NUMERICAL BOUNDARY CONDITIONS FOR ODE

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Abstract. We consider consistent finite difference approximations of ordinary differential equations, and in particular, parasitic solutions. A framework is introduced, representing a discrete solution as a sum of the true solution and a number of parasitic solutions. We show that within this framework, finite difference equations can be analysed using theory of ordinary differential equations, simplifying the analysis considerably. As an example we give a simple recipe on how to construct numerical boundary conditions such that the solution converges with expected accuracy.

Key words. Parasitic solutions, Numerical boundary conditions, Green's functions

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1. Introduction. When approximating differential equations by high order finite difference schemes one needs to introduce numerical boundary conditions, since wide difference stencils cannot be applied at points close to boundaries. Usually, one uses extrapolation techniques or one-sided difference approximations to overcome this problem. Using these approaches, which essentially are the same, one often finds that the solution of the finite difference equation converges to the solution of the differential equation with expected accuracy. However, sometimes accuracy is lost, and in other cases, the discrete solution even fail to converge.

Kreiss studied finite difference discretisations of ordinary differential equations in great detail [9]. He proved that convergence follows from consistency and stability, and derived algebraic conditions implying that an approximation is stable. He also derived sharp estimates of the accuracy. Independently, Grigorieff developed essentially the same theory [6]. Thus, there is a general theory available, and one may, after some often tedious work, find out whether a particular approximation is stable or not.

We do not try to generalise the results of Kreiss. Instead, we derive a complementary theory that intends to give a good understanding of the finite difference method. For example, our framework leads to a simple recipe on how to construct numerical boundary conditions that yields solutions with expected accuracy. For readers mainly interested in the construction of numerical boundary conditions, we suggest skipping directly to Section 8. Also, the example given in Section 9 may be of interest.

We consider a finite difference approximation

$$\begin{aligned} P_h v &= f_h, \\ B_{k,h} v &= g_{k,h}, \quad k = 1, \dots, p+q, \end{aligned} \tag{1.1}$$

of a boundary value problem

$$\begin{aligned} Pu &= f, \\ B_k u &= g_k, \quad k = 1, \dots, p, \end{aligned} \tag{1.2}$$

where P is a differential operator of order p and P_h is a finite difference operator with stencil width $p+q+1$. Equation (1.2) requires p boundary conditions, and the approximation (1.1) requires an additional q numerical boundary conditions.

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We assume the two problems to be related by the consistency property, implying that every solution of $Pu = f$ is an approximate solution of $P_h v = f_h$. The solutions of the two problems may, in spite of consistency, behave very differently. If they do, standard theory tells us that the missing property is stability, in the sense that v should depend continuously on f_h and $g_{k,h}$. With consistency and stability, the solution of (1.1) converge to the solution of (1.2).

One major difference between (1.1) and (1.2) is that there are p linearly independent solutions of $Pu = 0$, but more than p linearly independent solutions of $P_h v = 0$ as soon as the stencil width of P_h exceeds $p+1$ points. It is even possible to distinguish between p solutions that corresponds to solutions of the differential equation and q extra, parasitic solutions. We show that this difference is the only reason why a discrete solution may fail to converge. With this result in mind, there are two equivalent ways of explaining lack of convergence. Either, one could say that the discretisation is unstable, or one could say that at least one parasitic solution fail to vanish as the grid is refined.

We believe that the introduction of a framework, where a discrete solution is represented as a sum of a true solution and a number of parasitic solutions, is fruitful in many different situations. This idea is not entirely new. In 1959, Dahlquist showed that the discretisation error for linear multi-step methods contains parasitic parts, and that these parts have smooth components that asymptotically satisfy modified differential equations [5]. The result can also be found in Henrici's book [8], see for example Theorem 5.12.

We prove the corresponding result for boundary value problems, and use, as Dahlquist did, the framework as a basis for stability considerations. However, we also argue that our point of view is beneficial in many other kinds of investigations. For example, if we realise that the role of numerical boundary conditions is to force parasitic solutions to vanish, the construction of numerical boundary conditions becomes a straightforward task.

In Appendix B we present another example of the benefits of our framework. Without too much effort, we manage to prove that the Green's function of the finite difference equation (1.1) remains bounded as the grid is refined. This is a quite powerful result that tells a great deal about the discrete solution.

Using this framework, we would like to investigate other areas. In particular, we are interested in the construction and analysis of preconditioners. A preconditioner is often constructed as an approximation of the inverse of a finite difference operator, and is used to improve convergence of iterative solvers. Approximating the inverse is of course the same as approximating the Green's function, although this rather theoretical point of view is usually not taken.

There are many ideas on how to construct and apply preconditioners. Some of these preconditioners show quite good performance, but the analysis of preconditioning techniques is often very hard to pursue. We believe that one of the reasons for this is that parasitic solutions are a part of the Green's function and that they play an important role. In future research, we hope that our new approach will give a better understanding of preconditioners.

The paper is organised as follows. The differential equation and the finite difference approximation are presented in Section 2 and 3. In Section 4 we review the standard theory of finite difference approximations, based on the concepts of consistency, stability and convergence. Section 5 states some lemmas. In Section 7 we present the main theorem, showing that the representation of discrete solutions introduced in Section 6 is adequate. The proof, which is based on Green's function theory, can be found in Appendices A, B and C. To illustrate the usefulness of our new approach, we discuss the construction of boundary conditions in Section 8. An example can be found in Section 9.

We end the paper with a summary and a discussion in Section 10. This section gives an overview of the theory presented in this paper.

2. Differential equation. Consider the differential equation

$$Pu = f, \quad x \in I, \tag{2.1}$$

where $I = (0,1)$ and $f \in C(\bar{I})$. Here, P is a linear differential operator of order p,

$$Pu(x) = \sum_{j=0}^{p} a_j(x) \frac{d^j u}{dx^j}(x),$$

with $a_j(x) \in C(\bar{I})$ and $a_p(x) \equiv 1$. The homogeneous version of Equation (2.1) has p linearly independent solutions [10], and we give p boundary conditions

$$B_k u = \sum_{j=0}^{p-1} c_{j,k}(0) \frac{d^j u}{dx^j}(0) + c_{j,k}(1) \frac{d^j u}{dx^j}(1) = g_k, \quad k = 1, \ldots, p, \tag{2.2}$$

for some constants $c_{j,k}(0)$, $c_{j,k}(1)$ and g_k, assuming they determine the solution uniquely. Boundary conditions involving higher order derivatives can be reduced to the form (2.2) by using (2.1).

As an example we consider the first order differential equation

$$\begin{aligned} \frac{du}{dx}(x) &= 0, \\ u(0) &= g. \end{aligned} \tag{2.3}$$

This problem has the unique solution $u(x) = g$. With constant coefficients it possible to draw a number of conclusions without too much effort. However, the theory covers the more general case with smooth coefficients.

We emphasise that (2.3) serves as a model problem for more general boundary value problems, since it may seem strange to regard Equation (2.3) as a boundary value problem. Initial value problems can usually be solved more efficiently using Runge–Kutta or linear multi-step methods.

However, out of curiosity we note that in some cases it may actually be advantageous to view initial value problems as boundary value problems, since numerical methods for boundary value problems usually have better stability properties. The Dahlquist barriers [4] limits the order of stable linear multi-step methods and there are corresponding results for explicit Runge–Kutta methods, see for example [3].

