

Analysis of Smoothing Operators in the Solution of Partial Differential Equations by Explicit Difference Schemes

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A smoothing technique for the "preconditioning" of the right-hand side of semi-discrete partial differential equations is analysed. For a parabolic and a hyperbolic model problem optimal smoothing matrices are constructed which result in a substantial amplification of the maximal stable integration step of arbitrary explicit time integrators when applied to the smoothed problem. This smoothing procedure is illustrated by integrating both linear and nonlinear parabolic and hyperbolic problems. The results show that the stability behaviour is comparable with that of the Crank-Nicholson method; furthermore, if the problem belongs to the problem class in which the time derivative of the solution is a smooth function of the space variables, then the accuracy is also comparable with that of the Crank-Nicholson method.

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1. INTRODUCTION

In a number of papers (cf. e.g., [2] and [4]), it has been observed that many initial-boundary value problems for partial differential equations of the form

$$\frac{\partial \mathbf{u}}{\partial t}(t, \mathbf{x}) = D(t, \mathbf{x}, \mathbf{u}(t, \mathbf{x})) \quad (1.1)$$

possess the property that the right-hand side $D(t, \mathbf{x}, \mathbf{u})$ is a smooth function of the space variable \mathbf{x} if the exact solution of the initial-value problem is substituted, even when the exact solution has large space derivatives. Here, D may be a (nonlinear) differential operator of parabolic or hyperbolic type.

The situation described above arises in cases where the solution of the initial-boundary value problem tends to a steady state solution:

$$\mathbf{u}(t, \mathbf{x}) \rightarrow \mathbf{r}(\mathbf{x}) + \mathbf{s}(t, \mathbf{x}) \quad \text{as } t \rightarrow \infty, \quad (1.2)$$

where $\mathbf{r}(\mathbf{x})$ is a rapidly varying function of \mathbf{x} and $\mathbf{s}(t, \mathbf{x})$ is a smooth function of (t, \mathbf{x}) . Evidently,

$$D(t, \mathbf{x}, \mathbf{r}(\mathbf{x}) + \mathbf{s}(t, \mathbf{x})) \rightarrow \frac{\partial \mathbf{s}}{\partial t}(t, \mathbf{x}),$$

so that the right-hand side becomes a smooth function of \mathbf{x} as $t \rightarrow \infty$ (see the examples in Section 4).

For such problems it was proposed in, e.g., [2] and [4] to smooth the right-hand side of the equation (1.1) with respect to \mathbf{x} , before applying a numerical integration method. The effect of smoothing the right-hand side of (1.1) becomes apparent when the space variable \mathbf{x} and the differential operator D in (1.1) are discretized: the resulting system of ordinary differential equations is *better conditioned* in the sense that the spectral radius of the Jacobian matrix of this system reduces considerably in magnitude by the smoothing process. It is well known that the usually large spectral radius of semi-

discrete partial differential equations makes *explicit* integration methods unattractive for solving these systems, because of the rather restrictive stability condition. However, if smoothing reduces the spectral radius sufficiently in magnitude, then explicit time integration methods become of interest.

The price we have to pay for the "preconditioning" of the system of semi-discrete equations, is a possible drop in accuracy of the space discretization. To make this more clear, we consider the quasi linear equation

$$\frac{\partial \mathbf{u}}{\partial t}(t, \mathbf{x}) = A(\mathbf{u}(t, \mathbf{x}))L\mathbf{u}(t, \mathbf{x}) + \mathbf{g}(t, \mathbf{x}), \quad (1.3)$$

where L is a linear differential operator with respect to \mathbf{x} , and A and \mathbf{g} are given functions; let A_Δ and L_Δ represent discretizations of A and L with Δ characterizing the accuracy of the discretization, and let S_Δ denote a (linear) smoothing operator. For example, in one space variable x , we may think of

$$L = \frac{\partial}{\partial x}, \quad L_\Delta \mathbf{u}(t, x) = \frac{1}{2\Delta}(E_\Delta - E_\Delta^{-1})\mathbf{u}(t, x), \quad S_\Delta \mathbf{u}(t, x) = \frac{1}{2}(E_\Delta + E_\Delta^{-1})\mathbf{u}(t, x),$$

where E_Δ is the forward shift operator defined by $E_\Delta \mathbf{u}(t, x) := \mathbf{u}(t, x + \Delta)$. Instead of solving (1.3), we try to solve the smoothed, semidiscrete equation

$$\frac{\partial \mathbf{u}}{\partial t}(t, \mathbf{x}) = S_\Delta A_\Delta(\mathbf{u}(t, \mathbf{x}))L_\Delta \mathbf{u}(t, \mathbf{x}) + S_\Delta \mathbf{g}(t, \mathbf{x}). \quad (1.4)$$

Let $\mathbf{v}(t, \mathbf{x})$ and $\mathbf{w}(t, \mathbf{x})$ denote the solutions of the initial-boundary value problem for the equations (1.3) and (1.4), respectively. Then, it is easily verified that the difference $\mathbf{v} - \mathbf{w}$ satisfies the equation

$$\begin{aligned} \frac{\partial}{\partial t}(\mathbf{v} - \mathbf{w}) &= S_\Delta A_\Delta(\mathbf{w})L_\Delta(\mathbf{v} - \mathbf{w}) + S_\Delta[A(\mathbf{v})L - A_\Delta(\mathbf{w})L_\Delta]\mathbf{v} \\ &+ [I - S_\Delta][A(\mathbf{v})L\mathbf{v} + \mathbf{g}]. \end{aligned} \quad (1.5)$$

This "error equation" shows the effect of the space discretization and of the smoothing operator on the accuracy by which \mathbf{w} approximates \mathbf{v} . The second term in the right-hand side of (1.5) represents the (smoothed) *space discretization error*, whereas the last term represents the *smoothing error*. Evidently, the smoothing error vanishes if $S_\Delta = I$ (no smoothing), it is small if $A(\mathbf{v})L\mathbf{v} + \mathbf{g}$ is a smooth function of \mathbf{x} , and it hardly affects the accuracy of \mathbf{w} if $A(\mathbf{v})L\mathbf{v} + \mathbf{g}$ is much smoother in \mathbf{x} than \mathbf{v} .

Thus, we expect that the introduction of smoothing operators into the right-hand side of the partial differential equation (1.1) will not severely decrease the accuracy provided that the exact solution of (1.1) varies much more rapidly with \mathbf{x} than its time derivative does.

