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Numerical Solution of Two-Point Boundary Value Problems

L. QUARTAPELLE AND S. REBAY

Istituto di Fisica del Politecnico di Milano,
Piazza Leonardo da Vinci, 32, 20133 Milan, Italy

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This paper presents an original formulation of two-point boundary value and eigenvalue problems expressed as a system of first-order equations. The fundamental difference between the new method and other methods based on a first-order approach is the introduction of conditions of an integral character to supplement the simultaneous set of first-order equations, which are hence never regarded as an initial value problem. The consideration of integral conditions leads to establish a class of *linear multipoint* schemes for the numerical solution of boundary value problems for ordinary differential equations. Furthermore, the global character of the integral conditions (nonlocality) combined with the block structure of the system of algebraic equations allow dealing with stiff problems by means of the classical procedure of iterative refinement introduced by Wilkinson. The properties of the numerical schemes are illustrated by the solution of linear and nonlinear problems and by the accurate and efficient determination of some eigensolutions of a difficult problem of hydrodynamic stability. The proposed method is conceptually simpler and numerically more convenient than existing initial value methods, while still retaining all the advantages of a formulation based on a first-order system.

INTRODUCTION

Numerical methods for solving ordinary differential equations supplemented with conditions at both extremes of the integration interval can be divided into two classes: methods which solve the second- or higher order equation directly as an elliptic problem in one dimension [1, Chap. 4; 2, Chap. 7; 3, Sect. 8.7.2], and initial value methods which transform the high-order differential equation into a system of first-order equations [1, Chap. 8; 3, Sect. 8.7.1; 4, p. 359]. Methods belonging to the first class can be applied to solve variable-coefficient and nonlinear problems (see, e.g., [2, p. 355]) and have been implemented using spline collocation to provide very efficient schemes for dealing with singular perturbation problems [5]. Nevertheless, a greater attention has been paid to methods relying on a first-order system, mainly because the corresponding schemes can be used to solve boundary value problems of any order and with an arbitrary order of accuracy. Among the various techniques proposed so far, four methods are the most frequently employed.

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In the *invariant imbedding* method [6, 7] the original ordinary differential problem is reinterpreted as a suitable cross section of a more general, partial differential, problem. The *superposition* or *shooting* method [8–10] is based on the evaluation of an influence matrix relating the values prescribed on the boundaries with the quantities to be determined at the initial point of the integration interval; the stabilized variant of this method for nonlinear problems, named multiple or parallel shooting, requires to solve n-fold versions of the first-order system, where n is the number of shooting points. The *compound-matrix* method [11–13] relies instead on the integration of first-order systems of equations for certain minors of the solution matrices, the number of minors depending on the differential order of the original equation. Finally, in the very recent *continuous orthonormalization* method [14–16] the linear independence of the solution components and the numerical stability during the integration process are assured by a nonlinearization procedure which in general increases the total number of first-order equations to be solved.

A feature common to all these methods is the use of numerical algorithms and computer software developed for the time integration of initial value problems. The solution of the differential equation with data prescribed at both interval extremes is then accomplished by integrating the various aforementioned first-order systems in both directions and by determining the lacking initial values so as to match the available final conditions (the most popular computer codes for boundary value problems are discussed in [17]). These methods have been greatly perfected in the last years and they can now be regarded as highly sophisticated numerical procedures capable of harnessing unstable initial value problems, including strongly oscillatory and extremely stiff problems. However, there are still situations where the inital value methods encounter numerical difficulties. For example, the orthonormalization method combined with an adaptive Runge–Kutta integration procedure experiences convergence difficulties when increasing the number of projection points beyond a certain limit, in the relatively simple linear problem considered as the first test case in [16]. Most difficulties of this type are due to the fact that "even for very well-conditioned boundary value problems the corresponding initial-value problems can be very ill-conditioned," to use the words of Fox [18]. This issue has been much debated in the literature [19–21], leading to the discovery of interesting relationships between the various methods of this kind, see also the recent monographs [22–24].

The aim of the present work is to describe a new numerical method for the solution of boundary value problems expressed in the form of a first-order system, making no reference to concepts pertaining to the class of initial value problems. As it turns out, the decision of not to decompose the problem into a collection of initial value subproblems is indeed very convenient in order to formulate the discrete approximations most appropriate for ordinary differential problems the originary nature of which is *elliptic*. Interestingly enough, such an investigation has been originated from some recent studies on the numerical solution of the vorticity-stream function equations for incompressible viscous flows [25–29]. It has been

shown that, when the fourth-order biharmonic equation for the stream function is replaced by two Poisson equations for the variables vorticity and stream function, the pair of no-slip conditions originally attached to the stream function translate into conditions of an integral character for the vorticity. Generally speaking, the integral conditions have the crucial property of preserving the functional equivalence of the lower order equation system with the original higher order differential problem. It is therefore logical to expect that conditions of a similar nature would arise when a high-order ordinary differential problem is formulated as a system of first-order equations. For example, in the typical case of separated-end conditions supplementing a second-order equation, the reduction of the differential order produces a very simple integral condition which expresses the normalization of the auxiliary variable in terms of the boundary values prescribed for the original unknown.

More generally, the occurrence of conditions not of the usual boundary value type is found to play a decisive role in the present context of ordinary differential equations. In fact, the integral conditions: (i) allow the establishment of a class of *linear multipoint* schemes which represent the extension to boundary value problems of the linear multistep schemes developed for initial value problems; (ii) can dispense with the use of pivoting, and (iii) make the iterative refinement of Wilkinson for ill-conditioned systems the only tool needed to deal with stiff and ill-posed problems. In practice, the proposed formulation is such that the solution of two-point boundary value problems expressed in first-order form becomes an ordinary matter of numerical linear and nonlinear algebra. At the same time, the profile of the block matrices is *bordered multidiagonal* and this structure can be easily preserved by properly choosing the direction in the elimination process. Therefore, the computational efficiency of the new algorithms is at least equivalent to that of the classical initial value techniques of the same order of accuracy.

All the essential features characterizing the new formulation are presented in this paper, the content of which is organized as follows. In section 1 the ordinary differential problem is formulated and the nonlocal character of the conditions supplementing the set of two simultaneous equations associated with a second-order boundary value problem is discussed for both separated and nonseparated conditions. Section 2 describes linear multipoint schemes with increasing order of accuracy for the solution of systems of first-order equations supplemented with conditions of an integral character. The fourth-order accurate scheme is described in some detail since it is believed to be a valuable alternative to the standard Runge–Kutta integration in the solution of boundary value problems. The section terminates by illustrating how the classical procedure of iterative refinement introduced by Wilkinson can be used in conjunction with the proposed schemes to solve stiff and ill-posed problems. Section 3 shows the form of the integral conditions for problems with differential order higher than two, mainly for the case of the fourth-order equation, i.e., the equation for an elastic beam according to the linearized Euler–Bernoulli theory. In Section 4 the proposed algorithms are employed in the solution of some examples, comprising linear and nonlinear

problems of increasing differential order and the Orr–Sommerfeld eigenvalue problem for plane Poiseuille flow. The last section is devoted to the concluding remarks.

1. First-Order Systems with Two-Point Conditions

Consider the linear system of first-order coupled equations

$$y' = A(x)\, y + r(x), \tag{1.1}$$

where y and r are m-vectors while A is an $m \times m$ matrix. The differential system (1.1) is to be solved over the finite and fixed interval $[a, b]$ subject to the so-called two-point boundary condition

$$Ly(a) + Ry(b) = \gamma, \tag{1.2}$$

where L and R are $m \times m$ matrices and γ is a known m-vector.

1.1 *Two-Point Conditions, Boundary Values, and Nonlocality*

When the rank of both L and R is equal to m, a case to be considered rather rare in the applications, condition (1.2) is called *nonseparated*. In this case, Eq. (1.2) prescribes a (linear) relationship between the values of the solution vector y at the end points $x = a$ and $x = b$ of the integration interval—the most nonlocal condition for a (vector-valued) function defined on the interval. With this understanding, denoting condition (1.2) as a "two-point boundary condition" appears confusing since Eq. (1.2) is not a *boundary condition* at all. To avoid such a misinterpretation, condition (1.2) will be here referred to simply as a *two-point condition*. The present formulation deals with the case of full-rank matrices L and R by taking Eq. (1.2) merely as it stands, namely as an algebraic equation relating the unknown vectors $y(a)$ and $y(b)$ (see below).

Most frequently, however, the ranks of L and R are deficient. This occurs when the values of some *components* of the vector unknown are prescribed at the end points $x = a$ and $x = b$. In the literature these types of conditions are referred to as *separated* boundary conditions.

In the simplest case $m = 2$, i.e., $y = (y^{(1)}, y^{(2)})$, two basically different kinds of separated conditions are encountered. The first form occurs when the values of *different* components are specified at the ends of the interval, e.g.,

$$y^{(1)}(a) = \alpha, \qquad y^{(2)}(b) = \beta. \tag{1.3}$$

Conditions (1.3) obviously represent a nonlocal conditioning for the vector unknown y since boundary data are available at both end-stations and for $y^{(1)}$ and $y^{(2)}$. This type of conditions will be dealt with as a particular case of the nonseparated condition (1.2).

