A nonstandard finite difference method for the solution of linear second order boundary value problems with nonsmooth coefficients

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A new three point highly accurate finite difference method for solving linear second order differential equations is proposed. The coefficients of the scheme are constructed via differentiations of the differential equation. The accuracy and efficiency of the method is compared with other well-known methods.

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1 Introduction

Consider the linear second order differential equation

$$-u'' + q(x)u = f(x), x \in (a, b), \tag{1}$$

where q, f are assumed to be sufficiently smooth on $[a, b]$ with the possible exception of a finite number of points. More precisely, let points $a = \tau_0 < \tau_1 < \ldots < \tau_M = b$ exist such that $q|_{(\tau_{j-1},\tau_j)}$, $f|_{(\tau_{j-1},\tau_j)} \in C^{m-1}[\tau_{i-1}, \tau_i]$ for some $m \geq 2$. Hence, any solution u of (1) belongs to $C^1[a, b]$ and $u|_{(\tau_{j-1},\tau_j)} \in C^{m+1}[\tau_{j-1}, \tau_j]$. In order to construct a finite difference method let a (nonuniform) mesh

$$\Delta_N : 0 = x_0 < x_1 < \ldots < x_N = b \tag{2}$$

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be given such that all breakpoints τ_j belong to Δ_N. In the traditional approach for the construction of finite difference schemes with higher accuracy, only sufficient smoothness of the solution is assumed, but the whole information from (1), namely the behaviour of the coefficients, is discarded. On the other hand, many problems of practical interest call for very fast, accurate, and reliable algorithms for solving them. The growing abilities of modern computer algebra systems allow to review the traditional approach in an attempt to construct algorithms using not only the coefficients of (1) but also their derivatives up to the necessary order. The aim of this paper is the construction of a highly accurate three point finite difference method for the approximate solution of (1).

Eq. (1) will be supplemented by initial conditions

$$u(a) = u_0, u'(a) = u'_0 \tag{3}$$

as well as separated boundary conditions

$$\begin{aligned} \alpha_1 u(a) + \beta_1 u'(a) &= \gamma_1, \\ \alpha_2 u(b) + \beta_2 u'(b) &= \gamma_2, \end{aligned} \tag{4}$$

where $\alpha_i^2 + \beta_i^2 > 0$, $\alpha_i \geq 0$, $(i = 1, 2)$, $\beta_1 \leq 0$, $\beta_2 \geq 0$.

2 Construction of the method

Let u be a solution of (1) and $m \geq 2$. Then $u \in C^1[a, b]$ and $u|_{(x_{i-1}, x_i)} \in C^{m+1}[x_{i-1}, x_i]$. Taylor expansion yields

$$u_{i+1} := u(x_{i+1}) = \sum_{k=0}^{m} \frac{u_{i+0}^{(k)}}{k!} h_{i+1}^k + O(h^{m+1}), i = 0, \ldots, N-1, \tag{5}$$

$$u_{i-1} := u(x_{i-1}) = \sum_{k=0}^{m} \frac{u_{i-0}^{(k)}}{k!} (-h_i)^k + O(h^{m+1}), i = 1, \ldots, N \tag{6}$$

where x_{i-1}, x_i, x_{i+1} are breakpoints of Δ_N (2), $h_i = x_i - x_{i-1}$, $h = \max\{h_i | i = 1, \ldots, N\}$. In (5), (6) the one-sided (right resp. left) derivatives of u at x_i are denoted by $u_{i+0}^{(k)}$ and $u_{i-0}^{(k)}$, respectively. Because of the linearity of (1), all derivatives $u_{i\pm0}^{(k)}$ can be expressed using u_i, u'_i and the derivatives of q and f for $k \geq 2$. Omitting the remainder it results

Table 1
Coefficients

	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
a	1	0	q_{i+0}	q'_{i+0}	$q''_{i+0}+q^2_{i+0}$
b	0	1	0	q_{i+0}	$2q'_{i+0}$
c	1	0	q_{i-0}	$-q'_{i-0}$	$q''_{i-0}+q^2_{i-0}$
d	0	-1	0	$-q_{i-0}$	$2q'_{i-0}$

$$u_{i+1} = A_i u_i + B_i u'_i + E_i^+(f) \tag{7}$$
$$u_{i-1} = C_i u_i + D_i u'_i + E_i^-(f) \tag{8}$$

where

$$\begin{array}{lll} A_i = \sum_{k=0}^m \frac{a_k(q)}{k!} h^k_{i+1}, & B_i = \sum_{k=0}^m \frac{b_k(q)}{k!} h^k_{i+1}, & E^+_i(f) = \sum_{k=2}^m \frac{f^+_k(q,f)}{k!} h^k_{i+1}, \\ C_i = \sum_{k=0}^m \frac{c_k(q)}{k!} h^k_i, & D_i = \sum_{k=0}^m \frac{d_k(q)}{k!} h^k_i, & E^-_i(f) = \sum_{k=2}^m \frac{f^-_k(q,f)}{k!} h^k_i. \end{array} \tag{9}$$