In [4] a few smoothing operators were tested and shown to have the expected effect. In this paper, we analyse smoothing operators more systematically, and we derive a family of optimal operators of second-order for a parabolic and a hyperbolic model problem. In addition, a family of fourth-order smoothing operators are constructed which are not optimal, but still result in a considerable reduction of the spectral radius of the Jacobian matrix.

The various smoothing operators are tested by integrating a few initial-value problems of parabolic and hyperbolic type, both linear and nonlinear. The results obtained clearly show that the two-stage *explicit* Runge-Kutta time integrators used in our experiments, when combined with a suitable smoothing operator, exhibit a stability behaviour which is comparable with that of the (*implicit*) Crank-Nicholson method, while the accuracy is hardly lower. Since a *smoothed* Runge-Kutta step is "cheaper" than a Crank-Nicholson step, particularly in the case of *nonlinear* problems, we conclude that, for the class of problems described above, explicit Runge-Kutta methods equipped with the right smoothing operators are preferable to the Crank-Nicholson method.

2. SMOOTHING OPERATORS

By restricting the semi-discrete (partial) differential equation (1.4) to a grid Ω_Δ in the x -space, we are led to a system of ordinary differential equations (method of lines). This system will be denoted by

$$\frac{d\mathbf{y}(t)}{dt} = S \mathbf{f}(t, \mathbf{y}(t)), \quad t \geq t_0, \quad (2.1)$$

where the matrix S corresponds to the smoothing operator S_Δ introduced in (1.4). More generally, by smoothing the right-hand side of (1.1) and by discretizing x and D , we will always obtain a system of the form (2.1).

2.1. Relaxing the stability condition by smoothing

If the system (2.1) is integrated by an *explicit* time integrator we are faced with a stability condition on the time step Δt of the form

$$\Delta t \leq \frac{\beta}{\rho(SJ)}, \quad J := \frac{\partial \mathbf{f}}{\partial \mathbf{y}}(t, \mathbf{y}(t)), \quad (2.2)$$

where $\rho(SJ)$ denotes the spectral radius of the matrix SJ , and β is a constant (the so-called *stability boundary*) completely determined by the time integrator.

Since the stability boundary of explicit methods is relatively small and $\rho(J)$ usually extremely large, the condition (2.2) may be extremely restrictive if no smoothing is applied (i.e., $S=I$). This may force the method to take steps Δt that are much smaller than accuracy would require. By an appropriate choice of the smoothing matrix S we can reduce the magnitude of $\rho(SJ)$ considerably.

In general, it is too ambitious to derive optimal smoothing matrices for an arbitrary Jacobian matrix J . Therefore, we shall consider the optimization problem for two model problems which characterize, respectively, a parabolic and a hyperbolic equation. First, however, we consider the order of accuracy of the smoothing operator, that is we require

$$S = I + O(\Delta^p) \quad (2.3)$$

as the spatial grid Ω_Δ is refined.

2.2. The order of accuracy of smoothing operators

Let the vector \mathbf{v} have components $v^{(j)}$ and define the shift operator E by

$$E v^{(j)} := v^{(j+1)}. \quad (2.4)$$

Let $Q_k(z)$ be a polynomial of degree k in z with $Q_k(1) = 1$. Then we may consider smoothing matrices S of the form

$$S \mathbf{v} = \mathbf{u} := \left(\frac{1}{2} [Q_k(E) + Q_k(E^{-1})] v^{(j)} \right), \quad Q_k(1) = 1. \quad (2.5)$$

We shall call this matrix a *smoothing matrix* or *smoothing operator of degree k* .

This operator should be sufficiently close to the identity operator I . In order to define the order of the smoothing operator (2.5) we apply S to the test vector $\mathbf{v} = (v^{(j)}) := (w(j\Delta x))$, where $w(x)$ is a sufficiently differentiable function of x . We find

$$\begin{aligned} S \mathbf{v} &= \left(\frac{1}{2} [Q_k(E) + Q_k(E^{-1})] w(j\Delta x) \right) \\ &= \left(\frac{1}{2} [Q_k(e^{\Delta x \frac{d}{dx}}) + Q_k(e^{-\Delta x \frac{d}{dx}})] w(j\Delta x) \right) \\ &= \left([Q_k(1) + \frac{1}{2}(Q'_k(1) + Q''_k(1))\Delta^2 x \frac{d^2}{dx^2} + O(\Delta^4 x)] w(j\Delta x) \right). \end{aligned}$$

DEFINITION 2.1. The smoothing operator (2.5) is said to be of order p if for all vectors $\mathbf{w} = (w(j\Delta x))$ with $w \in C^p$ we have

$$S\mathbf{w} = \mathbf{w} + O(\Delta^p x) \text{ as } \Delta x \rightarrow 0. \quad \square$$

The following theorem is easily proved:

THEOREM 2.1. The smoothing operator (2.5) is at least of order $p = 2$; it is of order $p = 4$ if $Q_k(z)$ satisfies $Q'_k(1) + Q''_k(1) = 0$. \square

EXAMPLE 2.1. A two-parameter family of second-order smoothing operators is generated by the polynomial

$$Q_2(z) = 1 - q_1 - q_2 + q_1 z + q_2 z^2.$$

The order can be raised to four if we choose $q_1 = -4q_2$. We observe that fourth-order smoothing operators always require $k \geq 2$. \square

EXAMPLE 2.2. Let S be defined by

$$Sv := \left(\frac{1}{16}(E + 2 + E^{-1})(E^2 + 2 + E^{-2})v^{(j)}\right).$$

It is easily verified that this operator can be represented in the form (2.5) with

$$Q_3(z) = \frac{1}{4} + \frac{3}{8}z + \frac{1}{4}z^2 + \frac{1}{8}z^3.$$

Since $Q_3(1) = 1$, this smoothing operator is second-order accurate. \square

3. CONSTRUCTION OF OPTIMAL SMOOTHING OPERATORS

In order to investigate the operator S defined by (2.5) we will use the test vectors

$$\mathbf{e} = (e^{lj}), \quad e^{(j)} := \exp(i\omega j\Delta x), \quad (3.1)$$

where $\omega \in \mathbb{R}$ and Δx is the space discretization parameter.