Also, the construction of stable high order methods for initial value problems may be a difficult task. Therefore, several methods have been proposed where initial value problems are viewed as boundary value problems, see for example [2]. These methods are typically developed for stiff problems, where good stability properties of the numerical method are required.

3. Finite difference approximation. We introduce a uniform grid $x_i = ih$, $i = 0, \dots, N$, where $N = 1/h$ is a positive integer. Equation (2.1) is approximated by

$$P_h v = f_h, \quad i \in I_h, \tag{3.1}$$

where f_h is a uniform approximation of f, that is,

$$\lim_{h \to 0} \max_{0 \le i \le N} |(f_h)_i - f(x_i)| = 0.$$

The difference operator P_h has the form

$$P_h v_i = \sum_{j=0}^{p} a_j(x_i) D^{(j)} v_i,$$

where

$$D^{(j)} v_i = \sum_{k=-m}^{n} b_k^{(j)} h^{-j} v_{i+k},$$

approximates d^j/dx^j for some constants $b_k^{(j)}$ and non-negative integers m and n. Finally, $I_h = \{m, \dots, N-n\}$.

The boundary conditions (2.2) are approximated by

$$B_{k,h} v = \sum_{j=0}^{p-1} c_{j,k}(0) D_{k,0}^{(j)} v_0 + c_{j,k}(1) D_{k,1}^{(j)} v_N = g_{k,h}, \tag{3.2}$$

where $|g_{k,h} - g_k| \to 0$ when $h \to 0$. Here,

$$D_{k,0}^{(j)} v_0 = \sum_{l=0}^{m+n-1} b_{l,k,0}^{(j)} h^{-j} v_l,$$

and

$$D_{k,1}^{(j)} v_N = \sum_{l=0}^{m+n-1} b_{l,k,1}^{(j)} h^{-j} v_{N-l},$$

are approximations of the jth derivative at $x = 0$ and $x = 1$ respectively, for some constants $b_{l,k,0}^{(j)}$ and $b_{l,k,1}^{(j)}$. Boundary conditions involving more than $m+n$ grid points can be reduced to the form (3.2) by using (3.1).

Equation (3.1) has $m+n$ linearly independent solutions [1]. Thus, if $m+n > p$, we need $m+n-p$ numerical boundary conditions. We introduce

$$B_{k,h} v = g_{k,h}, \quad k = p+1, \dots, m+n, \tag{3.3}$$

of the same form as (3.2). One way of choosing the extra boundary conditions (3.3) is to let $B_{k,h} v$ and $g_{k,h}$ approximate $Pu(x)$ and $f(x)$ at $x = 0$ or $x = 1$. More generally, $B_{k,h}$ approximates some functional B_k, and $g_{k,h}$ approaches some number g_k.

For model problem (2.3) we use the approximation

$$\begin{aligned} D_0 v_i &= 0, \quad i = 1, \dots, N-1, \\ v_0 &= g, \\ D_- v_N &= 0. \end{aligned} \tag{3.4}$$

Thus, we have used a one-sided finite difference approximation of the differential equation at $x = 1$ as a numerical boundary condition.

4. Consistency, stability and convergence. We now review known theory about convergence in a Banach space with norm

$$||v|| = \max_{0 \le i \le N} |v_i|.$$

The finite difference equation is said to be *consistent* if for every smooth function $u(x)$

$$\begin{aligned} P_h u(x_i) &= Pu(x_i) + h^s \tilde{f}_i, \\ B_{k,h} u &= B_k u + h^{t_k} \tilde{g}_k, \quad k = 1, \dots, m+n, \end{aligned}$$

for some uniformly bounded $\tilde{f}$, bounded $\tilde{g}_k$, $s \ge 1$ and $t_k \ge 1$. It is *stable* if there exists a constant C such that

$$||v|| \le C \left(||f_h|| + \sum_{k=1}^{m+n} |g_{k,h}| \right).$$

The function v is said to *converge* to u if

$$\lim_{h \to 0} ||R_h u - v|| = 0,$$

where $(R_h u)_i = u(x_i)$.

THEOREM 4.1. *Assume a consistent and stable approximation. Then, the solution of the finite difference equation (3.1), (3.2) and (3.3) converges to the (smooth) solution of the differential equation (2.1) and (2.2).*

Proof. The error $R_h u - v$ satisfies (3.1), (3.2) and (3.3) with f_h and $g_{k,h}$ replaced by $R_h f + h^s \tilde{f} - f_h$ and $g_k + h^{t_k} \tilde{g}_k - g_{k,h}$, and convergence follows from stability. □

Returning to our example, a Taylor expansion shows that

$$\begin{aligned} D_0 u(x_i) &= \frac{du}{dx}(x_i) + \mathrm{O}(h^2), \\ u(x_0) &= u(0), \\ D_- u(x_N) &= \frac{du}{dx}(1) + \mathrm{O}(h), \end{aligned}$$

for every smooth u. Thus, the finite difference equation (3.4) is a consistent approximation of the differential equation (2.3).

The characteristic equation of the finite difference equation (3.4)

$$r^2 - 1 = 0$$

has two roots, $r_1 = 1$ and $r_2 = -1$, and the general solution takes the form

$$v_i = c_0 + (-1)^i c_1,$$

where the constants c_0 and c_1 are determined by the boundary conditions. A simple calculation shows that $c_0 = g$ and $c_1 = 0$, and we conclude that the discretisation is stable.

Since the approximation is both consistent and stable, it follows from Theorem 4.1 that v converge to u. In fact, we just showed that $v_i = g$. Thus, for this simple example the discrete solution coincides with the exact solution even for finite h.

5. Preliminaries. In the following sections we need two lemmas given here. We define the characteristic polynomials

$$\hat{D}^{(j)}(z) = \sum_{k=-m}^{n} b_k^{(j)} h^{-j} z^{k+m}, \quad j = 0, \ldots, p.$$

LEMMA 5.1. *If $D^{(j)}$ is a consistent approximation of d^j/dx^j, there are exactly j zeros of $\hat{D}^{(j)}(z)$ satisfying $z = 1$.*

Proof. By Taylor expansion,

$$D^{(j)}u(x_i) = \sum_{l=0}^{j} \sum_{k=-m}^{n} b_k^{(j)} \frac{k^l h^{l-j}}{l!} \frac{d^l u}{dx^l}(x_i) + \mathrm{O}(h).$$

Since the operator $D^{(j)}$ is a consistent approximation of d^j/dx^j, it follows that

$$\sum_{k=-m}^{n} b_k^{(j)} k^l = \begin{cases} 0, & l = 0, \ldots, j-1, \\ l!, & l = j. \end{cases} \tag{5.1}$$

For $z = 1$, the lth derivative of $\hat{D}^{(j)}(z)$,

$$\frac{d^l}{dz^l}\hat{D}^{(j)}(z) = \sum_{k=-m}^{n} b_k^{(j)} h^{-j} \frac{(k+m)!}{(k+m-l)!} z^{k+m-l}, \quad l = 0, \ldots, j-1,$$

is a linear combination of expressions of the form (5.1), and consequently equals zero. On the other hand, the jth derivative contains one term different from zero, and we conclude that $z = 1$ is a zero of multiplicity j. ☐

For $z \neq 0$ we define the modified finite difference operator

$$P_{z,h} v_i = \sum_{j=0}^{p} a_j(x_i) \sum_{k=-m}^{n} b_k^{(j)} h^{p-1-j} z^k v_{i+k}. \tag{5.2}$$