The second form of separated conditions arises when no data are available for one component, say $y^{(1)}$, whereas the values of only the other component $y^{(2)}$ are prescribed at both ends of the interval, namely,

$$y^{(2)}(a) = \alpha, \qquad y^{(2)}(b) = \beta. \tag{1.4}$$

This type of separated-end conditions is structurally different from the previous one and plays a crucial role in the present formulation. It is encountered whenever the second-order boundary value problem

$$Y'' = F(Y', Y, x), \qquad Y(a) = \alpha \text{ and } Y(b) = \beta, \tag{1.5}$$

for the scalar unknown Y is reformulated as a system of two first-order equations by introducing the auxiliary variable $Z = Y'$. Then, from the definition of the new unknown Z and the two boundary conditions imposed on the original unknown Y, it is straightforward to obtain

$$\int_a^b Z\,dx = \int_a^b Y'\,dx = Y\,|_a^b = Y(b) - Y(a) = \beta - \alpha. \tag{1.6}$$

Therefore, the second-order problem (1.5) is equivalent to the following system of two first-order equations

$$\begin{aligned} &Z' = F(Z, Y, x), && \int_a^b Z\,dx = \beta - \alpha, \\ &Y' = Z, && Y(a) = \alpha \text{ or } Y(b) = \beta. \end{aligned} \tag{1.7}$$

Each variable of system (1.7) is supplemented with its own condition: the first equation is supplemented with an integral condition, here simply a normalization condition in terms of the boundary data prescribed for the original unknown Y, whereas the second equation can be solved subject to either boundary condition for Y. For example, if the left boundary condition $Y(a) = \alpha$ is imposed, the defining equation $Z = Y'$ and the integral condition for Z give

$$Y(b) = Y(a) + \int_a^b Z\,dx = \alpha + \beta - \alpha = \beta, \tag{1.8}$$

so that the right boundary condition for Y is also satisfied. The *elliptic* character of the second-order problem (1.5) implies an *integral* and hencefore *nonlocal* character in the conditions for the system of first-order equations (1.7). By summarizing, the unusual property of nonlocality is found to be attached to all types of conditions for the system (1.1), irrespective of their separated or nonseparated character.

1.2. *An Alternative Interpretation*

The integral condition (1.6) can be also interpreted in the light of the general theory of the compatibility conditions formulated by Lanczos [30]. Let the problem defining the single unknown Y,

$$Y' = Z, \qquad Y(a) = \alpha, \qquad Y(b) = \beta, \tag{1.9}$$

be considered as an independent problem to be solved after the function Z has been already determined. The data for such a problem, i.e., the source term $Z(x)$ and the boundary values α and β, cannot be specified in an independent manner because only one integration constant is allowed in the solution of a first-order differential equation. Since there are two boundary conditions, problem (1.9) can admit a solution only on condition that the data $Z(x)$, α and β satisfy a *compatibility* relationship, usually known as the Fredholm criterion or alternative. Following Lanczos' analysis, an *overdetermined* problem associated with a given differential operator is subject to compatibility conditions which require that the right-hand side of the equation be orthogonal (for homogeneous boundary data) to the linear manifold spanned by the solutions of the homogeneous adjoint problem [30, Chap. 4]. The argument is a direct consequence of the Green identity for the differential operator of the considered equation and its adjoint. The application of this general principle to the problem (1.9) is immediate and relies on the well-known formula of integration by parts, that is,

$$\int_a^b (X'Y + XY')\, dx = [XY]\,|_a^b, \tag{1.10}$$

where $X(x)$ and $Y(x)$ are arbitrary differentiable functions. The differential operator associated with problem (1.9) is the first derivative supplemented with boundary conditions at *both* the extremes of the interval $[a, b]$. By virtue of the integration-by-parts formula, the adjoint operator is the first derivative with a negative sign and *without* any boundary condition. It follows that in the specific case examined here the linear manifold to be used in the orthogonality relationship contains only the constant functions. Therefore, there is only one linearly independent condition stemming from the orthogonality principle and it assumes the following form

$$\int_a^b Z\, dx = Y(b) - Y(a) = \beta - \alpha. \tag{1.11}$$

The nonhomogeneous character of condition (1.11) is a consequence of the fact that the boundary conditions of the overdetermined problem (1.9) are nonhomogeneous. Such a compatibility condition is coincident with the integral condition (1.6) derived previously.

It can be noted that the reduction of the second-order equation into the form of a first-order system is not unique. In fact, the set of equations will depend on the

form of the relationship used to define the auxiliary or intermediate variable Z and to each specific definition it will correspond a different form of the integral condition associated with that variable. Anyway, whenever separated conditions of type (1.4) are prescribed, an integral condition will be established to supplement the system of first-order equations which, in the general case of a nonlinear problem, will be written in the form

$$y' = f(y, x). \tag{1.12}$$

It is important to recognize that the very presence of a condition not of the usual boundary value (local) type prevents the interpretation of the first-order system (1.12) as an initial value problem and therefore discourages the use of marching-in-time or step-by-step integration procedures. On the contrary, the structure of the discrete approximations introduced in this paper depends essentially on the fact that the integration associated with the considered problem is *definite* and that the conditions supplementing the first-order system have a nonlocal character. By construction, these approximations will be appropriate also in the presence of full-rank two-point conditions (1.2) as well as conditions of *multipoint* type.

2. Linear Multipoint Schemes

It has been shown that the differential system (1.1), or its nonlinear equivalent (1.12), is supplemented always with conditions of a nonlocal character. They can be the nonseparated two-point conditions (1.2), the separated conditions (1.3), or the integral condition (1.6). The complete problem is now descretized by means of the finite difference method over a uniform mesh of size $h = (b-a)/(N-1)$, namely

$$x_j = a + (j-1)h, \qquad j = 1, 2, ..., N. \tag{2.1}$$

Due to the *integral*-value character of the problem in the proposed formulation, the first-order system will be discretized using only *central* differences.

2.1. *Second-Order Scheme*

A second-order accurate scheme is obtained by approximating the differential system (1.1) at the mid-way point $x_{j+1/2}$ and using a two-point computational molecule over the entire interval, to give

$$\frac{y_{j+1} - y_j}{h} = \frac{1}{2}\left[A(x_j)\, y_j + A(x_{j+1})\, y_{j+1}\right] + \frac{1}{2}\left[r(x_j) + r(x_{j+1})\right], \qquad 1 \leqslant j \leqslant N-1. \tag{2.2}$$

This scheme is well known and is called *trapezoidal rule*, see, e.g., [9, p. 28]. In the present work, the system of algebraic equations in the $m \times N$ unknowns $(y_1, y_2, ..., y_N)$ is made complete by including the two-point condition (1.2), which in discretized form becomes

$$Ly_1 + Ry_N = \gamma. \tag{2.3}$$

In the case of separated-end conditions as in (1.4), one component of the vector equation (2.3) is replaced by a discretized version of the integral condition (1.6). To guarantee the second-order accuracy of the approximation, the following quadrature formula is employed for the considered component, say $y^{(1)}$,

$$(\tfrac{1}{2} y_1^{(1)} + y_2^{(1)} + \cdots + y_{N-1}^{(1)} + \tfrac{1}{2} y_N^{(1)})\, h = \beta - \alpha. \tag{2.4}$$

After multiplication by h, Eq. (2.2) gives

$$(-1 - \tfrac{1}{2}hA_j)\, y_j + (1 - \tfrac{1}{2}hA_{j+1})\, y_{j+1} = \tfrac{1}{2}h(r_j + r_{j+1}), \qquad 1 \leqslant j \leqslant N-1, \tag{2.5}$$

where $A_j \equiv A(x_j)$ and $r_j \equiv r(x_j)$. According to (2.3)–(2.5), the equations of the second-order scheme constitute a linear system of mN algebraic equations, the matrix of which has a block structure, with nonzero $m \times m$ blocks on the main diagonal, on the lower codiagonal and on a single (full) row. If the equation corresponding to the two-point or integral condition is placed at the top of the system of equations, one obtains the block *bordered bidiagonal* matrix shown in Fig. 1. all the coefficients displayed being actually $m \times m$ matrices.

When an integral condition (2.4) is present, $g_j \neq 0$ for all j. In the case of nonseparated conditions (2.3), $g_1 = L$ and $g_N = R$, whereas $g_2 = g_3 = \cdots = g_{N-1} = 0$.

$$\begin{array}{cccccccc}
g_1 & g_2 & g_3 & \cdot & \cdot & g_{N-1} & g_N \\
a_1 & b_2 & & & & & \\
 & a_2 & b_3 & & & & \\
 & & \cdot & \cdot & & & \\
 & & & \cdot & \cdot & & \\
 & & & & a_{N-2} & b_{N-1} & \\
 & & & & & a_{N-1} & b_N
\end{array}$$

FIG. 1. Profile of a bordered bidiagonal matrix.

All the coefficients g_j, $1 \leqslant j \leqslant N$, are however still retained in the profile of the matrix during its (block) factorization in order to take into account automatically the nonlocal effect brought about by the condition (2.3). It can be noted in passing that retaining this full row in the matrix profile accomplishes quite naturally and in a general form what is achieved through an artifact by the multiple shooting method in the particular case of separated-end conditions, see [9, p. 5]. The profile of the matrix of the linear system in the present formulation is thus always the same, independently of the separated or nonseparated character of the conditions. The scheme appears to be *fully implicit* due to the presence of one full row. However, this feature does not compromise the computational efficiency of the method. In fact, the linear system associated with the bordered bidiagonal matrix can be solved by a Gaussian elimination which preserves the profile simply by starting at the bottom and proceeding to the top row (UL factorization).

The key property of Eqs. (2.2) making the trapezoidal scheme *combined* with the integral condition a *linear multipoint* scheme for boundary value problems lies in the fact that, by summing the discrete equations (2.2) all together, the left-hand side yields the difference $y_N - y_1$, whereas the right-hand side provides an approximation to the definite integral coincident with the quadrature formula (2.4). The relevance of such a property in the discretization of boundary value problems expressed as a simultaneous set of first-order equations has not been realized so far, although higher order multipoint schemes are obtained simply by searching for algebraically consistent approximations to the first derivative and the definite integral.