DEFINITION 3.1. Let $C(z)$ be the polynomial

$$C(z) = \sum_{l=0}^r c_l z^l.$$

Then we associate to C the polynomial \hat{C} defined by

$$\hat{C}(z) := \sum_{l=0}^r c_l T_l(z), \quad T_l(z) := \cos(l \arccos z).$$

THEOREM 3.1. The smoothing operator S satisfies the eigenvalue equation

$$S\mathbf{e} = \hat{Q}_k(\xi)\mathbf{e}, \quad \xi := \cos(\omega\Delta x).$$

PROOF. On substitution of \mathbf{e} into (2.5) we obtain

$$\begin{aligned} S\mathbf{e} &= \frac{1}{2}[Q_k(e^{i\omega\Delta x}) + Q_k(e^{-i\omega\Delta x})]\mathbf{e} \\ &= \frac{1}{2} \sum_{l=0}^k q_l (e^{il\omega\Delta x} + e^{-il\omega\Delta x})\mathbf{e} \\ &= \sum_{l=0}^k q_l \cos(l\omega\Delta x)\mathbf{e} = \sum_{l=0}^k q_l T_l(\xi)\mathbf{e}. \quad \square \end{aligned}$$

Thus, the test vector \mathbf{e} is an eigenvector of S with eigenvalue $\hat{Q}_k(\xi)$. The behaviour of the polynomial $\hat{Q}_k(z)$ on the interval $[-1, 1]$ determines the properties of the smoothing operator S (notice that $-1 \leq \xi \leq 1$). For instance, if $\hat{Q}_k(z)$ is small in magnitude for $z \rightarrow -1$, then S will damp the high frequencies in the Fourier expansion of the vector $\mathbf{v} = (w(j\Delta x))$.

In the actual derivation of the smoothing operator S from a given polynomial $\hat{Q}_k(z)$ the following corollary of Theorem 3.1 is often convenient.

COROLLARY 3.1. Let $\hat{Q}_k(z)$ be a polynomial expression in terms of the functions $T_0(z), T_1(z), \dots, T_k(z)$:

$$\hat{Q}_k(z) = \mathfrak{S}(T_0(z), \dots, T_k(z)). \quad (3.2a)$$

Then the generated smoothing operator is given by

$$S\mathbf{v} = (\mathfrak{S}(\frac{E^0 + E^0}{2}, \dots, \frac{E^k + E^{-k}}{2})\mathbf{v}^{(j)}). \quad (3.2b)$$

PROOF. From Theorem 3.1 it follows that the smoothing operator \bar{S} generated by (3.2a), has the eigenvalues

$$\hat{Q}_k(\xi) = \mathfrak{S}(T_0(\xi), \dots, T_k(\xi)), \quad \xi = \cos(\omega\Delta x).$$

On the other hand, because $T_j(\xi)$ is an eigenvalue of $(E^j + E^{-j})/2$, it follows from (3.2b) that the operator S has the same eigenvalues. Since S and \bar{S} are both polynomial operators in E and E^{-1} with identical eigenvalues, they are necessarily identical. \square

EXAMPLE 3.1. Suppose that

$$\hat{Q}_6(z) = 2T_2(z)T_1(z) - T_3^2(z).$$

Then, S is defined by

$$S\mathbf{v} = ((\frac{1}{2}(E^2 + E^{-2})(E + E^{-1}) - \frac{1}{4}(E^3 + E^{-3})^2)\mathbf{v}^{(j)}). \quad \square$$

The following result is similarly proved by means of Theorem 3.1.:

COROLLARY 3.2. Let the polynomials $\hat{Q}^{(j)}(z)$ generate smoothing operators $S^{(j)}$, and let a and b be scalars. Then the polynomial

$$\hat{Q}(z) := a\hat{Q}^{(1)}(z) + b\hat{Q}^{(2)}(z)\hat{Q}^{(3)}(z)$$

generates the smoothing operator

$$S := aS^{(1)} + bS^{(2)}S^{(3)}. \quad \square$$

The next theorem expresses the order conditions in terms of the polynomial $\hat{Q}_k(z)$.

THEOREM 3.2.(a) The smoothing operator generated by $\hat{Q}_k(z)$ is of second-order if $\hat{Q}_k(1) = 1$, and of fourth-order if, in addition, $\hat{Q}'_k(1) = 0$.

(b) If $\hat{Q}_k(1) = 1$ and $\hat{Q}'_k(1) \neq 0$, then the polynomial

$$\hat{P}_{2k}(z) := 1 - \alpha + \alpha\hat{Q}_k(z)[2 - \hat{Q}_k(z)]$$

generates a fourth-order smoothing operator for all values of α .

PROOF. (a) Since $T_l(1) = 1$ and $T'_l(1) = l^2$ we have

$$Q_k(1) = \sum_{l=0}^k q_l = \sum_{l=0}^k q_l T_l(1) = \hat{Q}_k(1)$$

and

$$\begin{aligned} Q'_k(1) + Q''_k(1) &= \sum_{l=0}^k q_l [l + l(l-1)] = \sum_{l=0}^k q_l l^2 \\ &= \sum_{l=0}^k q_l T'_l(1) = \hat{Q}'_k(1). \end{aligned}$$

From these relations and Theorem 2.1 assertion (a) of the theorem easily follows.

(b) The polynomial $\hat{P}_{2k}(z)$ is easily shown to satisfy for all α the conditions for fourth-order accuracy stated in (a). \square

Once the polynomial \hat{Q}_k has been specified, the smoothing operator S is easily found, either by using Definition 3.1 (to obtain Q_k) and formula (2.5) (to obtain S), or by using the above Corollaries 3.1 and 3.2.

In order to construct an effective operator S , in the sense that $\rho(SJ)$ is substantially smaller than $\rho(J)$, we need some additional information on the spectrum of J . We shall distinguish Jacobian matrices with *negative* eigenvalues arising in *parabolic* equations and *imaginary* eigenvalues arising in *hyperbolic* equations.