LEMMA 5.2. *If $u(x)$ is a smooth function and z is a simple zero of $\hat{D}^{(p)}(z)$, $z \neq 0$ and $z \neq 1$, then*

$$P_{z,h} u(x_i) = P_z u(x_i) + O(h),$$

where

$$P_z u(x) = a_{p,z} \frac{du}{dx}(x) + a_{p-1,z}(x) u(x), \tag{5.3}$$

and

$$a_{p,z} = \sum_{k=-m}^{n} b_k^{(p)} k z^k, \quad a_{p-1,z}(x) = a_{p-1}(x) \sum_{k=-m}^{n} b_k^{(p-1)} z^k.$$

Proof. Follows from a Taylor expansion, z being a zero of $\hat{D}^{(p)}(z)$ and $a_p(x) \equiv 1$. ☐

6. Parasitic solutions and a new framework. We begin this section by considering our example. Recall that

$$Pu = \frac{du}{dx},$$

and

$$P_h v = D_0 v.$$

The characteristic polynomial

$$\hat{D}_0(z) = \frac{z^2 - 1}{2h}$$

has two zeros, $z_1 = 1$ and $z_2 = -1$, which is consistent with Lemma 5.1. The general solution has the form

$$v_i = c_0 + (-1)^i c_1.$$

Note that only the first term corresponds to a solution of the differential equation. The second term does not have a counterpart in the solution of the differential equation, and is said to be parasitic.

Once the constants c_0 and c_1 have been determined by the boundary conditions, the solution is known, illustrating that finding a solution is straightforward as long as the difference equation has constant coefficients. In general, a first order difference operator contains a zeroth order term $a_i v_i$, where a_i depends on i. The situation is then completely different, and we cannot use the familiar method of characteristics.

From theory of differential equations, we know that the principal part of a differential operator plays an important role. It determines the overall behaviour of the solution, and a low order disturbance of the differential operator will not changes the characteristics of the solution. The same is true for difference operators. With this in mind we suggest that one should look for a solution of the slightly more general form

$$v_i = (c_0)_i + (-1)^i (c_1)_i,$$

where c_0 and c_1 no longer are constants. Since we have altered a low order term in the difference operator, we keep the same general form of the solution, but expect a perturbation of c_0 and c_1. For small alterations, c_0 and c_1 probably still behave "almost like constants".

In general, finding $(c_0)_i$ and $(c_1)_i$ is just as difficult as determining v_i, and we have not gained anything simply by assuming a particular form of the solution. The idea is therefore to concentrate on the asymptotic behaviour of the solution and try to find the asymptotes of $(c_0)_i$ and $(c_1)_i$. We argue that $(c_0)_i$ and $(c_1)_i$ behave "almost like constants", and that the asymptotes are smooth functions. Therefore, we look for an asymptotic solution of the form

$$u_i = u^{(0)}(x_i) + (-1)^i u^{(1)}(x_i),$$

where $u^{(0)}(x)$ and $u^{(1)}(x)$ are smooth functions.

The asymptotes $u^{(0)}(x)$ and $u^{(1)}(x)$ may be easier to find. It is straightforward to derive a system of differential equations that governs the two functions, and if the system is easy to solve, we are done. Otherwise, we still have the theory of differential equations at our disposal that can be used to investigate the system and its solution. This is the main advantage of our approach; even if a lot of theory have been developed for difference equations, the theory of differential equations is often more powerful and may simplify our analysis considerably.

We now show how to derive the system of differential equations for our model problem. We begin by noting that $u_i = u^{(0)}(x_i) + (-1)^i u^{(1)}(x_i)$ implies

$$D_0 u_i = D_0 u^{(0)}(x_i) + (-1)^i (-D_0 u^{(1)}(x_i)). \tag{6.1}$$

This motivates the introduction of a modified finite difference operator

$$P_{\text{-}1,h} v = -D_0 v,$$

which, of course, is a consistent approximation of

$$P_{\text{-}1} u = -\frac{du}{dx},$$

a result that coincides with Lemma 5.2.

Next, we realise that if $u^{(0)}(x)$ and $u^{(1)}(x)$ are smooth, the two terms in (6.1) are linearly independent. Therefore, we can separate the original finite difference equation $D_0 v = 0$ into two equations that are consistent approximations of

$$\begin{aligned} \frac{du^{(0)}}{dx} &= 0, \\ -\frac{du^{(1)}}{dx} &= 0. \end{aligned} \tag{6.2}$$

The boundary condition $v_0 = g$ translates directly into

$$u^{(0)}(0) + u^{(1)}(0) = g, \tag{6.3}$$

but the condition $D_{\text{-}} v_N = 0$ needs to be examined more carefully. A Taylor expansion shows that

$$\begin{aligned} D_{\text{-}} u_N &= \frac{u^{(0)}(x_N) - u^{(0)}(x_{N-1})}{h} + (-1)^N \frac{u^{(1)}(x_N) + u^{(1)}(x_{N-1})}{h} \\ &= \frac{du^{(0)}}{dx}(1) + (-1)^N \left(\frac{2}{h} u^{(1)}(1) - \frac{du^{(1)}}{dx}(1) \right) + \mathrm{O}(h). \end{aligned}$$

This expression approaches zero only if

$$u^{(1)}(1) = 0. \tag{6.4}$$

To summarise, (6.2), (6.3) and (6.4) is a system of differential equations for the unknown functions $u^{(0)}(x)$ and $u^{(1)}(x)$, where the coupling is in the boundary conditions only. Once again we find that both $u^{(0)}(x)$ and $u^{(1)}(x)$ are constants, and from the boundary conditions follows $u^{(0)}(x) = g$ and $u^{(1)}(x) = 0$, implying $u_i = g$. Thus, by means of Taylor expansions, we have derived a system of differential equations that governs the smooth components $u^{(0)}(x)$ and $u^{(1)}(x)$ of the asymptotic solution.

We now leave our example and consider the general case. As proven in Lemma 5.1, there are $m + n - p$ zeros of the characteristic polynomial of the principal part of the finite difference operator satisfying $z \neq 1$. Let $q = m + n - p$, and number the zeros so that $z_j \neq 1$, $j = 1, \dots, q$, and $|z_j| \leq 1$, $j = 1, \dots, q_l$. We assume z_j, $j = 1, \dots, q$, to be distinct since this will simplify the presentation considerably.

The main result of this paper is that the solution of the finite difference equation (3.1), (3.2) and (3.3) approaches u given by

$$u_i = u^{(0)}(x_i) + \sum_{j=1}^{q_l} z_j^i h^{p-1} u^{(j)}(x_i) + \sum_{j=q_l+1}^{q} z_j^{i-N} h^{p-1} u^{(j)}(x_i), \tag{6.5}$$

when h tends to zero, where $u^{(0)}, \dots, u^{(q)}$ satisfy a system of differential equations

$$\begin{array}{rcll} Pu^{(0)} &=& f, & \\ P_{z_j} u^{(j)} &=& 0, & j = 1, \dots, q, \\ B'_k u &=& g'_k, & k = 1, \dots, m+n. \end{array} \tag{6.6}$$

Thus, we view the discrete solution as a sum of a true solution and a number of parasitic solutions. If for example $u^{(j)}(x) \equiv 0$, $j = 1, \dots, q$, we have convergence.