For convenience, the first coefficients of (9) are given in Table 1. Obviously, $B_i > 0$, $D_i < 0$ for sufficiently small h. Hence, u'_i can be eliminated in (7), (8). The resulting three point difference scheme is

$$B_i u_{i-1} - (B_i C_i - A_i D_i) u_i - D_i u_{i+1} = E_i(f), i = 1, \ldots, N-1, \tag{10}$$

where $E_i(f) = B_i E^-_i(f) - D_i E^+_i(f)$. Note that $B_i = O(h_{i+1})$, $D_i = O(h_i)$ such that (10) is badly scaled. For practical implementations, (10) should be scaled by $(h_{i+1}+h_i)^{-1}$. Besides this property remark that the classical three point scheme is obtained if m is chosen to be 2. So our scheme is a generalization of the latter one.

The initial condition (3) leads to the additional equation

$$u_1 = A_0 u_0 + B_0 u'_0 + E^+_0(f) \tag{11}$$

with given u_0, u'_0. Similarily, the boundary conditions (4) give rise to the approximations

$$(\alpha_1 B_0 - \beta_1 A_0) u_0 + \beta_1 u_1 = \gamma_1 B_0 + \beta_1 E^+_0(f) \tag{12}$$
$$\beta_2 u_{N-1} + (\alpha_2 D_N - \beta_2 C_N) u_N = \gamma_2 D_N + \beta_2 E^-_N(f). \tag{13}$$

Eq. (11) – (13) should be formally multiplied by h_1 and h_N, respectively, in order to have the same scaling as in (10).

Table 2
Intervals of periodicity $(0, R)$

m	2	4	6	8	10
R	2	12	7.57	21.48	31.70

In order to ensure the stability of the scheme assume that

$$q(x) > 0, x \in [a, b] \tag{14}$$

is true. Condition (14) assures that the system matrices of (10), (11) as well as those of (10), (12), (13) are strictly diagonally dominant L-matrices for sufficiently small h. Moreover, one can easily show that the L^∞-norms of their inverses are bounded by Ch^{-3}. Since the discretization error of (10) is $O(h^{m+2})$, the convergence order of the scheme is $O(h^{m-1})$. Because of these properties, the linear systems can be solved stably and efficiently by the marching method [6], for instance.

Note that an exact three point finite difference scheme was already suggested by Samarskij [6]. However, the coefficients of this scheme are expressed by integrals of q and f and by linear combinations of fundamental solutions of the associated initial value problem, which are hard to find in general. For this reason the scheme has not found widespread use.

The main difficulty for realizing our method consists in the evaluation of all the necessary derivatives of q and f. For larger values of m, this process can be cumbersome and errorprone. Therefore, it is desirable to use some sort of symbolic manipulation. Moreover, another possibility is the approximation of these functions by piecewise sufficiently smooth and accurate interpolations.

In order to investigate asymptotic properties of finite difference methods it is common to use the test problem

$$-u'' = \omega^2 u$$

for $\omega > 0$. Since u is analytical in this case, our scheme can be used with $m = \infty$, which leads to

$$-u_{i-1} + 2\cos \omega h u_i - u_{i+1} = 0, i = 1, \ldots, N-1$$

on an equidistant mesh (2). The solutions of this equation system are $\exp(\pm \mathrm{i}\omega h)$, which means that our scheme is P-stable [5]. For finite values of m, the intervals of periodicity are collected in Table 2.

3 Application to the numerical solution of eigenvalue problems

There has been much interest in problems requiring the efficient and accurate computation of a large number of eigenvalues of Sturm-Liouville problems. They can be written in the form

$$
\begin{aligned}
-u'' + (q(x) - \lambda)u &= 0, \\
\alpha_1 u(a) + \beta_1 u'(a) &= 0, \\
\alpha_2 u(b) + \beta_2 u'(b) &= 0.
\end{aligned}
\tag{15}
$$

If finite element or finite difference methods are used to approximate the eigenvalues λ_k of (15) by the eigenvalues $\lambda_k^{(N)}$ of an algebraic eigenvalue problem of dimension N, the error $|\lambda_k - \lambda_k^{(N)}|$ $(k = 1, 2, \ldots, N)$ is known to increase rapidly with k. Lots of recent efforts have been devoted to finding more accurate approximations [1–3,7,8]. One immediate application of our scheme is the eigenvalue problem (15). In this case the coefficients of (10) as well as those of (11)–(13) contain the eigenvalue λ in a nonlinear fashion. So we are given a nonlinear eigenvalue problem. It can be solved by some iterative procedure, e.g., continuous analogues of Newton's method [9,11] or shooting like methods [4] with respect to λ. It should be mentioned that an important property of our nonlinear difference scheme is that, for sufficiently large m, *all* eigenvalues can be approximated accurately in contrast to standard methods, which can give the first N eigenvalues, only. In particular, if q is analytical, our method with $m = \infty$ yields the exact eigenvalues of (15) up to computer precision [10].