3.1. Smoothing of parabolic problems

If symmetric space discretizations are used in parabolic problems then J is usually of the form

$$Jv = \left(\frac{1}{2}[K(E) + K(E^{-1})]\right)v^{(j)}, \quad (3.3a)$$

where K is a polynomial. In the same manner as we associated to Q_k the polynomial \hat{Q}_k (cf. Theorem 3.1), we can associate to K the polynomial \hat{K} , to obtain the eigenvalue equation

$$Je = \hat{K}(\zeta)e, \quad e := (e^{ij\omega\Delta x}), \quad \zeta := \cos(\omega\Delta x). \quad (3.3b)$$

EXAMPLE 3.2. Consider the *parabolic model problem*

$$u_t = u_{xx} + g(x, t).$$

The standard three-point discretization leads to a system of differential equations of which the j -th equation reads:

$$\frac{dy^{(j)}}{dt} = \frac{1}{\Delta^2 x} [E - 2 + E^{-1}]y^{(j)} + g^{(j)}(t);$$

it is easily seen that the matrix J can be characterized by the polynomial

$$K(z) = -\frac{2}{\Delta^2 x}(1-z).$$

The polynomial $\hat{K}(z)$ turns out to be identical with $K(z)$. \square

EXAMPLE 3.3. If the equation above is discretized by the standard fourth-order five-point discretization we obtain the polynomial

$$K(z) = -\frac{1}{6\Delta^2 x}(z^2 - 16z + 15)$$

and

$$\hat{K}(z) = -\frac{1}{3\Delta^2 x}(z^2 - 8z + 7) = -\frac{1}{3\Delta^2 x}(z-1)(z-7). \quad \square$$

Let us return to our problem of minimizing $\rho(SJ)$ occurring in the stability condition (2.2). It follows from Theorem 3.1 and (3.3) that

$$\rho(SJ) = \max_{-1 \leq \xi \leq 1} |\hat{Q}_k(\xi) \hat{K}(\xi)|. \quad (3.4)$$

Thus, the right-hand side has to be minimized taking into account the order condition in Theorem 3.1. Moreover, the polynomial \hat{Q}_k should be nonnegative on $[-1, 1]$ (otherwise SJ would have positive eigenvalues).

In general, it is too ambitious to solve this minimax problem for arbitrary eigenvalue functions $\hat{K}(\xi)$. Therefore, we shall write, instead,

$$\rho(SJ) \leq \max_{-1 \leq \xi \leq 1} [(1-\xi)\hat{Q}_k(\xi)] \cdot \max_{-1 \leq \xi \leq 1} \left[\frac{\hat{K}(\xi)}{\xi-1} \right], \quad (3.5)$$

and solve the minimax problem for the polynomial $(1-\xi)\hat{Q}_k(\xi)$, which is independent of the parabolic equation under consideration. This approach is justified by the observation that the resulting polynomial \hat{Q}_k does generate optimal second-order smoothing operators in the case of the parabolic model problem of Example 3.2. In nonmodel problems (where $\hat{K}(\xi)$ contains the factor $\xi-1$), the resulting polynomial \hat{Q}_k is not optimal, but it gives rise to the same reduction factor of the spectral radius as in the model problem.

On the basis of (3.5) the stability condition (2.2) becomes

$$\Delta t \leq \mu \beta \min_{-1 \leq \xi \leq 1} \frac{\xi-1}{2\hat{K}(\xi)}, \quad (3.6a)$$

where we introduced the *amplification factor*

$$\mu := \left[\max_{-1 \leq \xi \leq 1} \frac{1}{2} (1-\xi)\hat{Q}_k(\xi) \right]^{-1}. \quad (3.6b)$$

Notice that $\mu = 1$ ($\hat{Q}_0 \equiv 1$) if no smoothing operators are applied.

3.1.1. Second-order smoothing operators

The following lemma is basic in our subsequent discussion:

LEMMA 3.1. *Of all polynomials $P_m(z)$ of degree m in z satisfying the conditions $P_m(1) = 0$, $P'_m(1) = -1$, and $P_m(z) \geq 0$ on $[-1, 1]$, the polynomial $P_m(z) := [1 - T_m(z)]/m^2$ has the smallest maximum norm on $[-1, 1]$.*

PROOF. The assertion of the lemma follows immediately from the various properties of the Chebyshev polynomial $T_m(z)$. \square

With the help of this lemma the following theorem is easily proved.

THEOREM 3.3. *Let the smoothing operator S be generated by the polynomial*

$$\hat{Q}_k(z) = \frac{1 - T_{k+1}(z)}{(k+1)^2(1-z)}. \quad (3.7)$$

Then, S is second-order accurate, and minimizes, for given k , the spectral radius $\rho(SJ)$ of the model problem in Example 3.2.

PROOF. It follows from Example 3.2 and from (3.4) that

$$\rho(SJ) = \frac{2}{\Delta^2 x} \max_{-1 \leq \xi \leq 1} \frac{1 - T_{k+1}(\xi)}{(k+1)^2}.$$

and from Lemma 3.1 that $\rho(SJ)$ is as small as possible, while $\hat{Q}_k(z)$ is nonnegative with $\hat{Q}_k(1) = 1$. \square

EXAMPLE 3.4. The first few polynomials Q_k corresponding to the optimal polynomials \hat{Q}_k specified in Theorem 3.3 are given by

$$\begin{aligned} Q_1(z) &= \frac{1}{2}(1+z), \\ Q_2(z) &= \frac{1}{9}(3+4z+2z^2), \\ Q_3(z) &= \frac{1}{8}(2+3z+2z^2+z^3). \end{aligned}$$

Notice that $Q_3(z)$ is identical with the polynomial $Q_3(z)$ derived in Example 2.2. \square

THEOREM 3.4. Let J satisfy the conditions (3.3) and let S be generated by (3.7). Then the amplification factor μ is given by $(k+1)^2$ so that

$$\Delta t \leq \beta(k+1)^2 \min_{-1 \leq \xi \leq 1} \frac{\xi-1}{2\hat{K}(\xi)}, \quad (3.6')$$

where $\hat{K}(\xi)$ is assumed to be negative.

PROOF. The proof is immediate from (3.7) and (3.6). \square

We recall that for $k=0$ the stability condition (3.6') corresponds to the "unsmoothed" method because $\hat{Q}_0(z) \equiv 1$. This indicates that the gain factor obtained by the smoothing technique is as large as $(k+1)^2$ independent of the particular problem under consideration.

EXAMPLE 3.5. Consider the model problem in Example 3.2. For this three-point discretization we have

$$\min_{-1 \leq \xi \leq 1} \frac{\xi-1}{2\hat{K}(\xi)} = \frac{\Delta^2 x}{4}.$$

Substitution into (3.6') yields the stability condition

$$\Delta t \leq \frac{1}{4}\beta(k+1)^2\Delta^2 x.$$

We recall that, by virtue of Theorem 3.3, there exists no smoothing operator of degree k which leads to a larger maximum stable step Δt . \square

EXAMPLE 3.6. Consider the discretization defined in Example 3.3. For this five-point discretization we have

$$\min_{-1 \leq \xi \leq 1} \frac{\xi-1}{2\hat{K}(\xi)} = \min_{-1 \leq \xi \leq 1} \frac{3\Delta^2 x}{2(7-\xi)} = \frac{3}{16}\Delta^2 x,$$

so that, by Theorem 3.4, the stability condition becomes

$$\Delta t \leq \frac{3}{16}\beta(k+1)^2\Delta^2 x. \quad \square$$

The following lemma is of interest in the actual implementation of smoothing operators.