In (6.6), the differential operators P_{z_j} are defined by (5.3), and the boundary conditions are derived in a way similar to the construction of P_{z_j}. One assumes a solution of the form (6.5) with $u^{(j)}$ smooth and define modified boundary functionals $B_{k,z_j,h}$ from

$$B_{k,h} u = B_{k,h} u^{(0)} + \sum_{j=1}^{q_l} B_{k,z_j,h} u^{(j)} + \sum_{j=q_l+1}^{q} z_j^{-N} B_{k,z_j,h} u^{(j)}.$$

By Taylor expansion one finds functionals B_{k,z_j} satisfying

$$B_{k,z_j,h} u^{(j)} = h^{r_k^{(j)}} B_{k,z_j} u^{(j)} + \mathrm{O}(h^{r_k^{(j)}+1}),$$

for some integer $r_k^{(j)}$. By scaling the boundary condition with some power of h and possibly with factors z_j^N for some of the j's, one usually finds a well defined functional B'_k operating on $u^{(0)}, \dots, u^{(q)}$ and satisfying

$$B'_{k,h} u = B'_k u + \mathrm{O}(h), \quad k = 1, \dots, m+n, \tag{6.7}$$

where $B'_{k,h}$ is the scaled boundary functional. Compare to the derivation of (6.4). In some cases, one needs to specify the way in which h tends to zero. For instance, consider the boundary condition $v_N = 0$, applied to our model problem. The asymptotic condition then reads $u^{(0)}(1) + (-1)^N u^{(1)}(1) = 0$, something that states two different things, depending on whether N is odd or even.

If $g'_{k,h} = (B'_{k,h} u / B_{k,h} u) g_{k,h}$ converges when h tends to zero, we define

$$g'_k = \lim_{h \to 0} g'_{k,h}, \quad k = 1, \dots, m+n.$$

We state for later reference that the system (6.6) has the property that if the solution is unique, it depends continuously on f and g'_k [10], that is, there exists a constant C such that

$$\max_{x \in \bar{I}} |u^{(j)}(x)| \leq C \left(\max_{x \in I} |f(x)| + \sum_{j=1}^{m+n} |g'_k| \right), \quad j = 0, \dots, q. \tag{6.8}$$

7. Main result. We now prove that the solution of the finite difference equation (3.1), (3.2) and (3.3) approaches u as defined in (6.5) and (6.6). We use the concepts of consistency and stability, and begin by addressing the former.

THEOREM 7.1. *For every set of smooth functions $u^{(j)}$, the function u, as defined in (6.5), satisfies*

$$\begin{aligned}P_h u_i =& P u^{(0)}(x_i) + \sum_{j=1}^{q_l} z_j^i P_{z_j} u^{(j)}(x_i) + \sum_{j=q_l+1}^{q} z_j^{i-N} P_{z_j} u^{(j)}(x_i) \\ &+ h^s \tilde{f}_i + \sum_{j=1}^{q_l} z_j^i h^{s_j} \tilde{f}_i^{(j)} + \sum_{j=q_l+1}^{q} z_j^{i-N} h^{s_j} \tilde{f}_i^{(j)}, \\ B'_{k,h} u =& B'_k u + h^{t_k} \tilde{g}_k, \quad k = 1, \dots, m+n,\end{aligned} \tag{7.1}$$

for some uniformly bounded $\tilde{f}$ and $\tilde{f}^{(j)}$, bounded $\tilde{g}_k$, $s \geq 1$, $s_j \geq 1$ and $t_k \geq 1$.

Proof. Follows from Lemma 5.2 and Equation (6.7). □

The proof of stability is a little bit longer, and we use Appendix A and B for deriving the theory. The proof is presented in Appendix C.

THEOREM 7.2. *Assume z_j, $j = 1, \dots, q$, to be distinct and different from zero. If (6.6) has a unique solution, there exists a constant C such that the solution of the finite difference equation (3.1), (3.2) and (3.3) satisfies*

$$||v|| \leq C \left(||f_h|| + \sum_{k=1}^{m+n} |g'_{k,h}| \right).$$

The main result now follows directly.

THEOREM 7.3. *Assume z_j, $j = 1, \dots, q$, to be distinct and different from zero. Let v be the solution of (3.1), (3.2) and (3.3), and let u be defined by (6.5) and (6.6). If (6.6) has a unique solution, then $||u - v|| \to 0$ when h tends to zero.*

Proof. From Theorem 7.1 follows that the difference $u_i - v_i$ satisfies (3.1), (3.2) and (3.3) with f_h and $g'_{k,h}$ replaced by

$$f(x_i) + h^s \tilde{f}_i + \sum_{j=1}^{q_l} z_j^i h^{s_j} \tilde{f}_i^{(j)} + \sum_{j=q_l+1}^{q} z_j^{i-N} h^{s_j} \tilde{f}_i^{(j)} - (f_h)_i,$$

and $g'_k + h^{t_k} \tilde{g}_k - g'_{k,h}$, and the result follows from Theorem 7.2. □

8. Constructing boundary conditions. The theory derived above can be used to prove convergence for a given finite difference discretisation, but it is also a useful tool in the construction of boundary conditions. Given a differential equation (2.1), (2.2) and a finite difference approximation (3.1), boundary conditions can be derived by assuming a solution of the form (6.5) and approximating

$$\begin{aligned} B_k u^{(0)} &= g_k, \quad k = 1, \dots, p, \\ u^{(j)}(0) &= 0, \quad j = 1, \dots, q_l, \\ u^{(j)}(1) &= 0, \quad j = q_l + 1, \dots, q, \end{aligned} \tag{8.1}$$

in a consistent way. The numerical boundary conditions will then in general not approximate the differential equation. However, by this choice (6.6) has a unique solution with $u^{(j)}(x) \equiv 0$, $j = 1, \dots, q$, if the original problem (2.1) and (2.2) has a unique solution, and Theorem 7.3 guarantees convergence.

We can also estimate the accuracy.

THEOREM 8.1. *Assume z_j, $j = 1, \dots, q$, to be distinct and different from zero, $f_h = R_h f$ and $g'_{k,h} = g'_k$. If the boundary conditions are consistent approximations of (8.1) and*

$$\begin{array}{rcll} P_h \varphi & = & P\varphi + h^s \tilde{f}, & \\ B'_{k,h}\varphi & = & B_k \varphi + h^s \tilde{g}_k, & k = 1, \dots, p, \\ B'_{k,h}\varphi & = & h^s \tilde{g}_k, & k = p+1, \dots, p+q, \end{array}$$

for every smooth φ, then the solution $u(x)$ of the differential equation (2.1) and (2.2), and the solution v of the finite difference equation (3.1), (3.2) and (3.3) satisfies $||R_h u - v|| = O(h^s)$.

