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The Use of Smoothing Techniques in the Method of Lines

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We describe a special space discretization method for parabolic partial differential equations which is based on conventional discretization techniques and smoothing matrices. This smoothed discretization method leads to systems of ODEs which are considerably less stiff than the ODEs obtained by conventional discretization methods. It turns out that the stiffness is reduced to an extent that ordinary predictor-corrector methods become feasible integration methods. By a few experiments we illustrate this new type of space discretization method.

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1. INTRODUCTION

We consider the numerical solution of the initial-value problem for systems of (nonlinear) ordinary differential equations (ODEs):

$$\frac{dy(t)}{dt} = f(t,y(t)), \quad y(t_0) = y_0, \tag{1}$$

which arises when time-dependent parabolic differential equations (PDEs) are semidiscretized in space. If conventional discretization methods are employed, then the eigenvalues of the Jacobian matrix $\partial f/\partial y$ are located in a negative interval $[-R,0)$ where R is usually extremely large. In such cases, we need a time integration method with a large real stability boundary.

One possibility is the use of implicit methods for which (often infinitely) large real stability boundaries can be easily realized. In order to solve the implicit relations one may resort to Newton's method and to numerical linear algebra techniques for handling the linear systems of equations defining the Newton corrections. However, this approach is often unattractive because of the algorithmic complexity when solving higher-dimensional problems or problems where the spatial discretization is based on extended stencils.

At the other end of the scale, we have conventional predictor-corrector (PC) methods which are extremely simple to implement for any number of dimensions and arbitrary spatial discretizations. Moreover, PC iteration can take full advantage of vector and parallel facilities. However, the price to be paid in computation time is high because of the small stability boundaries and, as a consequence, the small integration steps needed to achieve stability.

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Yet another possibility is the (explicit) SGPC method proposed in [2] which is in fact a generalized PC method combined with the technique of residue smoothing. In the case of special PC pairs, this method possesses relatively large real stability boundaries. In particular, an extrapolation formula (EPF) of back values as the predictor and a backward differentiation formula (BDF) as the corrector leads, when used in a SGPC method, to impressive stability boundaries. We shall refer to these special PC pairs as EP-BD pairs. SGPC methods are more complicated than PC methods but, just as PC methods, they can take full advantage of vector and parallel facilities, while, unlike PC methods, stability is obtained for much larger integration steps. A drawback of these methods is that, within the class of BDF correctors, only the lower-order BDFs can be used as correctors, but the higher-order BDFs cannot. But perhaps more important is that the SGPC methods developed so far are only applicable to parabolic problems and it seems to be rather difficult to construct such methods with large *imaginary* stability boundaries. This topic is still under investigation.

Therefore, in this paper, we consider another approach in which the spatial discretization method is adapted, rather than the time integration method. Starting with a conventional semidiscretization (1), this approach replaces (1) by the smoothed equation

$$\frac{dy(t)}{dt} = Sf(t,y(t)), \quad y(t_0) = y_0, \tag{1'}$$

where S is an explicitly defined (nonsingular) matrix which is chosen such that the stiffness of the semidiscretization is relaxed, and therefore the stability characteristics of the the time integrator used become less crucial. It turns out that S is a sort of smoothing matrix. By requiring that S->I as the spatial grid is refined, we may consider (1') as a special semidiscretization of the original problem. However, the solution of (1') has the property that its time derivative is a slowly varying function of the spatial grid points. This is the price we have to pay for relaxing the stiffness of the spatial discretization, because the accuracy of the discretization is reduced in the case where the time derivative of the solution of the original problem (1) does not slowly vary with the spatial variables.

The idea of *explicit* right-hand side smoothing was introduced in [4] for solving efficiently the shallow water equations. A theoretical analysis of the smoothing matrices employed in the present paper may be found in [1]. Further references for the use of *implicit* smoothing techniques are given in [2].

2. SMOOTHING MATRICES

In this section we briefly summarize the definition and characteristics of smoothing matrices. Following [1], we assume that

$$S = P(D), \tag{2}$$

where D is a difference matrix with eigenvalues in the interval [-1,0] and P(z) is a polynomial satisfying the condition P(0)=1. The eigenvalues of S can be monitored by choosing the polynomial P(z) appropriately in the interval [-1,0]. Typically, the Fourier components in the discrete Fourier expansion of grid functions are just the eigenvectors of D and the Fourier components of high frequency correspond to eigenvalues of D close to -1. By this observation, we are led to polynomials P(z) which equal 1 in z=0 and become smaller in magnitude as z varies from 0 to -1. There are of course many possibilities to achieve this. For instance, the shifted Chebyshev polynomial of degree m

$$\frac{1}{2} c_m \left[1 + T_m\left(\frac{1 + d + 2z}{1 - d}\right)\right], \quad c_m := \frac{2}{T_m\left(\frac{1 + d}{1 - d}\right) + 1} \tag{3}$$

satisfies the above requirements and assumes values in the interval $[0,c_m]$ if $-1 \le z \le -d$. Thus, by choosing, e.g., d=3/4, we obtain an *exponential* damping factor $c_m = 2/[T_m(7)+1] \approx 4 \exp(-2.6m)$ for all frequencies corresponding to eigenvalues of D in [-1,-3/4].