4 A numerical example

In this section some results are presented in order to illustrate the performance of our method. Consider the resonance problem for the Schrödinger equation

$$-u'' + (V(x) - E)u = 0$$

with the Woods-Saxon potential

$$V(x) = \frac{\tilde{u}_0}{1+z} - \frac{\tilde{u}_0 z}{a(1+z)^2}$$

with $z = \exp[(x - \tilde{x}_0)/a]$, $\tilde{u}_0 = -50$, $a = 0.6$ and $\tilde{x}_0 = 7.0$. As in [1] the finite domain $0 \leq x \leq 15$ is chosen for the purpose of illustration. The boundary

Table 3
Absolute errors in 10^{-6} units

E_i	h	Ref. [3]	Ref. [1]	Ref. [1]	Ref. [8]	this paper
53.588872	1/16	108	6	110	0	0
	1/32	18	0	2	0	0
	1/64	3	0	0	0	0
341.495874	1/16	174675	977	103	5	0
	1/32	3354	70	13	1	0
	1/64	438	1	2	0	0
989.701916	1/16	(*)	98623	2039	8	1
	1/32	(*)	3044	117	2	0
	1/64	10685	44	4	0	0
Accuracy of the methods		$O(h^6)$	$O(h^8)$	exponentially fitted		$O(h^{10})$

(*): In these cases, the error is larger than 1 in magnitude.

conditions for this problem are

$$u(0) = 0, u(x) = \cos \sqrt{E}x \text{ for large } x.$$

In our scheme, we have chosen $m = 10$. The results are compared to those obtained by a method of Cash and Raptis [3], by the eighth order method of Allison, Raptis and Simos [1], by the exponentially fitted schemes of Ixaru and Rizea [1] and of Simos [7,8]. In all methods, equidistant grids with stepsize h are used. The results are shown in Table 3.

More extensive numerical comparisons using also discontinuous potentials will be published elsewhere.

5 Conclusion

The expected advantages of the proposed method are as follows:

(i) Very simple and effective construction on nonuniform partitions;
(ii) capability to integrate differential equations (1) with discontinuous coefficients;
(iii) construction of schemes up to high order with the possibility to easily implement error estimators;
(iv) approximation of arbitrary eigenvalues independent of the meshsize.

On the other hand, for larger values of m the efficient computation and stable evaluation of the coefficients of the scheme may become a nontrivial task.

References

[1] A.C. Allison, A.D. Raptis and T.E. Simos, An eighth-order formula for the numerical integration of the one-dimensional Schrödinger equation, *J. Comput. Phys.* **97** (1991) 240–248

[2] L.V. Berghe and H.D. Meyer, Accurate computation of higher Sturm-Liouville eigenvalues, *Numer. Math.* **59** (1991) 243–254

[3] J.R. Cash and A.D. Raptis, A high order method for the numerical solution of the one-dimensional Schrödinger equation, *Comput. Phys. Commun.* **33** (1984) 299–304

[4] L. Fox and D.E. Meyer, *Numerical Solution of Ordinary Differential Equations* (Oxford University Press, New York, 1990)

[5] J.D. Lambert and I.A. Watson, Symmetric multistep methods for periodic initial value problems, *J. Inst. math. Appl.* **18** (1976) 189–202

[6] A.A. Samarskij, *The Theory of Difference Schemes* (Nauka, Moskva, 1977, in Russian)

[7] T.E. Simos, An explicit four-step phase-fitted method for the numerical integration of second-order initial-value problems, *J. Comput. Appl. Math.* **55** (1994) 125–133

[8] T.E. Simos, A family of four-step exponentially fitted predictor-corrector methods for the numerical integration of the Schrödinger equation, *J. Comput. Appl. Math.* **58** (1995) 337–344

[9] T. Zhanlav, *Generalized Continuous Analogues of Newton's Method And Spline Methods for Solving Nonlinear Problems in Theoretical Physics* (JINR, Dubna, 1992, Doctoral thesis)

[10] T. Zhanlav and B. Batgerel, On an exact finite-difference scheme for solving eigenvalue problems, *Scientific notes of Nat. Univ. of Mongolia* (to appear)

[11] T. Zhanlav and I.V. Puzynin, The convergence of iterations based on a continuous analogue of Newton's method, *USSR Comput. Math. Math. Phys.* **32** (1992) 729–737