Proof. With boundary conditions (8.1), system (6.6) obviously has a unique solution with $u^{(j)}(x) \equiv 0$, $j = 1, \dots, q$, and $u^{(0)}(x)$ being the solution of the original problem (2.1) and (2.2), provided that the original problem has a unique solution. Therefore, $f_h = R_h f$ and $g'_{k,h} = g'_k$ implies that the error $e_i = u_i - v_i = u^{(0)}(x_i) - v_i$ satisfies

$$\begin{aligned} P_h e &= h^s \tilde{f}, \\ B'_{k,h} e &= h^s \tilde{g}_k, \end{aligned}$$

and the result follows from Theorem (7.2). $\square$

We now apply this technique to our model problem. Recall that

$$u_i = u^{(0)}(x_i) + (-1)^i u^{(1)}(x_i).$$

According to (8.1), we should look for a consistent approximation of

$$\begin{aligned} u^{(0)}(0) &= g, \\ u^{(1)}(1) &= 0. \end{aligned}$$

A Taylor expansion shows that

$$\begin{aligned} \frac{3}{4}u_0 + \frac{1}{2}u_1 - \frac{1}{4}u_2 &= u^{(0)}(0) + \mathrm{O}\left(h^2 \frac{d^2u^{(0)}}{dx^2}(0) + h\frac{du^{(1)}}{dx}(0)\right), \\ \frac{1}{4}u_N - \frac{1}{2}u_{N-1} + \frac{1}{4}u_{N-2} &= u^{(1)}(1) + \mathrm{O}\left(h^2 \frac{d^2u^{(0)}}{dx^2}(1) + h\frac{du^{(1)}}{dx}(1)\right). \end{aligned}$$

Thus,

$$\begin{aligned} \frac{3}{4}v_0 + \frac{1}{2}v_1 - \frac{1}{4}v_2 &= g, \\ \frac{1}{4}v_N - \frac{1}{2}v_{N-1} + \frac{1}{4}v_{N-2} &= 0, \end{aligned}$$

is a consistent approximation, with approximation order two for the $u^{(0)}$-part and one for the $u^{(1)}$-part. According to Theorem (8.1), consistency is sufficient for the $u^{(1)}$-part, and this set of boundary conditions gives a second order accurate solution.

By using the difference equation it is possible to write the conditions as

$$\begin{aligned} \frac{1}{2}(v_0 + v_1) &= g, \\ \frac{1}{2}(v_N - v_{N-1}) &= 0. \end{aligned}$$

9. Numerical example. As an example, we consider the differential equation

$$\begin{aligned} \frac{d^2u}{dx^2}(x) - x\,u(x) &= 0, \\ u(0) &= \mathrm{Ai}(0), \\ u(1) &= \mathrm{Ai}(1), \end{aligned}$$

with solution $u(x) = \mathrm{Ai}(x)$, where $\mathrm{Ai}(x)$ is the Airy-function.

We discretise the second derivative using a fourth order approximation

$$D^{(2)}v_i = \frac{-v_{i-2} + 16v_{i-1} - 30v_i + 16v_{i+1} - v_{i+2}}{12h^2},$$

and the zero order term is approximated simply by $-x_i v_i$.

In this example, the $D^{(2)}$ operator is the principal part of the difference operator, and for later use we state that as Lemma 5.1 predicts, the corresponding characteristic polynomial has two roots equal to one. The two remaining roots are $z_1 = 7 - 4\sqrt{3}$ and $z_2 = 7 + 4\sqrt{3}$.

We consider two sets of boundary conditions. The first set reads

$$\begin{aligned} v_0 &= \mathrm{Ai}(0), \\ D_+D_-v_1 - x_1 v_1 &= 0, \\ D_+D_-v_{N-1} - x_{N-1}v_{N-1} &= 0, \\ v_N &= \mathrm{Ai}(1). \end{aligned}$$

Extrapolation techniques and one-sided finite difference approximations are the two most common ways of constructing numerical boundary conditions. Here, we illustrate that the two techniques are related.

It is not possible to apply $D^{(2)}$ to v_1 since the function v_i is not defined at $i = -1$. If we use cubic extrapolation to express v_{-1} in terms of well defined values within the domain, $D^{(2)}v_1$ turns into $D_+D_-v_1$. The fact that D_+D_- also approximates the second derivative illustrates the relation between the two techniques. The numerical boundary condition at the right boundary was constructed in the same way.

Note that the cubic extrapolation procedure is only third order accurate. However, for numerical boundary conditions, the accuracy can lowered one order, without destroying the expected convergence rate. See for instance the discussion in [7], where mixed initial boundary value problems are considered. For sharp error estimates regarding the numerical solution of two point boundary value problems, we refer to [9].

To find out whether this first set of boundary conditions yields a stable approximation and hence a converging solution, we may use the theory by Kreiss [9], or the theory derived in this paper. Here, we leave out the calculations and examine the choice of boundary conditions by a numerical experiment. As shown in Table 9.1, the finite difference solution converge to the true solution, and the convergence is of order four.

TABLE 9.1

The error as a function of N for the first set of boundary conditions.

N	16	32	64	128	256
$\|\|R_h u - v\|\|$	$6.9 \cdot 10^{-7}$	$4.5 \cdot 10^{-8}$	$2.9 \cdot 10^{-9}$	$1.8 \cdot 10^{-10}$	$1.2 \cdot 10^{-11}$
$\|\|R_h u - v\|\|/h^4$	0.045	0.048	0.049	0.049	0.050

The second set of boundary conditions we suggest is

$$\begin{aligned} v_0 &= \mathrm{Ai}(0), \\ \frac{97+56\sqrt{3}}{144}(v_0 - 4v_1 + 6v_2 - 4v_3 + v_4) &= 0, \\ \frac{97+56\sqrt{3}}{144}(v_N - 4v_{N-1} + 6v_{N-2} - 4v_{N-3} + v_{N-4}) &= 0, \\ v_N &= \mathrm{Ai}(1). \end{aligned}$$

These conditions are based on the idea introduced in Section 8 and approximate

$$\begin{aligned} u^{(0)}(0) &= \mathrm{Ai}(0), \\ u^{(1)}(0) &= 0, \\ u^{(2)}(1) &= 0, \\ u^{(0)}(1) &= \mathrm{Ai}(1). \end{aligned}$$

Since

$$u_0 = u^{(0)}(0) + hu^{(1)}(0) + z_2^{-N} hu^{(2)}(0),$$

the first condition is consistent. The approximation of the $u^{(0)}$-part is of infinite order and the $u^{(1)}$-part is of first order. The $u^{(2)}$-part approaches zeros faster than every power of h since $|z_2| > 1$.

The second condition was derived by choosing $c_0, \ldots, c_4$ such that a Taylor expansion gives

$$c_0 u_0 + \cdots + c_4 u_4 = hu^{(1)}(0) + \mathrm{O}\left(h^4 \frac{d^4 u^{(0)}}{dx^4}(0) + h^2 \frac{du^{(1)}}{dx}(0)\right)$$

Here, we have left out the $u^{(2)}$-part, since this term contains the factor z_2^{-N}. After scaling with h^{-1}, this choice obviously gives a consistent approximation. However, the order of approximation for the $u^{(0)}$-part is only three and Theorem 8.1 does not guarantee convergence of order four. Now, since this is a numerical boundary condition the third order approximation will not destroy the rate of convergence. Once again, we refer to [9] for error estimates.

The same technique was used for the third and fourth condition. At the right boundary, the $u^{(1)}$-part can be left out, since these terms contains expressions of the form z_1^N and since $|z_1| < 1$.

According to Table 9.2, numerical results verify that the solution is fourth order accurate.

TABLE 9.2
The error as a function of N for the second set of boundary conditions.

N	16	32	64	128	256
$\|\|u-v\|\|$	$9.5 \cdot 10^{-6}$	$6.3 \cdot 10^{-7}$	$4.0 \cdot 10^{-8}$	$2.6 \cdot 10^{-9}$	$1.6 \cdot 10^{-10}$
$\|\|u-v\|\|/h^4$	0.62	0.66	0.68	0.69	0.70

Finally, we note that our approach produces numerical boundary conditions that look very much like cubic interpolation.