2.2. *Fourth-Order Scheme*

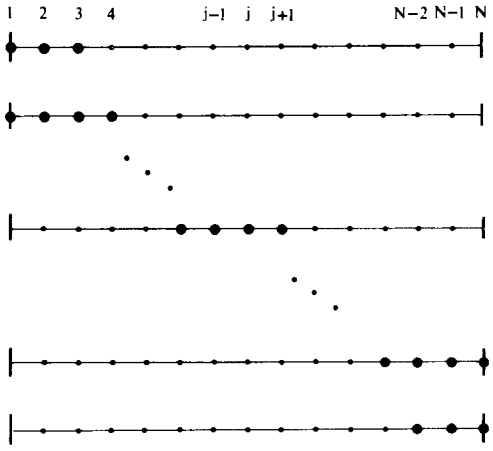

FIG. 2. Computational molecules of the fourth-order scheme for boundary value problems.

therefore to make use of formulas of symmetric type. This restriction combined with the need of obtaining the correct number of discrete equations indicates that the approximation of the equation $y' = f(y, x)$ must be evaluated midway between the grid points. It follows that the (general) computational molecule of a scheme for first-order systems associated with boundary value problems contains an even number of grid points. The advantages of discretizing first-order equations midway between the grid points have been already pointed out by Fox [1, p. 141]. In the case under examination, this location of the approximation becomes mandatory due to the definite character of the integration in order to obtain the correct number of equations.

The computational molecule for the first scheme with an order of accuracy higher than the second will contain four points, except near to the boundary, where a three-point molecule, as illustrated in Fig. 2, is to be used. For instance, at the left end of the interval, the linear three-point,[1] fourth-order accurate formula

$$-\tfrac{1}{2}y_1 + \tfrac{1}{2}y_3 = h(\tfrac{1}{6}f_1 + \tfrac{4}{6}f_2 + \tfrac{1}{6}f_3) \tag{2.6}$$

will be used, where $f_j \equiv f(y_j, x_j)$. At any internal location, the equation $y' = f(y, x)$ will be approximated by the linear four-point general relationship

$$\alpha_0 y_j + \alpha_1 y_{j+1} + \alpha_2 y_{j+2} + \alpha_3 y_{j+3} = h(\beta_0 f_j + \beta_1 f_{j+1} + \beta_2 f_{j+2} + \beta_3 f_{j+3}), \tag{2.7}$$

for $1 \leqslant j \leqslant N-3$. The coefficients α_k and β_k, $k = 0, 1, 2, 3$, are given in [31, p. 43] as a function of two parameters a and b:

$$\begin{aligned} \alpha_0 &= -\tfrac{1}{2}b & \beta_0 &= \tfrac{1}{48}(1 + a + 9b) \\ \alpha_1 &= +\tfrac{1}{2}(a + b) & \beta_1 &= \tfrac{1}{48}(-5 - 13a + 19b) \\ \alpha_2 &= -\tfrac{1}{2}(1 + a) & \beta_2 &= \tfrac{1}{48}(19 - 13a - 5b) \\ \alpha_3 &= +\tfrac{1}{2} & \beta_3 &= \tfrac{1}{48}(9 + a + b). \end{aligned} \tag{2.8}$$

Here, the normalization $\sum_k \beta_k = (1 - a + b)/2$ has been adopted. For arbitrary values of a and b, approximation (2.7) is fourth-order accurate, whereas for the particular value $a = -\frac{38}{11}$ and $b = 1$ it becomes sixth-order accurate. However, the overall accuracy of the scheme will be necessarily limited by the lower accuracy of the three-point approximation to be used near the boundaries. Therefore, the values of a and b will be chosen so as to reproduce the effect of the definite integration, exactly, namely, $y_N - y_1$. To this end, the summation of the left-hand sides of all the discrete equations must give a complete *cancellation* of the coefficients of the unknowns $(y_1, y_2, \ldots, y_N)$ except for the first and the last ones, y_1 and y_N. From

[1] In the present context of boundary value problems, the linear approximation formulas are denoted by the number of points used, instead of the number of steps as usual in the literature on initial value problems.

Eqs. (2.6)–(2.8) one obtains $a=0$ and $b=1$. Then, the linear four-point formula (2.7) becomes

$$-\tfrac{1}{2}y_j+\tfrac{1}{2}y_{j+1}-\tfrac{1}{2}y_{j+2}+\tfrac{1}{2}y_{j+3} = h(\tfrac{5}{24}f_j+\tfrac{7}{24}f_{j+1}+\tfrac{7}{24}f_{j+2}+\tfrac{5}{24}f_{j+3}). \tag{2.9}$$

Furthermore, the summation of the right-hand sides of all the discrete equations (i.e., Eq. (2.6) plus Eqs. (2.9) for $1\leqslant j\leqslant N-3$ and the equation similar to Eq. (2.6) valid for the right end of the interval) will provide an approximation to the definite integral with a consistent order of accuracy. In fact, the summation is found to give the expression

$$\frac{h}{24}(9f_1+28f_2+23f_3+24f_4+24f_5 + \cdots +24f_{N-3}+23f_{N-2}+28f_{N-1}+9f_N). \tag{2.10}$$

The coefficients in (2.10) are coincident with the weights of the Gregory quadrature formula with *end corrections* of degree of precision three reported by Fox [1, p. 19],

$$\begin{aligned}\frac{1}{h}\int_a^b y\,dx &= \frac{1}{2}y_1+y_2+y_3+\cdots+y_{N-1}+\frac{1}{2}y_N \\ &\quad+\left(\frac{1}{12}\Delta-\frac{1}{24}\Delta^2\right)y_1+\left(-\frac{1}{12}\nabla-\frac{1}{24}\nabla^2\right)y_N \\ &= \frac{1}{24}(9y_1+28y_2+23y_3+24y_4 \\ &\quad+\cdots+24y_{N-3}+23y_{N-2}+28y_{N-1}+9y_N),\end{aligned} \tag{2.11}$$

where Δ and ∇ are the forward and backward difference operators. Therefore, in the fourth-order accurate scheme this formula will be consistently used to approximate integral conditions of the type $\int_a^b y^{(1)}\,dx=\beta-\alpha$, whenever they are present. The patterns of all the coefficients α_k and β_k of the resulting scheme are shown in Fig. 3. The first row of the matrix is left void since the first equation of the (block) linear system is associated with the two-point or integral conditions.

Expression (2.11) has been derived by assuming that the two special three-point computational molecules do not overlap, namely, $N\geqslant 6$. Actually, the values of the coefficients in the left-hand side of Eqs. (2.6) and (2.9) are such that the aforementioned cancellation holds irrespective of the overlapping of the special molecules, namely, it holds also when $N=4$ or $N=5$. In these particular cases, a fourth-order

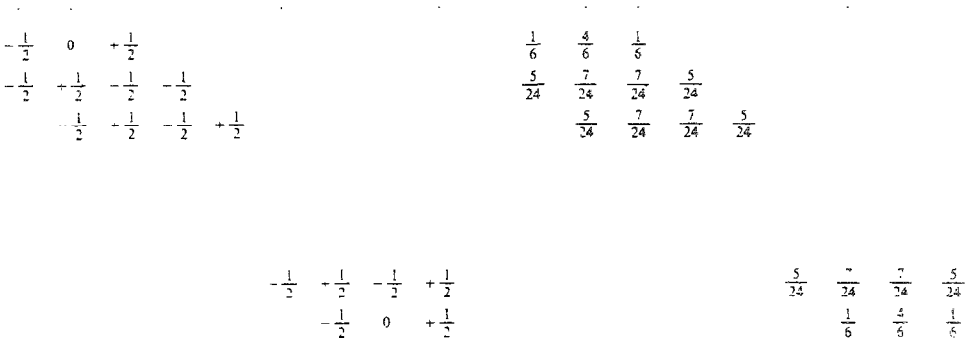

FIG. 3. Fourth-order scheme: Pattern of the coefficients α_k and β_k.

approximation is still possible provided that the quadrature formula (2.11) is replaced by the following modified integration rules

$$N=4: \frac{1}{h}\int_a^b y\,dx=\frac{1}{24}(9y_1+27y_2+27y_3+9y_4);$$
$$N=5: \frac{1}{h}\int_a^b y\,dx=\frac{1}{24}(9y_1+28y_2+22y_3+28y_4+9y_5). \tag{2.12}$$

It is important to remark that, once the discretized equations have been established, their form is valid irrespective of the type of separated or nonseparated conditions. In the particular case of separated-end conditions with the value of a single component prescribed at both the extremes, if the proper discrete equations are used, it is equivalent to impose the two boundary conditions or, alternatively, the integral condition together with either of the two boundary conditions. The choice involving the explicit use of the integral condition is, however, the optimal one since it avoids by construction the need of pivoting during the factorization process, each component of the unknown $y=(y^{(1)}, y^{(2)}, \ldots, y^{(m)})$ being provided with its own condition.

The numerical scheme based on Eqs. (2.6), (2.9) and on the condition (2.11) or possibly (2.3) is a *nonmarching* method for solving first-order systems $y'=f(y, x)$ stemming from boundary value problems for ordinary differential equations. The scheme has a fourth-order accuracy *uniformly* over the entire integration interval. Surprisingly enough, the special computational molecules employed near the boundaries are essential to define a higher order approximation for boundary value problems instead of being a factor of complication as in the case of initial value problems. It is noted that the general computational molecule within the interval is based on four points, very similarly to the most common, fourth-order accurate, Runge–Kutta integration method. However, the proposed method is basically different from any Runge – Kutta scheme. In fact, the linear multipoint approximation

is, on the one hand, *centred* and *fully implicit*, in compliance with the nonlocal character of the conditions supplementing the first-order system, and, on the other hand, *coupled*, due to the block structure of the system of discrete equations. In the case of a linear problem, the matrix profile of the linear system of algebraic equations is *bordered quadridiagonal* and is shown in Fig. 4.