Another possibility (cf. [1]) is the polynomial

$$\frac{T_{m+1}(1 + 2z) - 1}{2(m+1)^2 z} \,. \tag{4}$$

This polynomial is also of degree m and satisfies the above requirements. It is bounded by 0 and $\min\{1,-1/[(m+1)^2 z]\}$ in the interval [-1,0]. Hence, (4) yields a *polynomial* damping factor.

In the second case, a nice factorization of S can be obtained for particular choices of m. This factorization is based on the following factorization property of Chebyshev polynomials:

$$T_{2j} = T_2(T_j) = 2\,(T_j)^2 - 1, \; j = 1, 2, \ldots .$$

Following [1], we define the matrices

$$S_j := \frac{T_{2^j}(I + 2D) - I}{2^{2j+1} D} = [I + 4^{j-1} D\, S_{j-1}]\, S_{j-1}, \; j = 1, \ldots q, \tag{5}$$

and we set $S=S_q$. From (5) it can be derived that $S_q = F_q.F_{q-1}. \ldots .F_1$, where the factor matrices F_j can be generated according to the recursion $F_{j+1}=[I-2F_j]^2$, with $F_1=S_1=I+D$. Thus, the smoothing operator $S=S_q$ is a polynomial operator of degree 2^q-1 in D and its application to some vector v requires only q matrix-vector multiplications by the factor matrices F_j. We did not yet investigate whether such an elegant factorization is also possible in the case (3).

3. RIGHT-HAND SIDE SMOOTHING

In order to see the difference of the conventional semidis-cretization (1) and the smoothed semidiscretization (1'), it is illustrative to determine the spectral radius R* associated with the smoothed right-hand side function $Sf=S_qf$ in the case of a model problem. As our model problem we choose a system of ODEs where $\partial f/\partial y$ and D are related according to

$$\frac{\partial f(t,y)}{R \partial y} = D. \tag{6}$$

Thus,

$$\frac{\partial S_q f(t,y)}{\partial y} = \frac{T_{2^q}(I + 2D) - I}{2^{2q+1}} R,$$

so that $R^* = R/4^q$. Therefore, in the case of the model problem (6), the time steps allowed by the stability condition are a factor 4^q larger when we solve (1') instead of (1). Our numerical experiments have shown that, to a large extent, this is also true for nonmodel problems. By virtue of the

considerable reduction of the spectral radius it is now feasible to look for *explicit* methods for solving (1').

4. IMPLEMENTATION OF SMOOTHING MATRICES

In the case of one-dimensional problems, we found that a suitable difference matrix D is given by

$$D = \frac{1}{4}\begin{vmatrix} 0 & & & & & & \\ 1 & -2 & 1 & & & & \\ & \cdot & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & 1 & -2 & 1 \\ & & & & & & 0 \end{vmatrix} . \qquad (7)$$

As required above, the eigenvalues of D are in the interval [-1,0] and Fourier components of high frequency do correspond to eigenvalues close to -1. A nice property of the matrix defined by (7) is the simple structure (essentially tridiagonal) of the corresponding matrices F_j, so that the application of the smoothing matrix S_q is relatively cheap. Moreover, the actual implementation of this smoothing procedure requires only a few FORTRAN lines [2].

In higher-dimensional problems, we did not yet succeed in finding suitable difference matrices D. For instance, if we use the natural generalization of (7) for higher dimensions, then the factor matrices F_j loose their simple structure, thus increasing the computational effort drastically. Therefore, we applied the 'one-dimensional' smoothing matrix defined above in the successive spatial directions. In general, the stiffness-reducing effect of such an approach is higher than in the one-dimensional case, that is, the reduction factor for the magnitude of the spectral radius is larger than 4^q as we found above for the model problem (6). In fact, for two-dimensional problems, the reduction factor is almost twice as large, i.e., $R^* = .55R/4^q$.

5. TIME INTEGRATION BY PC METHODS

In principle, any explicit integration method can be applied for integrating (1'). Although right-hand side smoothing with large q reduces the spectral radius substantially, it is not always efficient using maximum q values because of a drop of accuracy, and therefore it is still recommendable to look for methods with increased real stability boundary. In this respect, the generalized PC methods based on the EP-BD pairs mentioned in the Introduction are attractive candidates. In this paper, however, for the sake of transparency, we shall explain the right-hand side smoothing technique by applying the conventional PC integration method to the smoothed system (1'). Because of the restricted storage requirements of EP-BD pairs and in view of the large systems we want to solve, we have confined our considerations to PC methods based on these pairs. This leads us straightforwardly to the method

$$y^{(j+1)} = b_0 \Delta t\, S_q\, f(t_{n+1}, y^{(j)}) + \Sigma_n, \quad j = 0, 1, \ldots \qquad (8)$$

for approximating the exact solution y(t) at $t=t_{n+1}$. Here, Σ_n is a sum of already computed quantities y_n, Δt denotes the integration step, b_0 is defined by the BDF used, and $y^{(0)}$ is an initial approximation

which is obtained by the EP method. Notice that the conventional PC method is obtained if we set $S_q=I$.