10. Summary and discussion. We consider a finite difference approximation

$$\begin{aligned} P_h v &= f_h, \\ B_{k,h} v &= g_{k,h}, \quad k = 1, \ldots, p+q, \end{aligned} \tag{10.1}$$

of a two point boundary value problem

$$\begin{aligned} Pu &= f, \\ B_k u &= g_k, \quad k = 1, \ldots, p, \end{aligned} \tag{10.2}$$

where P is a differential operator of order p and P_h is a finite difference operator with stencil width $p+q+1$. Equation (10.2) requires p boundary conditions, and (10.1) requires an additional q numerical boundary conditions.

We show that the finite difference equation (10.1) is closely related to a certain system of differential equations

$$\begin{array}{rcll} Pu^{(0)} &=& f, & \\ P_{z_j} u^{(j)} &=& 0, & j = 1, \ldots, q, \\ B'_k u &=& g'_k, & k = 1, \ldots, p+q. \end{array} \tag{10.3}$$

From theory of ordinary differential equations, we know that the solutions of (10.3) depend continously on f and g'_k. Interestingly enough, it follows as a consequence that v also depends continuously on f and g'_k, and using this property we prove that v approaches the function

$$u^{(0)}(x_i) + \sum_{j=1}^{q_l} z_j^i h^{p-1} u^{(j)}(x_i) + \sum_{j=q_l+1}^{q} z_j^{i-N} h^{p-1} u^{(j)}(x_i), \tag{10.4}$$

when h tends to zero. Here, $u^{(0)}, \ldots, u^{(q)}$ satisfy (10.3), and z_j are the characteristic roots different from one of the principal part of the finite difference operator P_h. The first term in (10.4) is the true solution and the other terms are parasitic.

There are three possible reasons why the discrete solution may fail to converge.

1. The finite difference equation (10.1) may not have a unique solution. In this case, there is no unique solution of (10.3).
2. The boundary data g'_k of system (10.3) may not exist. Recall that the numbers g'_k are the limits as h tends to zero of boundary data $g_{k,h}$, scaled in a certain way. In this case, (10.3) is not even well defined.
3. If (10.3) has a unique solution, it may still happen that at least one of the functions $u^{(j)}(x)$, $j = 1, \ldots, q$, is different from zero. If $p = 1$, the parasitic part will not vanish when h tends to zero.

In all three cases it is sufficient to study the system (10.3).

In this context, it is easy to construct boundary conditions that give a convergent solution. One could for instance use consistent approximations of

$$\begin{array}{rcll} B_k u^{(0)} &=& g_k, & k = 1, \ldots, p, \\ u^{(j)}(0) &=& 0, & j = 1, \ldots, q_l, \\ u^{(j)}(1) &=& 0, & j = q_l + 1, \ldots, q. \end{array} \tag{10.5}$$

We derive estimates of the accuracy showing that full approximation order is necessary only for the true boundary conditions.

The choice of boundary conditions is in no way unique. There are many sets of conditions that give solutions converging with expected order of accuracy. By numerical experiments we compare a set of heuristically constructed boundary conditions with a set that approximates (10.5). Even though the rate of convergence is the same for both methods, the heuristic approach gives an error that is about 10 times smaller.

There are probably more clever ways of choosing the set of boundary conditions and we intend to look into this in the future. However, we would like to stress that our main goal is to achieve a better understanding of the finite difference method, and that this understanding may be used in many different applications. Our study of numerical boundary conditions intends to illustrate the power of the new theory. Recall that we have actually provided a simple recipe on how to construct a set boundary conditions that we know, a priori, will give us the expected rate of convergence.

The only theorem in this paper that requires more than a few lines to prove, states that the solution of the finite difference equation (10.1) depends continuously on f and g_k'. It is interesting to note that the proof uses theory of ordinary differential equations in great extent, but almost no theory of difference equations. This is possible since (10.3) contains differential equations governing the behaviour not only of the true solution, but also of the parasitic solutions.

The proof of the theorem is in two steps. First, we show that the Green's function of the finite difference equation (10.1) remains bounded when h tends to zero. This follows essentially from the fact that the solutions of (10.3) are bounded. The second step is to construct a function φ such that $w = v - \varphi$ satisfies the semi-homogenous problem

$$\begin{aligned} P_h w &= f_h - P_h \varphi, \\ B'_{k,h} w &= 0, \quad k = 1, \dots, p+q. \end{aligned} \tag{10.6}$$

As a consequence of the fact that the solutions of (10.3) depend continuously on boundary data, the function φ has the same kind of continuous dependency. Since the Green's function, which defines an inverse of (10.6), is bounded, w depends continously on the right hand side, and the result follows for $v = w + \varphi$.

The little need of theory of difference equations raises hope that it might be possible to investigate partial finite difference equations from a similar point of view. The theory of partial differential equations is of course a much more complicated matter, and we cannot hope for any general statements about convergence. However, it might be possible to derive a system of partial differential equations, corresponding to (10.3), that governs not only the true solution, but also the parasitic solutions. Furthermore, we hope to understand when stability of the finite difference equation is inherited from this system. It would then be possible to prove convergence in those cases where the behaviour of the system is understood.

In one dimension it seems to be quite easy to construct numerical boundary conditions. Qualified guesses usually works just fine. In several dimensions, however, the situation is almost the opposite. Anyone who have tried to use high order approximations knows that the construction of numerical boundary conditions is a difficult task. Heuristic approaches often fail. This is one of the reasons why Padé approximations and other compact schemes have become popular.

Extending the theory to partial finite difference equations, and searching for a recipe on the construction of boundary conditions in several dimensions is a subject of future research.

Appendix A. Green's function and adjoint equation. The remaining part of the paper is devoted to the proof of Theorem 7.2. The proof uses the well known theory of Green's functions, and in this section we discuss some of their properties.

A *Green's function* $G_{i,j}$ is for every $j \in I_h$ a solution of the problem

$$\begin{aligned} P_h G_{i,j} &= 0, & i \neq j, \\ P_h G_{i,j} &= h^{-1}, & i = j, \\ B_{k,h} G_{i,j} &= 0, & k = 1, \dots, m+n. \end{aligned}$$

Given a set of linearly independent solutions and some linearly independent boundary conditions, the Green's function can be constructed, and existence follows.

It is easy to verify that if $G_{i,j}$ is a Green's function, then

$$v_i = \sum_{j \in I_h} G_{i,j} (f_h)_j \, h,$$

is a solution of the semi-homogenous problem

$$\begin{aligned} P_h v &= f_h, \\ B_{k,h} v &= 0, \quad k = 1, \dots, m+n. \end{aligned} \tag{A.1}$$

The *formal adjoint* P_h^* of P_h, as defined in Section 3, is given by

$$P_h^* v_i = \sum_{j=0}^{p} \sum_{k=-m}^{n} b_k^{(j)} h^{-j} a_j(x_{i-k}) v_{i-k}.$$

The importance of this definition lies in the fact that summation by parts yields

$$\sum_{i \in I_h} \mu_i P_h \nu_i \, h = \sum_{i \in I_h} (P_h^* \mu_i) \nu_i \, h, \tag{A.2}$$

for every μ and ν equal to zero for $i \in \{0, \dots, m-1, N-n+1, \dots, N\}$. We also define the *adjoint* to (A.1) by

$$\begin{aligned} P_h^* v &= f_h^*, \\ B_{k,h}^* v &= 0, \quad k = 1, \dots, m+n, \end{aligned} \tag{A.3}$$

where $B_{k,h}^* v = 0$ denote a set of $m+n$ boundary conditions such that (A.2) holds for every μ and ν satisfying $B_{k,h}^* \mu = 0$ and $B_{k,h} \nu = 0$. According to the next theorem, the Green's function satisfies the direct problem in its first variable and the adjoint problem in its second variable.