The equation corresponding to the integral or two-point conditions is placed at the top of the linear system. With such an ordering, the fill-in of the matrix is avoided by starting the elimination at the bottom and proceeding to the top row of the matrix (UL factorization). Thus, in the proposed method there is no need for sophisticated procedures of Gaussian elimination, such as those described in [24].

2.3. *Sixth-Order Scheme*

The linear multipoint scheme with a sixth-order accuracy can be derived using a similar reasoning. In this case, the general computational molecule contains six points and there are two special molecules at each extreme of the interval, one with five points and another with four points. The coefficients α_k and β_k of the smallest molecule are fixed by the condition of a sixth-order accuracy and are given by

$$
\begin{array}{ccccccccccc}
g_1 & g_2 & g_3 & g_4 & g_5 & \cdot & \cdot & g_{N-2} & g_{N-1} & g_N \\
b_1 & c_2 & d_3 & & & & & & & \\
a_1 & b_2 & c_3 & d_4 & & & & & & \\
 & a_2 & b_3 & c_4 & d_5 & & & & & \\
 & & \cdot & \cdot & \cdot & \cdot & & & & \\
 & & & \cdot & \cdot & \cdot & \cdot & & & \\
 & & & & \cdot & \cdot & \cdot & \cdot & & \\
 & & & & & a_{N-4} & b_{N-3} & c_{N-2} & d_{N-1} & \\
 & & & & & & a_{N-3} & b_{N-2} & c_{N-1} & d_N \\
 & & & & & & & a_{N-2} & b_{N-1} & c_N
\end{array}
$$

FIG. 4. Profile of a bordered quadridiagonal matrix.

expressions (2.8) with $a = -\frac{38}{11}$ and $b = 1$. After the renormalization $\sum_k \beta_k = 1$, one obtains

$$\begin{aligned} -\alpha_1 &= \alpha_4 = \tfrac{11}{60}, & -\alpha_2 &= \alpha_3 = \tfrac{27}{60}, \\ +\beta_1 &= \beta_4 = \tfrac{1}{20}, & +\beta_2 &= \beta_3 = \tfrac{9}{20}. \end{aligned} \tag{2.13}$$

The values of the coefficients α_k for the two larger molecules are determined using the parametric representation of the five-point formula given in [31] and by imposing the condition of cancellation introduced previously. The values of the coefficients α_k and β_k for the five-point molecule are easily found to be, using the normalization $\sum_k \beta_k = 1$,

$$\begin{aligned} -\alpha_1 &= \alpha_5 = \tfrac{49}{120}, & \alpha_2 &= -\alpha_4 = \tfrac{38}{120}, & \alpha_3 &= 0, \\ +\beta_1 &= \beta_5 = \tfrac{47}{360}, & \beta_2 &= +\beta_4 = \tfrac{166}{360}, & \beta_3 &= -\tfrac{66}{360}, \end{aligned} \tag{2.14}$$

[illegible] coefficients for the six-point molecule are

$$-\alpha_1 = \alpha_6 = \tfrac{49}{120}, \qquad \alpha_2 = -\alpha_5 = \tfrac{65}{120}, \qquad -\alpha_3 = \alpha_4 = \tfrac{70}{120}. \tag{2.15}$$

The values of the coefficients β_k of the general six-point molecule are finally determined by the condition that the summation of the right-hand side of the discrete equations gives the same weights as the Gregory quadrature formula with degree of precision five [1, p. 19], namely,

$$\begin{aligned} \frac{1}{h}\int_a^b y\,dx = {} & \frac{1}{2}y_1 + y_2 + y_3 + \cdots + y_{N-1} + \frac{1}{2}y_N \\ & + \left(\frac{1}{12}\Delta - \frac{1}{24}\Delta^2 + \frac{19}{720}\Delta^3 - \frac{27}{1440}\Delta^4\right) y_1 \\ & + \left(-\frac{1}{12}\nabla - \frac{1}{24}\nabla^2 - \frac{19}{720}\nabla^3 - \frac{27}{1440}\nabla^4\right) y_N \\ = {} & \frac{1}{1440}(475y_1 + 1902y_2 + 1104y_3 + 1586y_4 \\ & + 1413y_5 + 1440y_6 + \cdots + 475y_N). \end{aligned} \tag{2.16}$$

After some calculations one finds the values

$$\beta_1 = \beta_6 = \tfrac{215}{1440}, \qquad \beta_2 = \beta_5 = \tfrac{375}{1440}, \qquad \beta_3 = \beta_4 = \tfrac{130}{1440}. \tag{2.15a}$$

It is not difficult to verify that the linear six-point formula based on the coefficient values given in (2.15) and (2.15a) constitutes a sixth-order accurate approximation of the equation $y' = f(y, x)$.

The derivation of the quadrature formula (2.16) assumes that the left and the

right special molecules do not overlap and hencefore $N \geqslant 10$. To obtain the sixth-order scheme valid also for $6 \leqslant N \leqslant 9$, the quadrature formula (2.16) must be changed by introducing the following modified weights

$$\begin{aligned} &N=6: \quad w_2 = w_5 = \tfrac{1875}{1440}, \quad w_3 = w_4 = \tfrac{1250}{1440}; \\ &N=7: \quad w_3 = w_5 = \tfrac{1077}{1440}, \quad w_4 = \tfrac{1732}{1440}; \\ &N=8: \quad w_4 = w_5 = \tfrac{1559}{1440}; \\ &N=9: \quad w_5 = \tfrac{1386}{1440}. \end{aligned} \tag{2.17}$$

2.4. *Wilkinson Refinement for Ill-Posed Problems*

The proposed discretization method provides an *algebraically exact* representation of the boundary value problem expressed in a first-order form. As a consequence, the solution of nonpathological equations is straightforward, as it has been confirmed by several test calculations including strongly oscillatory and nonlinear problems. However, when the differential equation is *stiff*, the resulting system of algebraic equations becomes *ill-conditioned.* In these cases, the procedure of *iterative refinement* introduced by Wilkinson can be used [32]. Such a procedure is very convenient in the present context of sparse bordered multidiagonal matrices since it requires to storing only two copies of the coefficient matrix and avoids the fill-in, as would occur instead using Gaussian elimination with partial or complete pivoting. Although the latter procedure is in principle preferable, the numerical results for several test problems indicate that the iterative refinement is what the linear multistep schemes basically need to deal with in most stiff and ill-conditioned situations. It must be noted that the residual associated with the full row imposing the integral conditions provides a numerical indicator whether or not the Wilkinson procedure is required, as shown in the following.

It is very easy to detect the occurrence of ill-conditioning when solving the linear system of equations

$$Ay = b \tag{2.18}$$

in the present formulation. The conditions supplementing the first-order system are imposed through the algebraic equation

$$\sum_{j=1}^{N} g_j y_j = \gamma, \tag{2.19}$$

where γ is the m-vector of the condition values. After the numerical solution $\bar{y}$ of Eq. (2.18) has been computed, one evaluates the vector

$$\bar{\gamma} = \sum_{j=1}^{N} g_j \bar{y}_j, \tag{2.20}$$

using *extended precision* arithmetics in the accumulation of the scalar product. The linear system of equations is ill-posed when the relative average error associated with the satisfaction of the conditions is found to be greater than the machine roundoff error. Therefore, the iterative refinement will be attempted whenever the condition

$$\frac{\langle \bar{\gamma} - \gamma \rangle}{\langle \gamma \rangle} > \text{machine roundoff} \tag{2.21}$$

is found to be satisfied, where $\langle \gamma \rangle \equiv m^{-1} \sum_{p=1}^{m} |\gamma^{(p)}|$. The refinement procedure of Wilkinson bears some resemblance with the *difference correction* method introduced by Fox in 1947 [33], and subsequently modified and extended by Pereyra in the form of a *iterated deferred correction* method (a discussion of such methods and related techniques is given in [18, 34]). Although Fox's method "was effectively in the spirit of the later idea for the iterative refinement of the solution of linear equations" [18], deferred correction methods are rather different from Wilkinson iterative refinement, considering that the former act to increase the order of accuracy of the approximation whereas the latter operates on a discretization with a fixed order of accuracy. It is also worth mentioning that Wilkinson procedure is an auxiliary component of the proposed method, because most problems do not require the refinement so that it is bypassed automatically, by virtue of the test (2.21). The iterative refinement is instead necessary only under very special circumstances, such as, for instance, to assure the theoretical rate of convergence of the schemes in the case of stiff equations (cf. examples (4.1.2f) and (4.2.1)–(4.2.2)), or to detect a situation in which the ill-conditioning is beyond the recovery capability of Wilkinson procedure (cf. example (4.2.3)).

3. Higher Order Equations

This section discusses the form of the integral conditions for boundary value problems of differential order higher than the second. The present exposition is limited to the case of linear equations of the *fourth* and *sixth* order. The conditions that will be formulated are valid also for nonlinear problems and the analysis can be easily extended to deal with equations of any order.

3.1. *Fourth-Order Equation*

The most general linear equation of the fourth order has the form

$$\psi'''' + f(x)\psi''' + g(x)\psi'' + h(x)\psi' + k(x)\psi = s(x), \tag{3.1}$$

where f, g, h, k, and s are known functions. The boundary conditions most frequently associated with this equation are

$$\begin{aligned} \psi(a) &= \alpha, \qquad \psi(b) = \beta, \\ \psi'(a) &= \alpha', \qquad \psi'(b) = \beta', \end{aligned} \tag{3.2}$$

where the values α, β, α', β' are prescribed. By introducing the variables $\phi = \psi'$, $\zeta = \psi''$, and $\xi = \psi'''$, Eq. (3.1) can be rewritten as a system of first-order equations. The conditions associated with the system are obtained as follows.