LEMMA 3.2. If $m = 2^q$ with $q > 0$, then

$$T_m(z) = 1 - m(1-z) \prod_{l=0}^{q-1} (1 + T_{2^l}(z)).$$

PROOF. It follows from the identity $T_{2l} = 2T_l^2 - 1$ that

$$\begin{aligned} 1 - T_m &= 1 - T_{2^q} = 2(1 - T_{2^{q-1}}^2) = 2(1 + T_{2^{q-1}})(1 - T_{2^{q-1}}) = \\ &\dots = 2^q(1 + T_{2^{q-1}})(1 + T_{2^{q-2}})\dots(1 + T_1)(1 - T_1). \end{aligned}$$

This proves the lemma. \square

By means of this lemma and Corollary 3.1 the following Theorem is immediate:

THEOREM 3.5. *Let $k = 2^q - 1$ with $q > 0$, then the smoothing operator based on (3.7) can be factorized according to*

$$Sv = \frac{1}{2^{2q}} \left(\prod_{l=0}^{q-1} [E^{2^l} + 2 + E^{-2^l}] v^{(l)} \right). \quad (3.8)$$

The operator (3.8) is identical to the smoothing operator proposed in WUBS [4]. In this factorized form it allows a rather efficient implementation on a computer.

3.1.2. Fourth-order smoothing operators

Suppose that we can solve the following minimax problem:

Problem 3.1. Of all polynomials $P_m(z)$ of degree m in z satisfying the conditions $P_m(1) = 0, P'_m(1) = -1, P''_m(1) = 0$ and $P_m(z) \geq 0$ on $[-1, 1]$, find the polynomial with the smallest maximum norm on $[-1, 1]$. \square

If such a minimax polynomial is found, then by defining

$$\hat{Q}_k(z) = \frac{P_{k+1}(z)}{1-z}, \quad k = m-1,$$

we obtain a polynomial satisfying the fourth-order conditions $\hat{Q}_k(1) = 1, \hat{Q}'_k(1) = 0$, being nonnegative on $[-1, 1]$, and maximizing the amplification factor in the stability condition (3.6).

Sofar, we did not succeed in deriving closed expressions for the optimal polynomials $P_{k+1}(z)$ and the corresponding maximal amplification factor μ . The derivation of these polynomials will be subject of future investigations.

An alternative is offered by Theorem 3.2(b). By starting with the one-parameter family of fourth-order polynomials

$$\hat{Q}(z) = 1 - \alpha + \alpha \hat{Q}^*(z)(2 - \hat{Q}^*(z)), \quad (3.9)$$

where $\hat{Q}^*(z)$ generates a second-order smoothing operator S^* , there is only one parameter to be optimized such that $(1-z)\hat{Q}(z)$ has a minimal maximum norm on $[-1, 1]$. In Table 3.1 the resulting amplification factors μ are listed for the case where $\hat{Q}^*(z)$ is given by (3.7). It seems that $\mu/(k+1)^2$, k denoting the degree of \hat{Q} , converges to a constant value (recall that this value is 1 in the second-order case).

We observe that the spectral radius $\rho(SJ)$ can be reduced further for $\alpha > 1$. However, then $\hat{Q}(z)$ is not nonnegative on $[-1, 1]$ anymore which leads to unstable discretizations.

Finally, we remark that the operator S generated by $\hat{Q}(z)$, i.e.,

$$S = (1-\alpha)I + \alpha S^*(2I - S^*), \quad (3.10)$$

is to a high degree factorizable if S^* is factorizable.

TABLE 3.1. μ -values for (3.9) with $\hat{Q}^*(z)$ defined by (3.7)

Degree k of S	α	μ	$\mu/(k+1)^2$
2	1	2.6	.29
4	1	4.7	.19
6	1	8.3	.17
8	1	12.7	.16

3.2. Smoothing of a hyperbolic model problem

Symmetric space discretizations of hyperbolic problems often lead to Jacobian matrices defined by

$$J\mathbf{v} = \left(\frac{1}{2}[K(E) - K(E^{-1})]\mathbf{v}^{(j)}\right), \quad (3.11a)$$

where K is a polynomial.

DEFINITION 3.2. Let $C(z)$ be defined as in Definition 3.1. Then \tilde{C} is defined by

$$\tilde{C}(z) := \sum_{l=1}^r c_l U_{l-1}(z),$$

where U_l is the Chebyshev polynomial of the second kind. \square

By means of this definition we can write the eigenvalue equation for the Jacobian matrix J in the form

$$J\mathbf{e} = \pm i \sqrt{1 - \xi^2} \tilde{K}(\xi) \mathbf{e}, \quad \mathbf{e} := (e^{ij\omega\Delta x}), \quad \xi := \cos(\omega\Delta x), \quad (3.11b)$$

where the sign is determined by the sign of $\sin(\omega\Delta x)$.

In order to prove this, let

$$K(z) := \sum_{l=0}^r c_l z^l.$$

Then

$$\begin{aligned} J\mathbf{e} &= \frac{1}{2}[K(e^{i\omega\Delta x}) - K(e^{-i\omega\Delta x})] \mathbf{e} \\ &= \frac{1}{2} \sum_{l=0}^r c_l (e^{il\omega\Delta x} - e^{-il\omega\Delta x}) \mathbf{e} \\ &= i \sum_{l=1}^r c_l \sin(l\omega\Delta x) \mathbf{e} = i \sum_{l=1}^r c_l \sin(\omega\Delta x) U_{l-1}(\cos\omega\Delta x) \mathbf{e} \\ &= \pm i \sqrt{1 - \xi^2} \sum_{l=1}^r c_l U_{l-1}(\xi) \mathbf{e}. \end{aligned}$$

