C.-N. scheme with two b.E. damping steps and for the b.E. scheme (Fig. 4).

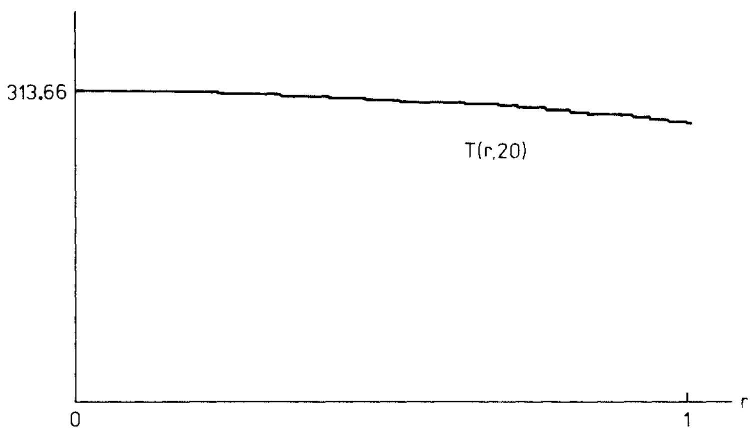

Fig. 3. Temperature distribution $T(r, 20)$

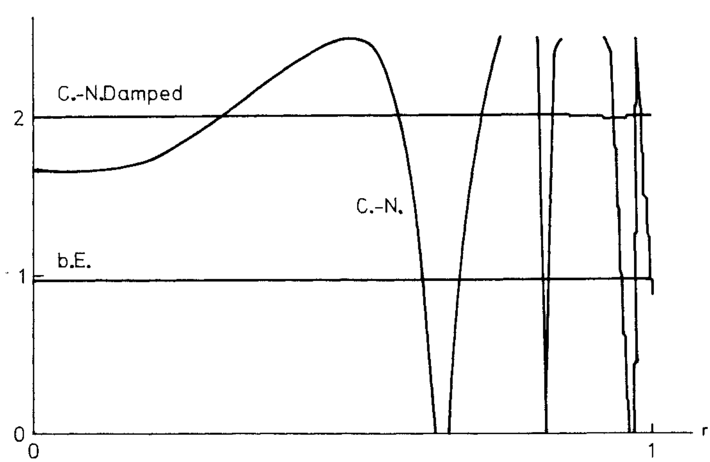

Fig. 4. Rates of convergence

3) Fluid Flow in a Spherical Gap

Fluid flow between two rotating spheres (or cylinders), the Taylor-problem, is one of the best studied model problems in fluid mechanics; for experimental and numerical results see Bartels [1] and the literature cited there. We consider here the situation when the fluid's motion between two concentric spheres is driven by a constant accelleration $\omega > 0$ of the inner sphere. The velocity vector $\vec{v} = \vec{v}(x, t)$ and the scalar pressure $p = p(x, t)$ of the fluid (assumed to be viscous and incompressible, as usual) are determined by the *Navier-Stokes equations*

$$\partial_t \vec{v} + \vec{v} \cdot \operatorname{grad} \vec{v} = \nu \Delta \vec{v} - \operatorname{grad} p, \quad (x, t) \in \Omega \times (0, \infty), \tag{3.7}$$

subject to the incompressibility condition, $\operatorname{div} \vec{v} = 0$, to the initial condition

$$\vec{v}(x, 0) = 0, \quad x \in \Omega, \tag{3.8}$$

and to the boundary condition

$$\vec{v}|_{r=r_a} = 0, \quad \begin{bmatrix} \vec{v} \cdot \vec{n} \\ \vec{v} \cdot \vec{t}_\phi \\ \vec{v} \cdot \vec{t}_\eta \end{bmatrix}\Bigg|_{r=r_i} = \begin{bmatrix} 0 \\ 0 \\ r_i \cos(\phi)\, \omega t \end{bmatrix}. \tag{3.9}$$

Here, r_a and r_i are the radii of the outer and the inner sphere, respectively, and (r, ϕ, η) are the usual spherical coordinates with direction unit vectors denoted by $\vec{n}$, $\vec{t}_\phi$ and $\vec{t}_\eta$.

For solving this problem numerically, one may use a second order finite element or finite difference discretization for the spatial variables (taking into account spatial symmetry) and the Crank-Nicolson scheme in time. Alternatively, the ADI-method could be used which reduces the work to solving two tridiagonal systems per time step. For both methods second order accuracy requires, roughly spoken, the second time and spatial derivatives, $\partial_t^2 \vec{v}$ and $\Delta \vec{v}$, to remain bounded for all time $t \downarrow 0$. However, in the present situation the solution has only a reduced regularity at $t = 0$, due to a non-compatibility of the initial and the driving boundary data. This is easily seen as follows. Suppose that $\partial_t \vec{v}$, $\Delta \vec{v}$ and $\operatorname{grad} p$ are continuous functions of $x \in \bar{\Omega}$ for $t \downarrow 0$. Then, letting $t \downarrow 0$ in (3.7) and observing $\vec{v}|_{t=0} = 0$, we find that

$$\partial_t \vec{v}|_{t=0} = -\operatorname{grad} p|_{t=0}, \quad x \in \Omega,$$

and, consequently, setting $p^0 = p|_{t=0}$,

$$\partial_n p^0|_{\partial\Omega} = 0, \qquad \partial_\eta p^0|_{r=r_i} = -r_i \cos(\phi)\, \omega.$$

On the other hand, multiplying (3.7) through by $\operatorname{grad} \phi$ and then letting $t \downarrow 0$, we conclude that

$$\int_\Omega \operatorname{grad} p^0 \cdot \operatorname{grad} \phi \, dx = 0$$

holds for every "test function" ϕ. This shows that p^0 is a harmonic function on Ω satisfying $\partial_n p^0|_{\partial\Omega}=0$, and hence, necessarily $p^0=\text{const.}$ on $\bar{\Omega}$. But this contradicts

$$\partial_n p^0|_{r=r_i} = -r_i \cos(\phi)\,\omega \neq 0,$$

so that even $\partial_t \vec{v}$ cannot remain bounded as $t\downarrow 0$ as a continuous function in $x\in\bar{\Omega}$; for a more rigorous analysis of this phenomenon see [6; Part I]. It should be noted that this loss of regularity as $t\downarrow 0$ also occurs for the (linear) Stokes equation when combined with the conditions (3.8) and (3.9).

In view of the foregoing, the Crank-Nicolson scheme cannot be expected to show more than first order accuracy unless some precautions are taken. Although, the analysis of this paper is restricted to linear problems, our smoothing device also applies to the weakly nonlinear problem (3.7)–(3.9), as will be proven in [6; Parts III and IV]. For times $t>0$, the full second order accuracy of the Crank-Nicolson scheme can be achieved by starting the computation with two backward Euler steps; for this, no restriction on the time step k in terms of the spatial mesh size h is needed.

4. Conclusion

It has been shown that high order time discretization schemes based on diagonal Padé formulas can successfully be used in solving linear convection-diffusion problems even with irregular initial or boundary data. Usually the high frequency error components incited by local singularities are propagated in time spoiling the global order of accuracy. As an example, the order of the standard Crank-Nicolson scheme may be reduced to zero in the case of rough initial data. This pollution effect can be suppressed by providing additional damping, here, merely by starting the computation with two backward Euler steps. The theoretical analysis and the numerical tests show that this procedure yields the full second order accuracy away from the singularities and does not increase the computational costs.

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