THEOREM A.1. *The Green's function $G_{i,j}$ and the Green's function $G_{i,j}^*$ of the adjoint equation satisfy $G_{i,j} = G_{j,i}^*$, $i, j \in I_h$.*

Proof. Since $G_{i,j}$ and $G_{i,j}^*$ are Green's functions,

$$\begin{aligned} 0 &= \sum_{k \in I_h} G_{k,i}^* P_h G_{k,j} \, h - \sum_{k \in I_h} (P_h G_{k,j}) G_{k,i}^* \, h \\ &= \sum_{k \in I_h} (P_h^* G_{k,i}^*) G_{k,j} \, h - \sum_{k \in I_h} (P_h G_{k,j}) G_{k,i}^* \, h \\ &= G_{i,j} - G_{j,i}^*, \end{aligned}$$

and the equality follows. ∎

Appendix B. Existence of a bounded Green's function. In this section, we show that a uniformly bounded approximation of the Green's function can be constructed, and as a consequence, that the Green's function itself is bounded. We say that $v_{i,j}$ is *uniformly bounded* if

$$\limsup_{h\to 0} \max_{0\le i,j\le N} |v_{i,j}| < \infty.$$

Let $y_r(x)$, $r = 1,\ldots,p$, be a set of linearly independent solutions of $Pu = 0$, and let $y_{p+r}(x)$ be a solution of $P_{z_r}u = 0$, $r = 1,\ldots,q$. For some constants $c_1,\ldots,c_{p+q}$ and $d_1,\ldots,d_{p+q}$ we introduce

$$\tilde{G}^{\text{left}}_{i,j} = \sum_{r=1}^{p} c_r\, y_r(x_i) + \sum_{r=1}^{q_l} c_{p+r}\, z_r^i h^{p-1} y_{p+r}(x_i) + \sum_{r=q_l+1}^{q} c_{p+r}\, z_r^{i-N} h^{p-1} y_{p+r}(x_i),$$

and

$$\tilde{G}^{\text{right}}_{i,j} = \sum_{r=1}^{p} d_r\, y_r(x_i) + \sum_{r=1}^{q_l} d_{p+r}\, z_r^i h^{p-1} y_{p+r}(x_i) + \sum_{r=q_l+1}^{q} d_{p+r}\, z_r^{i-N} h^{p-1} y_{p+r}(x_i).$$

We require

$$\begin{aligned} \tilde{G}^{\text{right}}_{i,j} &= \tilde{G}^{\text{left}}_{i,j}, \quad i = j-m+1,\ldots,j+n-1, \\ \tilde{G}^{\text{right}}_{j+n,j} &= \tilde{G}^{\text{left}}_{j+n,j} + \left(\sum_{j'=0}^{p} a_{j'}(x_j) b_n^{(j')} h^{1-j'}\right)^{-1}, \end{aligned} \tag{B.1}$$

and

$$B'_{k,h}\tilde{G} = 0, \quad k = 1,\ldots,m+n, \tag{B.2}$$

where

$$\tilde{G}_{i,j} = \begin{cases} \tilde{G}^{\text{left}}_{i,j}, & i = 0,\ldots,j-1, \\ \tilde{G}^{\text{right}}_{i,j}, & i = j+1,\ldots,N, \end{cases}$$

with $\tilde{G}_{j,j} = \tilde{G}^{\text{left}}_{j,j}$ if $n > 0$, and $\tilde{G}_{j,j} = \tilde{G}^{\text{right}}_{j,j}$ otherwise. Some simple algebra shows that by this construction,

$$\begin{aligned} P_h\tilde{G}_{i,j} &= \mathrm{O}(h), & i &\ne j, \\ P_h\tilde{G}_{i,j} &= h^{-1} + \mathrm{O}(h), & i &= j, \\ B'_{k,h}\tilde{G} &= 0, & k &= 1,\ldots,m+n, \end{aligned}$$

for every $j \in I_h$. Thus, $\tilde{G}$ is an approximation of the Green's function.

Next, we prove that $\tilde{G}_{i,j}$ is uniformly bounded. From theory of ordinary differential equations we know that $y_r(x)$, $r = 1,\ldots,p+q$, are continuous functions on the closed interval $\bar{I}$, and therefore bounded. Thus, it is sufficient to prove that $c_1, \ldots, c_{p+q}$ and $d_1, \ldots, d_{p+q}$ given by (B.1) and (B.2) remain bounded when $h \to 0$.

Condition (B.1) is a system of equations

$$Ae = b, \tag{B.3}$$

where $e = (d_1 - c_1, \ldots, d_{p+q} - c_{p+q})^T$ and $b = (0, \ldots, 0, \mathrm{O}(h^{p-1}))^T$.

A Taylor expansion at $x = x_{j-m+1}$ shows that

$$A = (A_1 W \;\; CA_2) + h^p B,$$

where B is an O(1) matrix. Here,

$$A_1 = \begin{pmatrix} 1 & x_0 & \cdots & \dfrac{x_0^{p-1}}{(p-1)!} \\ \vdots & \vdots & & \vdots \\ 1 & x_{m+n-1} & \cdots & \dfrac{x_{m+n-1}^{p-1}}{(p-1)!} \end{pmatrix}.$$

The *Wronskian matrix*

$$W = \begin{pmatrix} y_1(x_{j-m+1}) & \cdots & y_p(x_{j-m+1}) \\ \vdots & & \vdots \\ \dfrac{d^{p-1}y_1}{dx^{p-1}}(x_{j-m+1}) & \cdots & \dfrac{d^{p-1}y_p}{dx^{p-1}}(x_{j-m+1}) \end{pmatrix},$$

is non-singular since $y_1, \ldots, y_p$ are linearly independent. We denote the first p rows of

$$C = \begin{pmatrix} z_1^0 & \cdots & z_q^0 \\ \vdots & & \vdots \\ z_1^{m+n-1} & \cdots & z_q^{m+n-1} \end{pmatrix},$$

by C_1, and the remaining q rows, the *Casoratian matrix*, by C_2. The diagonal matrix

$$A_2 = h^{p-1} \begin{pmatrix} z_1^{j-m+1} y_{p+1}(x_{j-m+1}) & & \\ & \ddots & \\ & & z_q^{j-m+1} y_{p+q}(x_{j-m+1}) \end{pmatrix},$$

is non-singular since $z_j \neq 0$, $j = 1, \ldots, q$, and the general solution of $P_z u = 0$ is

$$u(x) = c \exp\left(-\int \frac{a_{p-1,z}(x)}{a_{p,z}(x)}\, dx\right),$$

implying $y_r(x) \neq 0$ for every $x \in I$, $r = p+1, \ldots, p+q$.