The derivative boundary conditions in (3.2) for ψ give two "Dirichlet" conditions for ϕ, namely, $\phi(a) = \alpha'$ and $\phi(b) = \beta'$. On the other hand, since $\phi = \psi'$ and the values of ψ on the boundaries are prescribed, ϕ satisfies also the integral condition $\int_a^b \phi \, dx = \beta - \alpha$. Thus, there are three possible conditions for ϕ, namely,

$$\phi(a) = \alpha' \qquad \text{or} \qquad \phi(b) = \beta' \qquad \text{or} \qquad \int_a^b \phi \, dx = \beta - \alpha.$$

The condition for the variable $\zeta = \psi''$ comes from the application of the *Green identity* for the second-order (total) derivative operator

$$\int_a^b (\phi\psi'' - \phi''\psi) \, dx = [\phi\psi' - \phi'\psi] \,|_a^b.$$

By taking any function η satisfying the equation

$$\eta'' = 0$$

and using the boundary conditions (3.2), this identity with $\phi = \eta$ gives the following integral condition for the variable ζ,

$$\int_a^b \zeta\eta \, dx = \gamma[\eta],$$

where

$$\gamma[\eta] \equiv \eta(b)\beta' - \eta(a)\alpha' - \eta'(b)\beta + \eta'(a)\alpha.$$

Note that the boundary term $\gamma[\eta]$ is a known quantity since it involves only the prescribed boundary values and the already determined function η (evaluated at $x = a$ and $x = b$). In particular, if η is chosen to be $\eta(x) \equiv 1$, the integral condition assumes the form of a normalization condition

$$\int_a^b \zeta \, dx = \beta' - \alpha'.$$

Such a condition could also have been obtained more directly from the equation $\zeta = \phi'$ using the boundary specifications for ϕ.

The condition for the third auxiliary variable $\xi = \psi'''$ results from the Green identity for the *third-order* derivative operator, namely,

$$\int_a^b (\phi\psi''' + \phi'''\psi)\, dx = [\phi\psi'' - \phi'\psi' + \phi''\psi]\,|_a^b.$$

For any function σ, the identity yields

$$\int_a^b \xi\sigma\, dx = \int_a^b \psi'''\sigma\, dx$$

$$= -\int_a^b \psi\sigma'''\, dx + [\psi''\sigma - \psi'\sigma' + \psi\sigma'']\,|_a^b.$$

Since no boundary condition is prescribed for ψ'', the function σ is to be taken as the solution of the problem

$$\sigma''' = 0, \qquad \sigma(a) = 0, \qquad \text{and} \qquad \sigma(b) = 0,$$

so that the Green identity becomes

$$\int_a^b \xi\sigma\, dx = -\gamma[\sigma'].$$

The function σ is defined up to an (inessential) arbitrary coefficient. If σ is chosen to be

$$\sigma(x) = \frac{(b-x)(x-a)}{(b-a)^2},$$

the integral condition for ξ assumes the specific form

$$\int_a^b \xi\sigma\, dx = \frac{\alpha' + \beta'}{b-a} - 2\,\frac{\beta - \alpha}{(b-a)^2}.$$

If one introduces the function

$$S(x) \equiv -f(x)\xi - g(x)\zeta - h(x)\phi - k(x)\psi + s(x),$$

for notational convenience, the formulation of problem (3.1)–(3.2) as first-order system becomes

$$\begin{aligned}
&\xi' = S(x), && \int_a^b \xi\sigma\, dx = \frac{\alpha' + \beta'}{b-a} - 2\,\frac{\beta - \alpha}{(b-a)^2},\\
&\zeta' = \xi, && \int_a^b \zeta\, dx = \beta' - \alpha',\\
&\phi' = \zeta, && \phi(a) = \alpha' \text{ or } \phi(b) = \beta' \text{ or } \int_a^b \phi\, dx = \beta - \alpha,\\
&\psi' = \phi, && \psi(a) = \alpha \text{ or } \psi(b) = \beta.
\end{aligned} \tag{3.3}$$

The system of equations can be also written in the following compact form

$$y' = A(x)\, y + r(x), \tag{3.4}$$

where

$$y = \begin{bmatrix} \xi \\ \zeta \\ \phi \\ \psi \end{bmatrix}, \quad A(x) = \begin{bmatrix} -f(x) & -g(x) & -h(x) & -k(x) \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad r(x) = \begin{bmatrix} s(x) \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{3.5}$$

The previous procedure for obtaining the integral conditions supplementing the system of first-order equations is applicable also to sets of boundary conditions different from those considered in Eqs. (3.2) such as, for instance, when the value of the second derivative of the unknown ψ is prescribed at one extreme of the interval.

3.2. *Sixth-Order Equation*

One can also extend the preceding analysis to the case of the sixth-order equation

$$\psi^{vi} = \sum_{k=0}^{5} f_k(x)\, \psi^{(k)} + s(x) \equiv S(x), \tag{3.6}$$

supplemented with the boundary conditions

$$\begin{aligned}
&\psi(a) = \alpha, && \psi(b) = \beta,\\
&\psi'(a) = \alpha', && \psi'(b) = \beta',\\
&\psi''(a) = \alpha'', && \psi''(b) = \beta''.
\end{aligned} \tag{3.7}$$

One has to consider the Green identity for the higher order derivative operators and to introduce the functions which belong to the kernel (null space) of these operators and satisfy suitable homogeneous boundary conditions. The first-order formulation of the problem defined by Eqs. (3.6)–(3.7) is easily found to be

$$\rho' = S(x), \qquad \int_a^b \rho v \, dx = 2\frac{\beta'' - \alpha''}{(b-a)^2} - 12\frac{\alpha' + \beta'}{(b-a)^3} + 24\frac{\beta - \alpha}{(b-a)^4},$$

$$\xi' = \rho, \qquad \int_a^b \xi\sigma \, dx = \frac{\alpha'' + \beta''}{b-a} - 2\frac{\beta' - \alpha'}{(b-a)^2},$$

$$\zeta' = \xi, \qquad \int_a^b \zeta \, dx = \beta'' - \alpha'',$$

$$\mu' = \zeta, \qquad \mu(a) = \alpha'' \text{ or } \mu(b) = \beta'' \text{ or } \int_a^b \mu \, dx = \beta' - \alpha',$$

$$\phi' = \mu, \qquad \phi(a) = \alpha' \text{ or } \phi(b) = \beta' \text{ or } \int_a^b \phi \, dx = \beta - \alpha,$$

$$\psi' = \phi. \qquad \psi(a) = \alpha \text{ or } \psi(b) = \beta,$$

where the functions $v(x)$ and $\sigma(x)$ are defined by

$$v(x) \equiv \frac{(x-a)^2 (b-x)^2}{(b-a)^4} \qquad \text{and} \qquad \sigma(x) \equiv \frac{(x-a)(b-x)}{(b-a)^2}.$$

It is important to note that integral conditions different from those explicitly given can be formulated for the variables ξ, ζ, and μ. The choice among the various alternative conditions of boundary value or integral value type is made completely free by the fact that the first unknown ρ is subject to a(n integral) condition involving all of the boundary data prescribed on ψ.

4. Numerical Examples

All the problems which follow have been solved on an IBM 43-81 computer using *double precision* arithmetic throughout and *extended precision* for the Wilkinson refinement procedure. The fourth-order linear multipoint scheme described in Section 2.2 has been used in most of the calculations, except where otherwise specified.

4.1. *Linear Problems with Constant Coefficients*

4.1.1. *System of Two Split Equations*

The first example is the simplest two-point boundary value problem, namely,

$$u'' = s(x), \qquad u(a) = \alpha, \qquad u(b) = \beta, \tag{4.1.1}$$

where $s(x)$ is a known function. The problem is formulated as a system of two first-order equations to give

$$\begin{aligned} v' &= s(x), \qquad \int_a^b v\,dx = \beta - \alpha, \\ u' &= v, \qquad u(a) = \alpha \text{ or } u(b) = \beta. \end{aligned} \tag{4.1.2}$$

These equations are said to be *split* in the sense that they can be solved in sequence, one after each other. They are solved in the case $s(x) = 4e^{2x}$, $u(x) = e^{2x}$, over the interval $[0, 1]$, using the second-order scheme described in Section 2.1. The L^2-error E_h of the numerical solutions for different values of h is reported in Table I.1 together with the order of convergence $\log_2(E_{2h}/E_h)$. Either of the two boundary conditions for u can be imposed in the solution of the second equation. The satisfaction of the integral condition in the solution of the first equation assures the two solutions u_L and u_R obtained by imposing the left or the right boundary condition are coincident, apart from the roundoff errors shown in Table I.1.

In the simple case of split equations solved by means of the second-order accurate scheme, the discrete equations for u read

$$u_j - u_{j-1} = \frac{h}{2}(v_{j-1} + v_j) \tag{4.1.3}$$

and could be interpreted as a scheme marching in a forward or backward direction, depending on the boundary condition which is actually imposed. This interpretation is, however, of no substance since the explicit character of the equations results accidentally from applying a two-point approximation to an uncoupled system. By contrast, the lack of dependence of the solution on the boundary condition actually imposed on the unknown u is a general property of the proposed linear multipoint schemes and holds also in the case of coupled equation systems.