EXAMPLE 3.7. Consider the hyperbolic model problem

$$u_t = u_x + g(x, t)$$

and its three-point discretization

$$\frac{dy^{(j)}}{dt} = \frac{1}{2\Delta x} [E - E^{-1}] y^{(j)} + g^{(j)}(t).$$

The Jacobian of this system is characterized by

$$K(z) = \frac{1}{\Delta x} z,$$

so that

$$\tilde{K}(z) = \frac{1}{\Delta x}. \quad \square$$

EXAMPLE 3.8. If the above equation is discretized by the fourth-order five-point discretization we obtain

$$K(z) = \frac{z}{6\Delta x} (8-z),$$

$$\tilde{K}(z) = \frac{1}{3\Delta x} (4-z). \quad \square$$

For hyperbolic problems we are faced with the problem of minimizing

$$\rho(SJ) = \max_{-1 \leq \xi \leq 1} \sqrt{1-\xi^2} |\hat{Q}_k(\xi) \tilde{K}(\xi)|, \quad (3.12)$$

taking into account the order conditions for \hat{Q}_k stated in Theorem 3.2. Notice that, in contrast to the minimax problem for parabolic problems, the polynomial \hat{Q}_k is not required to be nonnegative on $[-1, 1]$. Consequently, the polynomials derived for parabolic problems are not optimal in the present case.

Instead of minimizing the right-hand side of (3.12) we shall write

$$\rho(SJ) \leq \max_{-1 \leq \xi \leq 1} \sqrt{1-\xi^2} |\hat{Q}_k(\xi)| \max_{-1 \leq \xi \leq 1} |\tilde{K}(\xi)| \quad (3.13)$$

and we solve the minimax problem for $\sqrt{1-\xi^2} \hat{Q}_k(\xi)$ independently of \tilde{K} (cf. the discussion given for (3.5)). Similarly to (3.6), we derive from (3.13) the stability condition

$$\Delta t \leq \mu \beta \min_{-1 \leq \xi \leq 1} \frac{1}{|\tilde{K}(\xi)|}, \quad \mu := \left[\max_{-1 \leq \xi \leq 1} \sqrt{1-\xi^2} |\hat{Q}_k(\xi)| \right]^{-1}. \quad (3.14)$$

Again, μ is chosen such that $\mu = 1$ if no smoothing is applied.

3.2.1. Second-order smoothing operators

The following lemma plays the role that Lemma 3.1 played for parabolic problems.

LEMMA 3.3. *Of all functions of the form $\sqrt{1-z^2} P_m(z)$ where $P_m(z)$ is a polynomial of degree m in z satisfying the condition $P_m(1) = 1$, the function $\sqrt{1-z^2} U_m(z)/(m+1)$ has the smallest maximum norm on $[-1, 1]$.*

PROOF. Since $U_m(1) = m+1$ the condition $P_m(1) = 1$ is satisfied. Furthermore, we deduce from the identity

$$|U_m(z)| \equiv \sqrt{\frac{1-T_{m+1}^2(z)}{1-z^2}},$$

that the function $\sqrt{1-z^2} U_m(z)$ satisfies the equal ripple property from which it can be concluded that this function is optimal. \square

By virtue of this lemma the following theorem is obvious.

THEOREM 3.6. Let the smoothing operator S be generated by the polynomial

$$\hat{Q}_k(z) = \frac{U_k(z)}{k+1}. \quad (3.15)$$

Then S is second-order accurate, and minimizes, for given k , the spectral radius $\rho(SJ)$ of the model problem in Example 3.7. \square

EXAMPLE 3.9. The first few polynomials $Q_k(z)$ generated by (3.15) are given by

$$\begin{aligned} Q_1(z) &= z, \\ Q_2(z) &= \frac{1}{3}(1+2z^2), \\ Q_3(z) &= \frac{1}{2}(z^3+z). \quad \square \end{aligned}$$

THEOREM 3.7. Let J satisfy the conditions (3.11) and let S be generated by (3.15). Then the amplification factor is given by $k+1$ leading to the stability condition

$$\Delta t \leq \beta(k+1) \min_{-1 \leq \zeta \leq 1} \frac{1}{|K(\zeta)|}. \quad (3.14')$$

PROOF. Substitution of (3.15) into (3.14) leads to (3.14'). \square

EXAMPLE 3.10. Consider the discretization of Example 3.8. Applying Theorem 3.7 we find that this five-point discretization is stable if

$$\Delta t \leq \frac{3}{5}\beta(k+1)\Delta x. \quad \square$$

As in the parabolic case the operator S generated by (3.15) can be factorized for special values of k . The counterpart of Lemma 3.2 is given by

LEMMA 3.4. If $m = 2^q$ with $q > 0$, then

$$U_{m-1}(z) = m \prod_{l=0}^{q-1} T_{2^l}(z).$$

PROOF. Using the identity $U_{2l-1} = 2U_{l-1}T_l$, (cf [1], p.782) we deduce that

$$U_{m-1} = U_{2^q-1} = 2U_{2^{q-1}-1}T_{2^{q-1}} = \cdots = 2^q \prod_{l=1}^q T_{2^{l-1}}$$

proving the assertion of the lemma. \square

The analogue of Theorem 3.5 is given by

THEOREM 3.8. Let $k = 2^q - 1$ with $q > 0$, then the smoothing operator based on (3.15) can be factorized according to

$$S\mathbf{v} = \frac{1}{2^q} \left(\prod_{l=0}^{q-1} [E^{2^l} + E^{2^{l-1}}] \right) \mathbf{v}^{(l)}. \quad \square \quad (3.16)$$

3.2.2. Fourth-order smoothing operators

For hyperbolic problems we have the following analogue of Problem 3.1.

Problem 3.2. Of all functions of the form $\sqrt{1-z^2} P_m(z)$ where $P_m(z)$ is a polynomial of degree m in z satisfying the conditions $P_m(1) = 1$ and $P'_m(1) = 0$, find the function with the smallest maximum norm on $[-1, 1]$. \square

If this problem is solved for $m = k$, we set $\hat{Q}_k(z) = P_k(z)$ to obtain the generating polynomial for a fourth-order smoothing operator with optimal amplification factor μ as defined in (3.14).

As in the parabolic case we did not yet find closed expressions for the optimal polynomials and we applied, instead, (3.9) with $\hat{Q}^*(z)$ given by (3.15). The analogue of Table 3.1 is presented by Table 3.2. Notice that here α is not restricted by a sign condition on $\hat{Q}^*(z)$. The resulting smoothing operators are given by (3.10) with S^* corresponding to \hat{Q}^* .