Let β be the real stability boundary of the PC method in the actual mode used for solving (1'), and let R denote the spectral radius of the Jacobian matrix $\partial f/\partial y$ at the point (t_n,y_n). Then, in the case of the model problem (6), the condition for linear stability reads

$$\Delta t \le \frac{\beta}{R^*} . \tag{9}$$

Let p* and p# respectively denote the orders of the EPF and the BDF, then the order p and the real stability boundary β of the EP_{p^*} - $BD_{p\#}$ method in $P(EC)^m$ mode are both functions of p*, p# and m. For a given order p, we computed the scaled (or effective) stability boundary $\beta(p^*,p\#,m)/m$ for all relevant values of the arguments. The methods yielding the maximum effective stability boundaries are listed below. In addition, as a reference, we have also listed a few PC methods with increased real stability boundary such as the methods of Crane-Klopfenstein (CK) and of Krogh, and the popular fourth-order Adams-Bashforth-Moulton method (cf. [3, p.106]).

p	Method	Mode	β/m
2	EP_1 - BD_3	PEC	2.22
3	EP_2 - BD_4	PEC	1.52
4	EP_3 - BD_5	PEC	1.13
5	EP_4 - BD_6	PEC	0.89
6	EP_3 - BD_6	$P(EC)^3$	0.53
4	CK	PECE	1.24
4	Krogh	PECE	0.90
4	AB_4 - AM_4	PECE	0.65
4	AB_4 - AM_4	PEC	0.16

6. NUMERICAL EXPERIMENTS

We present results obtained by the second-order EP_1 - BD_3, the fourth-order EP_3 - BD_5 method in PEC mode, and the sixth-order EP_3 - BD_6 method in $P(EC)^3$ mode when applied to the special semi-discretization (1'). Our test example is the nonlinear problem

$$u_t = u^2 \Delta u + g(x_1,x_2,t), \quad 0 \le x_1,x_2 \le 1, \quad 0 \le t \le 2 \tag{10a}$$

where g and the initial and Dirichlet-boundary conditions are taken from the exact solution

$$u(x_1,x_2,t) = \frac{1}{2}[\sin(x_1 + x_2 + 9t) + \sin(9(x_1 + x_2))]. \tag{10b}$$

By the standard symmetric 3-point finite difference discretization of the right-hand side on a uniform grid with mesh sizes $\Delta x_1=\Delta x_2=\Delta$, we obtain a system of $(1 - 1/\Delta)^2$ ODEs. The associated spectral radius R is as large as $8/\Delta^2$ so that conventional explicit integration methods applied to this system require a number of right-hand side evaluations of $O(\Delta^{-2})$. However, by integrating the smoothed

system, the number of right-hand side evaluations is an order of magnitude smaller. In the table below, we have listed the maximum absolute errors at the endpoint t=2 obtained by the EP_1 - BD_3 method. By presenting the error in the form 10^{-d}, we give the value of d which may be considered as the number of correct decimal digits. In brackets, we have indicated the amount of work needed to perform the integration with maximal stable time step; as work unit we chose 1 (smoothed) right-hand side evaluation. Furthermore, we added the results obtained by the classical nonlinear ADI method performing 2 Newton iterations for each implicit relation; here, the work unit is 1 Newton iteration.

Δ	q=0	q=1	q=2	q=3	q=4	q=5	ADI
1/16	2.2 (2000)	2.3 (240)	2.0 (80)	1.2 (36)	0.5 (16)	-	2.0 (192)
1/32	2.8 (8000)	2.8 (800)	2.8 (200)	2.0 (80)	1.0 (30)	0.5 (16)	2.3 (320)

Since for q=0 we retain the unsmoothed semidiscretization, we may conclude from these results that the smoothed semidiscretization leads to considerably less computational effort and that reduction of accuracy starts only for relative large values of q. But the more interesting fact is that the EP-BD method is much cheaper than ADI, and that the EP-BD method enables us to get at an extremely cheap rate an inaccurate but stable solution, whereas the ADI method always furnishes the full accuracy associated with the grid used, however, at a high price. This is even more so in case of the higher-order EP-BD methods. The next table illustrates this phenomenon.

	EP_3 - BD_5			EP_3 - BD_6		
Δ	q=3	q=4	q=5	q=3	q=4	q=5
1/16	1.1 (50)	1.1 (16)	-	1.6 (120)	1.1 (48)	-
1/32	-	1.8 (60)	1.1 (16)	-	1.7 (120)	1.1 (48)

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