4.1.2. *Systems of Two Coupled Equations*

Consider now the Helmholtz-like problem in one dimension,

$$u'' + \omega^2 u = s(x), \qquad u(a) = \alpha, \qquad u(b) = \beta, \tag{4.1.4}$$

TABLE I.1

Boundary Value Problem Leading to a System of Two Split Equations, Second-Order Accurate Scheme

N	L^2 error	Convergence order	$\delta = u_R - u_L$
11	0.181(−2)		$2\times10^{-15} \leqslant \delta \leqslant 3\times10^{-15}$
21	0.475(−3)	1.93	$1\times10^{-15} \leqslant \delta \leqslant 5\times10^{-15}$
41	0.122(−3)	1.96	$0 \leqslant \delta \leqslant 8\times10^{-15}$
81	0.308(−4)	1.99	$4\times10^{-15} \leqslant \delta \leqslant 2\times10^{-16}$

TABLE I.2a

Comparison of Solutions Obtained by Imposing the Left or Right Boundary Condition, Second-Order Accurate Scheme

x	Exact solution	Numerical solution	$u_R - u_L$	x	Exact solution	Numerical solution	$u_R - u_L$
0.00	1.0000	1.0000	-10^{-16}	0.50	2.7182	2.7132	10^{-15}
0.05	1.1051	1.1044	0	0.55	3.0041	2.9990	10^{-15}
0.10	1.2214	1.2199	0	0.60	3.3201	3.3150	0
0.15	1.3498	1.3476	0	0.65	3.6692	3.6644	0
0.20	1.4918	1.4890	0	0.70	4.0551	4.0506	0
0.25	1.6487	1.6453	0	0.75	4.4816	4.4776	10^{-15}
0.30	1.8221	1.8182	10^{-15}	0.80	4.9530	4.9495	0
0.35	2.0137	2.0094	0	0.85	5.4739	5.4711	10^{-15}
0.40	2.2255	2.2208	0	0.90	6.0496	6.0476	0
0.45	2.4596	2.4546	10^{-15}	0.95	6.6858	6.6848	0
0.50	2.7182	2.7132	10^{-15}	1.00	7.3890	7.3890	0

TABLE I.2b

Linear Problem with Constant Coefficients (Oscillatory Case), Second-Order Accurate Scheme

N	L^2 error	Maximum absolute error	Convergence order
101	0.327(−1)	0.472(−1)	
201	0.809(−2)	0.117(−1)	2.02
401	0.202(−2)	0.291(−2)	2.00
801	0.504(−3)	0.728(−3)	2.00
1601	0.126(−3)	0.182(−3)	2.00

TABLE I.2c

Linear Problem with Constant Coefficients (Oscillatory Case), Fourth-Order Accurate Scheme

N	L^2 error	Maximum absolute error	Convergence order
200	0.151(+1)	0.22(+1)	
400	0.563(−1)	0.85(−1)	4.75
800	0.337(−2)	0.51(−2)	4.06
1600	0.209(−3)	0.32(−3)	4.01
3200	0.130(−4)	0.20(−4)	4.00

TABLE I.2c *bis*

First-Order System of Two Weakly Coupled Equations;
Dependence of the Error on the Parity of the Number of Mesh Points

N	L^2 error	Convergence order	N	L^2 error	Convergence order
100	0.610(−1)		101	0.110(+1)	
200	0.299(−2)	4.35	201	0.606(−1)	4.18
400	0.181(−3)	4.05	401	0.358(−2)	4.08
800	0.113(−4)	4.00	801	0.217(−3)	4.04
1600	0.713(−6)	3.99	1601	0.133(−4)	4.03

ter of the conditions. For instance, in the aforementioned example with $\omega^2 = 10^4$, exactly the same errors of Table I.2c are obtained using one point more or less than in the reported calculations. On the contrary, when the coupling is weak, the value of the error for N even may become smaller than for (a comparable) N odd. For example, the numerical results for problem (4.1.7) in the weakly coupled case $\omega^2 = 10^2$ using even and odd grids are compared in Table I.2c *bis*. The errors for N odd are larger than the errors for N even by more than an order of magnitude. It must be noted, however, that the theoretical convergence rate is achieved on the two distinct sets of even and odd grids.

In the case of fully uncoupled equations, the singularity makes it impossible to use the fourth-order accurate multipoint scheme with an odd number of grid points. The spurious mode associated with the singularity of the matrix is found to be a $2h$-wave ($h = 1/(N-1)$), namely,

$$u_j = \begin{cases} 0 & \text{for } j \text{ odd}, \\ 1 & \text{for } j = 2 + 4k, \\ -1 & \text{for } j = 4k, \end{cases}$$

where $k = 1, 2, 3, \ldots$.

The same oscillatory example (4.1.7) has also been solved by means of the sixth-order accurate scheme described in Section 2.3, obtaining results always exhibiting the expected order of convergence. Such a scheme has been employed on a grid of 1600 points to compute the solutions for several values of ω^2. The corresponding results are reported in Table I.2d. For $\omega^2 = 10^4$ the maximum absolute error is 0.33×10^{-6} to be compared with the value 0.32×10^{-3} of the fourth-order accurate scheme.

Exponential case. Another linear example with constant coefficients considered in [16] is the problem

$$u'' - \tilde{\omega}^2 u = s_0 \cos(\gamma x), \qquad u(0) = 1 \text{ and } u(1) = 0. \tag{4.1.8}$$

TABLE I.2d

Linear Problem with Constant Coefficients (Oscillatory Case), Sixth-Order Accurate Scheme

ω^2	L^2 error	Maximum absolute error
10^2	0.22(−11)	0.62(−11)
10^3	0.39(−9)	0.56(−9)
10^4	0.21(−6)	0.33(−6)
10^5	0.18(−3)	0.38(−3)

TABLE I.2e

Linear Problem with Constant Coefficients (Exponential Case)

N	L^2 error	Maximum absolute error	Convergence order
200	0.221(−2)	0.557(−2)	
400	0.123(−3)	0.291(−3)	4.17
800	0.744(−5)	0.170(−4)	4.05
1600	0.461(−6)	0.130(−5)	4.01

TABLE I.2f

Linear Problem with Homogeneous Boundary Conditions

N	L^2 error	Maximum absolute error	Convergence order
Without Wilkinson refinement			
100	0.17(−4)	0.38(−4)	—
200	0.68(−6)	0.18(−5)	—
400	0.18(−5)	0.11(−4)	—
800	0.23(−6)	0.15(−5)	—
1600	0.52(−6)	0.33(−5)	—
With Wilkinson refinement (two iterations)			
100	0.17(−4)	0.38(−4)	
200	0.67(−6)	0.18(−5)	4.67
400	0.31(−7)	0.89(−7)	4.45
800	0.17(−8)	0.47(−8)	4.18
1600	0.10(−9)	0.27(−9)	4.05
3200	0.64(−11)	0.15(−10)	4.01

The analytical solution is

$$u(x) = C_1 e^{\tilde{\omega}x} + C_2 e^{-\tilde{\omega}x} - \frac{s_0}{\tilde{\omega}^2 + \gamma^2} \cos(\gamma x). \tag{4.1.8a}$$

The solution is still oscillatory but now it contains rapidly growing and decaying components as $\tilde{\omega}$ becomes large. Problem (4.1.8) with $\tilde{\omega}^2 = 10^4$, $\gamma = 80.$ and $s_0 = 10^4$, has been solved by means of the fourth-order scheme and the numerical errors are reported in Table I.2e. The convergence rate is again achieved quite regularly. Compared with orthonormalization [16], for the same value of N, the linear multipoint method is less accurate but one has to remember that the number of mesh points actually used in the Runge–Kutta integration is a multiple of the number of declared grid points.

Homogeneous boundary conditions. In all the previous examples, the linear multipoint schemes provide accurate and convergent results without any need to resort to the Wilkinson refinement procedure. The next problems illustrate instead the importance of the iterative refinement in order to guarantee the convergence for general equations and boundary conditions. Stoer and Bulirsch have considered the following nonhomogeneous equation supplemented with homogeneous boundary data [35], see also [36 or 19],

$$\begin{gathered} u'' - \tilde{\omega}^2 u = \tilde{\omega}^2 \cos^2(\pi x) + 2\pi^2 \cos(2\pi x), \\ u(0) = 0 \qquad \text{and} \qquad u(1) = 0, \end{gathered} \tag{4.1.9}$$

with solution

$$u(x) = (1 + e^{-\tilde{\omega}})^{-1} \left[e^{\tilde{\omega}(x-1)} + e^{-\tilde{\omega}x} \right] - \cos^2(\pi x). \tag{4.1.9a}$$

Problem (4.1.9) with $\tilde{\omega} = 20$ has been solved by means of the fourth-order accurate scheme. The errors of the numerical solutions obtained without and with Wilkinson refinement are compared in Table I.2f which shows the impressive gain in accuracy assured by only two iterations. In comparison with the results provided by various initial value methods reported in [19], the proposed method requires less points for obtaining solutions of low accuracy and a comparable number of points for getting very accurate solutions.