TABLE 3.2. μ -values for (3.9) with $\hat{Q}^*(z)$ defined by (3.15)

Degree k of S	α	μ	$\mu/(k+1)$
2	.67901	1.38	.46
4	.83512	2.06	.41
6	.84250	1.96	.28
8	.95280	2.56	.28

4. NUMERICAL EXPERIMENTS

In WUBS [4] a few first experiments are reported for hyperbolic problems using smoothing techniques in combination with conventional time integrators. Here, we present further experiments, both for parabolic and hyperbolic problems. All examples are chosen such that conventional explicit time integrators (without smoothing) require unrealistically small time steps.

The examples are, respectively,

$$u_t = u_{xx} + g_1(t, x), \quad (4.1)$$

$$u_t = u^2 u_{xx} + g_2(t, x), \quad (4.2)$$

$$u_t = u_x + g_3(t, x), \quad (4.3)$$

$$u_t = \frac{1}{2}(u^2)_x + g_4(t, x), \quad (4.4)$$

where the forcing functions $g_j(t, x)$ are chosen in such a way that

$$u(t, x) = \frac{1}{2}[\sin(x+t) + \sin(\omega x)], \quad \omega \in \mathbf{N} \quad (4.5)$$

presents the exact solution. The initial condition is taken from the exact solution, and periodic boundary conditions are imposed at $x=0$ and $x=2\pi$. In all examples the integration interval is given by $[0, T]$, where T is specified in the tables of results.

The semi-discrete equations are obtained by using, respectively, the three-point discretizations of the Examples 3.2 and 3.7, and the five-point discretizations of the Examples 3.3 and 3.8. The spatial grid is given by the points $x_j = j\Delta x$, $j = 1, 2, \dots, 2\pi/\Delta x$, where Δx is chosen such that the forcing function and the initial function can adequately be represented.

The time integrators used (in combination with smoothing operators specified in the tables of results) are given by the explicit Runge-Kutta methods (for the notation used see LAPIDUS & SEINFELD [3]):

RKP:	0	0	
	1/8	1/8	
	1/2	0	1/2
		0	0 1
RKH:	0	0	
	1/2	1/2	
	1/2	0	1/2
		0	0 1

Both methods are second-order accurate: RKP is used for the parabolic problems (4.1) and (4.2) with stability boundary $\beta = 6.26$ in the stability condition (3.6); RKH is used for the hyperbolic problems (4.3) and (4.4) with stability boundary $\beta = 2$ in the stability condition (3.14). These conditionally stable methods were respectively applied with the parabolic smoothers generated by (3.7) and Table 3.1, and with the hyperbolic smoothers generated by (3.15) and Table 3.2.

As reference method we apply the implicit Crank-Nicholson method which can be represented by the array:

CN:	0	0	0
	1	1/2	1/2
		1/2	1/2

This method is also second-order accurate, but it is unconditionally stable both for parabolic and hyperbolic problems (i.e., $\beta = \infty$), and, therefore, it requires no smoothing in order to stabilize the integration process.

The integration steps Δt are chosen as large as allowed by the stability condition of the smoothed RKP or RKH methods.

In the tables of results we list the degree k of the smoothing operator used, the total number of steps $N := T/\Delta t$, and the number of correct significant digits obtained in $t_N = T$, i.e., the value of

$$sd := \min(-\log_{10} |y_N^k - u(T, x_j)|).$$

4.1. Problem (4.1)

This problem is given by (4.1) with solution (4.5) and with $\omega = 16$. The solution is therefore rapidly oscillating, while its time derivative is slowly varying with x ; hence, the problem belongs to the problem class for which the smoothing technique described in the preceding sections should be effective. In order to represent the initial condition and the forcing function adequately on the spatial grid we choose $\Delta x = \pi/192$.

The results obtained are listed in the Tables 4.1a and 4.1b (see Section 4.5). They show that the smoothed RKP method performs stably for all integration steps. Compared with the maximal step allowed by the "unsmoothed" RKP method (i.e. $k=0$), the gain factors for second and fourth-order smoothing are at least 64 and 32, respectively. The accuracy is hardly reduced by the smoothing procedure, except for the case where fourth-order space discretization is combined with second-order smoothing (here, an increase of the degree of the smoothing operator by 1 decreases the number of correct digits by about .25 if k is small and by about .15 if k becomes larger). In all other cases, the accuracy is comparable with that of the CN method.

4.2 Problem (4.2)

This problem is a *nonlinear* modification of problem (4.1), again with $\omega = 16$. The results listed in the Tables 4.2a and 4.2b show a similar behaviour as for the linear problem (4.1), provided that the degree of the smoothing operator is not too large ($k \leq 5$ for second-order smoothing and $k \leq 10$ for fourth-order smoothing). The respective amplification factors of the maximal stable integration step are at least 35 and 18.

4.3 Problem (4.3)

The results for the linear hyperbolic problem (4.3) with $\omega = 16$ (see the Tables 4.3a and 4.3b) again show that the smoothed RKH method performs stably for all integration steps, while the accuracy is not or only marginally less than the accuracy obtained by the CN method. The amplification factors of the maximal stable integration steps are at least 8 and 4 for second-order and fourth-order smoothing, respectively. Notice that, in contrast to the results obtained for the parabolic problems (4.1) and (4.2), the numerical error is not only determined by space discretization and smoothing errors, but also contains a time discretization error.

4.4. Problem (4.4)

When we integrated the nonlinear problem (4.4) with $\omega = 16$, rather low accuracies were obtained on a spatial grid with $\Delta x = \pi/192$, and instabilities developed in the case of fourth-order smoothers. Due to this low accuracy, the *numerical* solution did not satisfy the requirement that its time derivative is a smooth function of x . In order to overcome this unwanted behaviour we should decrease Δx , or equivalently, in order to stay within our budget available for these numerical experiments, we may decrease ω . Choosing $\omega = 8$ we obtained the results listed in the Tables 4.4a and 4.4b. We now have stability for all integration steps and accuracies which are even higher than those produced by the CN method.