An approximate inverse of A can be constructed. Define a matrix D,

$$D = h^{-p} \begin{pmatrix} D_1 & 0 \\ D_2 & I \end{pmatrix},$$

where the elements on row $j+1$ of D_1 are proportional to h^{p-j} and satisfy

$$h^{-p} \sum_{k=1}^{p} [D_1]_{j+1,k} u(x_{k-1}) = \frac{d^j u}{dx^j}(x_0) + \mathrm{O}(h^p), \quad j = 0, \ldots, p-1,$$

and the elements of D_2 are independent of h and satisfy

$$h^{-p}\sum_{k=1}^{p}[D_2]_{j,k}u(x_{k-1}) + h^{-p}u(x_{p-1+j}) = \frac{d^p u}{dx^p}(x_0) + \mathrm{O}(h^p),$$

$j = 1, \ldots, q$. These difference operators differentiate polynomials of degree less then p exact, so

$$DA_1 = \begin{pmatrix} I \\ 0 \end{pmatrix}.$$

Since both $(D_2 \;\; I)$ and C have linearly independent rows, it follows that the rows of $D_2C_1 + C_2$ are linearly independent. Therefore, $(D_2C_1 + C_2)^{-1}$ exists. Let

$$Q = \begin{pmatrix} W^{-1} & 0 \\ 0 & A_2^{-1}(D_2C_1 + C_2)^{-1} \end{pmatrix} D.$$

After multiplying both sides of (B.3) from the left with Q, e satisfies

$$e + h\tilde{B}e = \tilde{b},$$

where $\tilde{B}$ and $\tilde{b}$ are $\mathrm{O}(1)$, and we conclude that $d_i - c_i = \mathrm{O}(1)$. Thus, Equation (B.1) can be used to express d_i in terms of c_i, and if d_i is $\mathrm{O}(1)$, so is c_i.

It remains to investigate (B.2). With $u^{(0)} = c_1\, y_1 + \cdots + c_p\, y_p$ and $u^{(r)} = c_{p+r}\, y_{p+r}$, $r = 1, \ldots, q$, we find that $B_k' u = g_k'$, $k = 1, \ldots, m+n$, can be written as a system of equations

$$A_b c = g,$$

where $g = (g_1', \ldots, g_{m+n}')^T$, and A_b is non-singular if (6.6) has a unique solution. From Taylor expansion and $d_i - c_i = \mathrm{O}(1)$ follows that (B.2) can be written

$$A_b c + hB_b c + \tilde{g} = 0,$$

where B_b and $\tilde{g}$ are $\mathrm{O}(1)$. Thus, (B.2) determines c_i uniquely, and c_i is $\mathrm{O}(1)$.

To conclude, we have proved the following theorem.

THEOREM B.1. *There exists a uniformly bounded function $\tilde{G}_{i,j}$ satisfying*

$$\begin{array}{rcll} P_h\tilde{G}_{i,j} & = & h\,\tilde{w}_{i,j}, & i \neq j, \\ P_h\tilde{G}_{i,j} & = & h^{-1} + h\,\tilde{w}_{i,j}, & i = j, \\ B_{k,h}'\tilde{G} & = & 0, & k = 1, \ldots, m+n. \end{array}$$

for every $j \in I_h$ and some uniformly bounded $\tilde{w}_{i,j}$.

Boundedness of the Green's function itself now follows directly.

THEOREM B.2. *The Green's function is uniformly bounded.*

Proof. Let $G_{i,j}^*$ denote the Green's function of the adjoint problem. From Theorem B.1 follows that

$$\begin{aligned} 0 &= \sum_{k\in I_h} G_{k,j}^* P_h\tilde{G}_{k,i}\, h - \sum_{k\in I_h} (P_h\tilde{G}_{k,i})G_{k,j}^*\, h \\ &= \sum_{k\in I_h} (P_h^* G_{k,j}^*)\tilde{G}_{k,i}\, h - \sum_{k\in I_h} (P_h\tilde{G}_{k,i})G_{k,j}^*\, h \\ &= \tilde{G}_{j,i} - G_{i,j}^* - \sum_{k\in I_h} \tilde{w}_{k,i}G_{k,j}^*\, h^2, \end{aligned}$$

for some uniformly bounded $\tilde{w}_{k,i}$. We find that

$$|G^*_{j,i}| \leq |\tilde{G}_{i,j}| + N \cdot \max_{0\leq k\leq N} |\tilde{w}_{k,i}|\,|\tilde{G}^*_{k,j}|\,h^2, \quad i,j \in I_h,$$

implying that $G^*_{i,j}$ is uniformly bounded and the result follows from Theorem A.1. ☐

Appendix C. Proof of Theorem 7.2.

Proof. By assumption, there is a unique function φ,

$$\varphi_i = \varphi^{(0)}(x_i) + \sum_{j=1}^{q_l} z_j^i h^{p-1}\varphi^{(j)}(x_i) + \sum_{j=q_l+1}^{q} z_j^{i-N} h^{p-1}\varphi^{(j)}(x_i),$$

satisfying

$$\begin{array}{rcll} P\varphi^{(0)} & = & 0, & \\ P_{z_j}\varphi^{(j)} & = & 0, & j = 1,\dots,q, \\ B'_k\varphi & = & g'_{k,h} - h^{t_k}\tilde{g}_k, & k = 1,\dots,m+n, \end{array}$$

and according to (6.8) there exists a constant C such that

$$||\varphi|| \leq C \sum_{k=1}^{m+n} |g'_{k,h} - h^{t_k}\tilde{g}_k|.$$

By this construction, $w = v - \varphi$ satisfies

$$\begin{aligned} P_h w &= f_h - P_h\varphi, \\ B'_{k,h} w &= 0, \quad k = 1,\dots,m+n. \end{aligned} \tag{C.1}$$

Let $G^*_{i,j}$ denote the Green's function of the adjoint to (C.1). Then,

$$w_i = \sum_{j\in I_h} (P^*_h G^*_{j,i}) w_j\, h = \sum_{j\in I_h} G^*_{j,i} P_h w_j\, h = \sum_{j\in I_h} G^*_{j,i}\left((f_h)_j - P_h\varphi_j\right)\, h.$$

According to Theorem B.2, $G^*_{i,j}$ is uniformly bounded. From Theorem 7.1 and the definition of φ follows that $P_h\varphi = \mathrm{O}(h)$. Also, φ is bounded in terms of boundary data. Hence, there exists a constant C such that

$$||v|| \leq C\left(||f_h|| + \sum_{k=1}^{m+n} |g'_{k,h}|\right),$$

which concludes the proof. ☐

REFERENCES

[1] R. P. Agarwal, *Difference equations and inequalities*, Marcel Dekker, Inc., New York, 1992.

[2] L. Brugnano and D. Trigiante, *Boundary value methods: the third way between linear multistep and Runge–Kutta methods*, Comput. Math. Appl., 36 (1998), pp. 269–284.

[3] J. C. Butcher, *The nonexistence of ten-stage eight order Runge–Kutta methods*, BIT, 25 (1985), pp. 521–540.

[4] G. Dahlquist, *Convergence and stability in the numerical integration of ordinary differential equations*, Math. Scand., 4 (1956), pp. 33–53.

[5] ———, *Stability and error bounds in the numerical integration of ordinary differential equations*, Nr. 130, Trans. Roy. Inst. Technol., Stockholm, 1959.

[6] R. D. Grigorieff, *Die Konvergenz des Rand- und Eigenwertproblems linearer gewöhnlicher Differenzengleichungen*, Numer. Math., 15 (1970), pp. 15–48.
[7] B. Gustafsson, *The convergence rate for difference approximations to general mixed initial boundary value problems*, SIAM J. Numer. Anal., 18 (1981), pp. 179–190.
[8] P. Henrici, *Discrete variable methods in ordinary differential equations*, John Wiley & Sons, Inc., New York–London, 1962.
[9] H.-O. Kreiss, *Difference approximations for boundary and eigenvalue problems for ordinary differential equations*, Math. Comp., 26 (1972), pp. 605–624.
[10] W. Walter, *Ordinary differential equations*, Springer–Verlag, 1998.