4.2. *Linear Problems with Variable Coefficients*

4.2.1. *Homogeneous Equation with a Gaussian Solution*

The first example with variable coefficients is the two-point boundary value problem

$$u'' - (x^2 - 1)u = 0, \qquad u(0) = 1 \qquad \text{and} \qquad u(b) = e^{-b^2/2}. \tag{4.2.1}$$

suggested by Scott and also considered in [22, p. 68]. The general solution of the differential equation is

$$u(x) = Ae^{-x^2/2} + Be^{-x^2/2} \int_0^x e^{y^2/2}\, dy. \tag{4.2.1a}$$

With the conditions prescribed in (4.2.1), the solution is $u(x) = e^{-x^2/2}$ for any value of b. However, when b is not small, e.g., $b > 6$, it becomes difficult to solve

TABLE II.1

Homogeneous Linear Equation with Variable Coefficients

N	L^2 error	Maximum absolute error	Convergence order
100	0.21(−4)	0.26(−4)	
200	0.96(−6)	0.12(−5)	4.5
400	0.52(−7)	0.60(−7)	4.2
800	0.31(−8)	0.34(−8)	4.1
1600	0.19(−9)	0.21(−9)	4.0

TABLE II.2

Holt Equation ($m = 0$, $\alpha = 1$)

x	Osborne $h = 1/100$	Chasing method $h = 1/100$	Fourth-order linear multipoint method $h = 1/40$	Fourth-order linear multipoint method $h = 1/80$
0	0.1000(+01)	0.9999876(+00)	0.9999999(+00)	0.100000000(+01)
1	0.2593(+00)	0.2693404(+00)	0.2593425(+00)	0.259342547(+00)
2	0.3455(−01)	0.3456397(−01)	0.3456405(−01)	0.345640463(−01)
3	0.1987(−02)	0.1988532(−02)	0.1988528(−02)	0.198852332(−02)
4	0.4590(−04)	0.4595871(−04)	0.4596120(−04)	0.459582911(−04)
5	0.4188(−06)	0.4125652(−06)	0.4137580(−06)	0.412596333(−06)
6	0.1409(−08)	0.1413020(−08)	0.1231637(−08)	0.140732769(−08)
7	0.1821(−11)	0.1827268(−11)	−0.1011097(−08)	−0.304898194(−10)
8	0.8825(−15)	0.8863389(−15)	−0.1448407(−08)	−0.462611063(−10)
9	0.1597(−18)	0.1605597(−18)	−0.1637120(−08)	−0.525582396(−10)
10	0.1058(−22)	0.1082885(−22)	−0.1352774(−08)	−0.444881792(−10)
11		0.2713141(−27)	0.1121146(−08)	0.331291618(−10)
12		0.2521085(−32)	0.6748801(−16)	0.158927845(−16)
13		0.8677126(−38)		
14		0.1105113(−43)		
15		0.5203999(−50)		
16		0.9055032(−57)		
17		0.5818867(−64)		
18		0.4179442(−72)		

the problem by means of *superposition* methods. This is not the case for the linear multipoint schemes combined with the Wilkinson refinement procedure. For instance, the fourth-order scheme applied to the problem with $b = 10$ yields solutions with the numerical errors indicated in Table II.1. The effect of two Wilkinson iterations is dramatic: the error is decreased by several orders of magnitude with respect to the simple scheme without iterative refinement and the convergence rate is h^4 instead of linear.

4.2.2. *Holt Equation*

A boundary value problem very similar to the previous one is the Holt equation [23, p. 55]

$$u'' - (2m + 1 + x^2)u = 0, \qquad u(0) = \alpha, \qquad u(\infty) = 0. \tag{4.2.2}$$

The case $m = 0$, $\alpha = 1$ has been solved by means of the fourth-order scheme. The right boundary condition is imposed at the large but finite distance $x_\infty = 12$ and two meshes with $h = 1/40$ and $h = 1/80$ are considered. The numerical results are compared in Tables II.2 with those calculated by Osborne and by means of the so-called *chasing* method [23] on the mesh $h = 1/100$.

The absolute local accuracy assured by the present method is greater than in earlier computations and is uniform over the integration interval. On the contrary, in the exponentially vanishing tail, the relative local error (ratio of the local value of the numerical error to the value of the exact solution) is smaller using the initial value schemes. Two Wilkinson iterations are performed in the considered example.

4.2.3. *A Problem with a Turning Point*

The last variable coefficient example is the problem [16]

$$\begin{aligned} \varepsilon u'' + xu' &= -\varepsilon\pi^2 \cos(\pi x) - \pi x \sin(\pi x), \\ u(-1) &= -2, \qquad u(1) = 0. \end{aligned} \tag{4.2.3}$$

The solution of the problem is

$$u(x) = \cos(\pi x) + \frac{\operatorname{erf}(x/\sqrt{2\varepsilon})}{\operatorname{erf}(1/\sqrt{2\varepsilon})}, \tag{4.2.3a}$$

which shows a *turning point* or sharp *transition layer* near $x = 0$ when $\varepsilon \to 0$. Finite element and finite difference methods are expected to fail for this problem and cannot compete with algorithms designed for solving singular perturbation problems. For instance, the computer code COLSYS [5], based on a spline collocation method with h^8-accuracy, solves the problem for $\varepsilon = 10^{-6}$ within an absolute error of 10^{-6} using a nonuniform grid of 256 subintervals. By contrast, the fourth-order multipoint scheme combined with the Wilkinson iterative method provides the results reported in Table II.3 for the case $\varepsilon = 10^{-4}$. The maximum

TABLE II.3

Variable Coefficient Problem with a Turning Point

N	L^2 error	Maximum absolute error	Iterations
600	0.212(−1)	0.282(−1)	2
800	0.117(−1)	0.158(−1)	2
1000	0.392(−2)	0.528(−2)	3
1200	0.152(−2)	0.272(−2)	6

absolute error for $N=1200$ is 0.27×10^{-2} and can be compared with the value 0.27×10^{-3} provided by the orthonormalization method using 2000 projection points and an adaptive sixth-order accurate Runge–Kutta integrator. Six Wilkinson iterations are performed in the case $N=1200$. For finer grids, the equation system becomes so ill-conditioned that the iterative refinement procedure fails to converge. Of course, better numerical results are allowed when the linear multipoint scheme is employed using a stretched interval via a transformation such as $X=(x+1)^4$ [16]. However, the attention is limited here to a straightforward application of the new schemes without problem-dependent modifications. Anyway, it should be not difficult to devise the adaptive transformations most convenient for dealing with problems displaying a singular behaviour (see the example 4.5).

4.3. *Nonlinear Problems*

The potential of the linear multistep methods in the nonlinear case is assessed by applying the standard Newton method to the solution of a number of nonlinear boundary value problems. The Jacobian is always evaluated analytically. It is worthwhile mentioning that in the proposed formulation the Newton method can handle any kind of nonlinear conditions $F(y(a), y(b))=\gamma$, straightforwardly; in this case the Jacobian of F enters the top row $(g_1, g_2, ..., g_N)$ of the matrix of the linearized problem. In any case, the matrix associated with the linearized system of equations has the same bordered multidiagonal profile encountered for linear problems. All the results shown in the present section have been obtained without any need to resort to the Wilkinson refinement procedure.

4.3.1. *A Singular Perturbation Problem*

A nonlinear example of singular perturbation type is the following boundary value problem [37, p. 436]

$$\varepsilon u''=1-(u')^2, \qquad 0\leqslant x\leqslant 1, \qquad u(0)=\alpha, \qquad u(1)=\beta, \tag{4.3.1}$$

the boundary data of which are assumed to satisfy the condition $|\alpha - \beta| < 1$. The derivative u' of the exact solution is given in terms of ε, α, and β by

$$u'(x) = \frac{(k-1)e^{2x/\varepsilon} - e^{2/\varepsilon} + k}{(k-1)e^{2x/\varepsilon} + e^{2/\varepsilon} - k}, \tag{4.3.1a}$$

where $k = e^{(\beta - \alpha + 1)/\varepsilon}$. The numerical results for this variable, which becomes discontinuous at $x = (\alpha - \beta + 1)/2$ as $\varepsilon \to 0^+$ [37, p. 436], are reported in Table III.1 for the case $\varepsilon = 0.05$, $\alpha = \frac{1}{2}$, and $\beta = 1$. Using the initial guess $u(x) = \alpha + (\beta - \alpha)x$ in the nonlinear procedure, the relative error becomes less than 10^{-10} in 9 iterations.

4.3.2. *An Equation with End Singularity*

The capability of the proposed approach in handling equations with singular coefficients is investigated against the following nonlinear problem [22, p. 36],

$$u'' + u'/x + \delta e^u = 0, \qquad u'(0) = 0, \qquad u(1) = 0. \tag{4.3.2}$$

The equation in (4.3.2) becomes singular at the left extreme $x = 0$ of the integration interval. In order to apply the fourth-order multipoint scheme to this problem, the discrete equations associated with molecules involving the singular point $x = 0$, namely, the left three-point molecule and the first four-point molecule, must be derived by approximating the (nonsingular) equation

$$2u'' + \delta e^u = 0, \qquad x \to 0. \tag{4.3.2'}$$

provided by the application of the l'Hospital rule to the original differential equation. The solution to the nonlinear problem (4.3.2) can be expressed in closed analytical form [22, p. 36]

$$u(x) = \ln \frac{8C}{(Cx^2 + \delta)^2}. \tag{4.3.2a}$$

The value of the integration constant C satisfies the equation $8C/(C + \delta)^2 = 1$. It can be readly shown that for δ in the range $0 < \delta < 2$ there are two distinct solutions. The two roots $C_\pm$ expressed in terms of the parameter δ are

$$C_\pm = 4 - \delta \pm 2\sqrt{2(2 - \delta)}.$$

TABLE III.1

Nonlinear Problem of Singular Perturbation Type

N	L^2 error	Maximum absolute error	Iterations
200	0.223(−5)	0.103(−4)	9
400	0.133(−6)	0.612(−6)	9
800	0.823(−8)	0.377(−7)	9

For $\delta = 2$, $C = 2$ and only one solution exists, whereas for $\delta > 2$ there is no solution. Starting from the initial guess $u(x) = 0$ and taking $\delta = 1$, the Newton method converges to the solution characterized by the root C_-. Four iterations are enough to obtain a relative error $< 10^{-12}$ in the nonlinear iteration. The errors of the numerical solutions with respect to the exact solution are given in Table III.2. They demonstrate the correctness of the proposed formulation of boundary value problems also in the presence of a singularity in the equation, without the need of matching the numerical solution to an analytic expansion in the neighborhood of the singularity. Again, the most convenient method for problems of this kind is the COLSYS code, which solves a problem almost identical to (4.3.2) with an error of