4.5. Tables of results

TABLE 4.1a. *sd*-values for problem (4.1) with $\omega = 16, T = 1.0, \Delta x = \pi/192$, and with second-order smoother based on (3.7)

k	3-point coupling			5-point coupling		
	N	RKP	CN	N	RKP	CN
0	2400	2.54	2.54	3200	4.59	4.59
1	600	2.54	2.54	800	4.34	4.58
2	270	2.53	2.54	355	4.10	4.58
3	150	2.53	2.54	200	3.90	4.58
4	96	2.52	2.54	130	3.73	4.56
5	68	2.51	2.54	90	3.58	4.54
6	49	3.26	2.54	66	3.46	4.50
7	38	2.49	2.54	50	3.35	4.44

TABLE 4.1b. sd -values for problem (4.1) with $\omega=16, T=1.0, \Delta x=\pi/192$, and with fourth-order smoother based on $\{(3.9), \alpha=1\}$

k	N	3-point coupling		N	5-point coupling	
		RKP	CN		RKP	CN
0	2400	2.54	2.54	3200	4.59	4.59
2	925	2.54	2.54	1250	4.59	4.59
4	540	2.54	2.54	710	4.59	4.59
6	300	2.54	2.54	400	4.58	4.58
8	192	2.54	2.54	260	4.58	4.58
10	136	2.54	2.54	180	4.58	4.57
12	98	2.54	2.54	132	4.57	4.56
14	76	2.54	2.54	100	4.55	4.55

TABLE 4.2a. sd -values for problem (4.2) with $\omega=16, T=1.0, \Delta x=\pi/192$, and with second-order smoother based on (3.7)

k	N	3-point coupling		N	5-point coupling	
		RKP	CN		RKP	CN
0	2400	0.62	0.62	3200	3.35	3.35
1	600	0.58	0.62	800	2.62	3.35
2	270	0.74	0.62	355	2.23	3.34
3	150	1.07	0.62	200	2.03	3.32
4	96	1.26	0.62	130	1.86	3.28
5	68	1.40	0.62	90	1.68	3.22

TABLE 4.2b. sd -values for problem (4.2) with $\omega=16, T=1.0, \Delta x=\pi/192$, and with fourth-order smoother based on $\{(3.9), \alpha=1\}$

k	N	3-point coupling		N	5-point coupling	
		RKP	CN		RKP	CN
0	2400	0.62	0.62	3200	3.35	3.35
2	925	0.52	0.62	1250	3.13	3.35
4	540	0.59	0.62	710	3.01	3.35
6	300	0.83	0.62	400	3.18	3.34
8	192	1.09	0.62	260	3.40	3.33
10	136	1.13	0.62	180	3.35	3.31

TABLE 4.3a. sd -values for problem (4.3) with $\omega = 16, T = 10, \Delta x = \pi/192$, and with second-order smoother based on (3.15)

k	3-point coupling			5-point coupling		
	N	RKH	CN	N	RKH	CN
0	310	2.19	1.96	472	3.57	3.54
1	155	2.08	1.97	236	2.83	3.05
2	104	1.94	1.81	160	2.46	2.75
3	78	1.79	1.77	120	2.20	2.52
4	62	1.66	1.82	95	2.00	2.33
5	52	1.54	1.58	80	1.84	2.19
6	43	1.42	1.49	67	1.70	2.03
7	39	1.33	1.47	58	1.58	1.91

TABLE 4.3b. sd -values for problem (4.3) with $\omega = 16, T = 10, \Delta x = \pi/192$, and with fourth-order smoother based on { (3.9), Table 3.2 }

k	3-point coupling			5-point coupling		
	N	RKH	CN	N	RKH	CN
0	310	2.19	1.96	472	3.57	3.54
2	220	2.16	2.16	350	3.39	3.45
4	145	2.10	2.41	240	3.10	3.06
6	150	2.11	2.10	260	3.16	3.13
8	115	2.04	2.28	180	2.86	2.88
10	110	2.03	2.02	185	2.88	2.91
12	85	1.93	1.83	135	2.62	2.64
14	85	1.93	1.83	145	2.68	2.68

TABLE 4.4a. sd -values for problem (4.4) with $\omega = 8, T = 4, \Delta x = \pi/192$, and with second-order smoother based on (3.15)

k	3-point coupling			5-point coupling		
	N	RKH	CN	N	RKH	CN
0	110	1.36	1.37	145	3.12	2.86
1	50	1.63	1.44	75	2.55	2.19
2	33	1.83	1.66	45	2.19	1.71
3	22	1.67	1.27	30	1.81	1.32
4	17	1.73	1.06	25	1.82	1.20
5	14	1.42	0.84	20	1.52	1.03

TABLE 4.4b. sd -values for problem (4.4) with $\omega=8, T=4, \Delta x = \pi/192$, and with fourth-order smoother based on {(3.9), Table 3.2}

k	3-point coupling			5-point coupling		
	N	RKH	CN	N	RKH	CN
0	110	1.36	1.37	145	3.12	2.86
2	75	1.53	1.38	115	3.09	2.65
4	50	1.65	1.44	70	2.54	2.13
6	45	1.69	1.48	70	2.57	2.13
8	35	1.27	1.62	55	2.10	1.90
10	30	1.34	1.61	40	1.74	1.59

5. CONCLUDING REMARKS

In this paper we analysed a smoothing technique for preconditioning a special class of semi-discrete partial differential equations. It turned out that, in order to obtain optimal smoothing matrices, one should distinguish between parabolic and hyperbolic equations. The resulting smoothing matrices are quite different. For instance, application of a smoothing matrix, which is optimal for the hyperbolic model problem, would lead to instabilities when applied to a parabolic problem. However, if the smoothing operator is appropriately chosen, a *substantial amplification of the maximal stable step size* is obtained, *irrespective of the (explicit) time integrators used*, while the additional computational effort is rather limited. The price to be paid for the less restrictive stability condition is (i) a *decrease of the accuracy for large degree smoothing matrices*, and (ii) the requirement that the *right-hand side function should be provided in grid points beyond the boundary*.

The reduced accuracy for large k has two sources: firstly, the smoothing technique analysed in this paper presupposes that the right-hand side function is a smooth function of the spatial variables and rapidly loses accuracy if not; secondly, the error constant of the smoothing operator increases with k^2 . On the other hand, the numerical experiments of the preceding section show that smoothing matrices of degree as high as 14 still do not reduce the accuracy very much if the problem belongs to the class of problems we are aiming at.

In Section 4, the need of providing right-hand side values outside the domain was solved by imposing periodic boundary conditions. In the case of other types of boundary conditions, a plausible approach is to generate these values by extrapolation. We repeated the series of experiments of Section 4 by employing *rational extrapolation* and we found a comparable stability behaviour and accuracy behaviour as well (polynomial extrapolation leads, of course, to severe instabilities). Alternatively, one may employ the Jacobian matrix of the right-hand side to achieve a correct amount of smoothing in the near boundary points. Both approaches will be subject of further investigations.

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