4.3.3. Blasius Equation

A very well-known equation of the boundary layer theory is the Blasius equation (see, e.g., [38, p. 135]),

$$\psi''' + \psi\psi'' = 0, \qquad \psi(0) = 0, \qquad \psi'(0) = 0, \qquad \psi'(\infty) = 1. \tag{4.3.3}$$

There are several ways of approaching the numerical solution of this boundary value problem. A first possibility is to introduce the variable *velocity* $u = \psi'$ and to write a system of *mixed-order* coupled equations for the variables u and ψ. A numerical scheme based on this representation of the problem is described in [38, p. 187]. Another possibility is to introduce the variable *vorticity* $\zeta = \psi''$ and to express the Blasius problem again as a mixed-order system for the variables ζ and ψ. A disadvantage of both mixed-order formulations is that the centering of the discretization for the different equations is not immediate, especially when higher order approximations are to be developed. This drawback is not present when the Blasius equation is instead formulated as a system of *three* first-order equations by introducing simultaneously the variables velocity $u = \psi'$ and vorticity $\zeta = u' = \psi''$, to give

$$\begin{aligned} \zeta' &= -\psi\zeta, & \int_0^\infty \zeta\, dx &= 1, \\ u' &= \zeta, & u(0) &= 0 \text{ or } u(\infty) = 1, \\ \psi' &= u, & \psi(0) &= 0. \end{aligned}$$

TABLE III.2

Nonlinear Problem with End Singularity

N	L^2 error	Maximum absolute error	Iterations
50	0.55(−7)	0.15(−6)	4
100	0.41(−8)	0.12(−7)	4
200	0.30(−9)	0.80(−9)	4
400	0.28(−10)	0.60(−10)	4

The fourth-order accurate scheme is used to solve such a system over the finite interval $[0, x_\infty]$ where $x_\infty = 5, 6, 7$, starting from the initial guess

$$\zeta(x) = \frac{1}{x_\infty}, \qquad u(x) = \frac{x}{x_\infty}, \qquad \psi(x) = \frac{x^2}{2x_\infty}.$$

Using up to 800 grid points, it is possible to determine the value of the wall vorticity $\zeta(0)$ with a precision of eight decimal figures (see Table III.3). The solution on the grid with 200 points and taking $x_\infty = 6$ is identical with the Howarth solution reproduced in [38, p. 139].

4.3.4. *Flow near a Rotating Disc*

Consider now the equations governing the steady flow of a viscous incompressible fluid which is set into motion by the rotation of a disc of infinite radial extent [38, p. 102]. They may be expressed as

$$\begin{aligned} F'' &= F'H + F^2 - G^2, \\ G'' &= G'H + 2FG, \\ H'' &= H'H + P', \\ H' &= -2F. \end{aligned} \tag{4.3.4}$$

Here, the prime denotes the derivative with respect to the variable ζ which expresses the dimensionless distance from the surface of the disc. The boundary conditions supplementing the system of equations are

$$\begin{aligned} F(0) &= 0, \qquad F(\infty) = 0, \\ G(0) &= 1, \qquad G(\infty) = 0, \\ H(0) &= 0. \end{aligned}$$

The last equation implies the equation $H'' + 2F' = 0$, which can be combined with the third equation to give $P' = -2F' - HH'$. Thus, the function $P(\zeta)$ can be expressed in terms of $F(\zeta)$ and $H(\zeta)$ by means of the relationship

TABLE III.3

Blasius Equation: Wall Vorticity

	$\zeta(0)$		
N	$x_\infty = 5$	$x_\infty = 6$	$x_\infty = 7$
100	0.46964510	0.46960041	0.46959985
200	0.46964514	0.46960049	0.46959998
300	0.46964514	0.46960049	0.46959999
400			0.46959999

$P = P_0 - 2F - H^2/2$, where P_0 is an arbitrary constant. It follows that the third equation can be eliminated from the system, obtaining a set of three coupled equations for the three unknowns F, G, and H, supplemented with the five specified boundary conditions. The problem is then reformulated as a system of five first-order differential equations by introducing the variables $E = F'$ and $K = G'$. After deriving the integral conditions for E and K from the boundary conditions originally prescribed, one obtains the set of equations and conditions

$$
\begin{aligned}
&E' = EH + F^2 - G^2, && \int_0^\infty E\, d\zeta = 0,\\
&F' = E, && F(0) = 0 \text{ or } F(\infty) = 0,\\
&K' = KH + 2FG, && \int_0^\infty K\, d\zeta = -1,\\
&G' = K, && G(0) = 1 \text{ or } G(\infty) = 0,\\
&H' = -2F, && H(0) = 0.
\end{aligned}
$$

Therefore, the introduction of the integral conditions allows providing each variable with its own condition. Now, defining the vectors

$$
y = \begin{bmatrix} E \\ F \\ K \\ G \\ H \end{bmatrix} \quad \text{and} \quad f(y) = \begin{bmatrix} EH + F^2 - G^2 \\ E \\ KH + 2FG \\ K \\ -2F \end{bmatrix},
$$

the nonlinear problem is rewritten in the canonical form $dy/d\zeta = f(y)$ and can be solved numerically by means of any one of the schemes previously described. For instance, the fourth-order accurate multipoint scheme is employed taking $\zeta_\infty = 20$ and using the four grids with $N = 50$, 100, 200, 400. The computed results are

TABLE III.4

Flow near a Rotating Disc

N	Err(G)	Err(H)	$E(0) = F'(0)$	$K(0) = G'(0)$
50	0.25(−1)	0.67(−1)	0.510585	−0.6152113
100	0.97(−3)	0.45(−2)	0.5102457	−0.61587339
200	0.37(−4)	0.15(−3)	0.5102336	−0.61591817
400	0.16(−5)	0.39(−5)	0.5102327	−0.61592174
[39]			0.510233	−0.6159220

compared in Table III.4 with the very accurate values provided by the following representation [39] of the exact solution for the variables H and G,

$$H(\zeta) = -\alpha + \sum_{n=1}^{\infty} A_n e^{-n\alpha\zeta}, \qquad G(\zeta) = \sum_{n=1}^{\infty} B_n e^{-n\alpha\zeta}.$$

The precise value of α is not known and its approximation depends on the number of terms which are retained in the summation. In the comparisons, the first 40 terms have been included, using for the coefficients A_n and B_n the values given in [39] which provides $\alpha = -H(\infty) = 0.884474$. Table III.4 indicates that the accuracy of the (fourth-order) solution over a mesh of 400 points is comparable with that one of the series expansion truncated after the first 40 terms.

4.4. *Higher Order Equations*

4.4.1. *Fourth-Order Nonlinear Equation*

The appropriateness of the integral conditions for higher order differential equations is first verified against the following nonlinear fourth-order equation

$$\psi'''' + [\psi''' \sin(\psi'' e^{\psi' \cos \psi}) + 1]^{-1} = s(x). \tag{4.4.1}$$

The nonlinear first-order system equivalent to Eq. (4.4.1) is integrated over the interval $[0, 1]$ assuming a solution of the form $\psi(x) = e^x$ and using Newton method. Starting from the initial guess $\psi \equiv 1$, four iterations are required to obtain a convergence error $< 10^{-12}$ with $N = 50, 100, 200$ points. The errors of the numerical solutions with respect to the exact solution are shown in Table IV.1. The theoretical order of convergence of the multipoint scheme is therefore achieved also in this higher order and highly nonlinear example.

4.4.2. *Sixth-Order Linear Equation*

This section on higher order nonhomogeneous problems is terminated by considering the following sixth-order, variable coefficient, equation,

$$\psi^{\mathrm{vi}} + x\psi^{\mathrm{v}} + \frac{1}{1+x}\psi'''' + \sin x\psi''' + e^x\psi'' + \cos x\psi' + e^{-x}\psi = s(x). \tag{4.4.2}$$

TABLE IV.1

Fourth-Order Nonlinear Equation

N	Maximum absolute error	L^2 error
50	0.529(−8)	0.337(−8)
100	0.321(−9)	0.208(−9)
200	0.199(−10)	0.129(−10)

Equation (4.4.2) is supplemented by the set of boundary conditions typical of a sixth-order problem as described in Section 3.2. The source term $s(x)$ is defined by choosing the solution to be $\psi(x) = e^{4x}$. The numerical results given in Table IV.2 indicate that the order of convergence of the linear multipoint scheme is not affected by the differential order of the problem provided the proper integral conditioning is taken into account.

4.5. *Orr–Sommerfeld Equation*

In view of the good numerical performances demonstrated by the fourth-order accurate scheme, it is employed also as a basic linear solver for the calculation of eigenvalues and eigenfunctions. This section describes the application of the methodology based on the use of integral conditions to a classical problem of hydrodynamic stability, namely, the determination of the most unstable mode in plane flow when the Reynolds number R is large.

The mathematical statement of this problem is the well-known Orr–Sommerfeld equation,

$$(D^2 - \alpha^2)^2 \psi - i\alpha R[V(x) - c](D^2 - \alpha^2)\psi + i\alpha R V''(x)\psi = 0, \tag{4.5.1}$$

supplemented with the no-slip boundary conditions

$$\psi(\pm 1) = 0, \qquad \psi'(\pm 1) = 0. \tag{4.5.2}$$

Here, the symbol D and the prime denote both the differentiation with respect to x, the coordinate normal to the plane walls, α is the wavenumber in the streamwise direction y, and c is the complex eigenvalue appearing in the expansion of the perturbation $\Psi(x, y, t) = \psi(x)\, e^{i\alpha(y - ct)}$. For Poiseuille plane flow, the unperturbed velocity $V(x)$ assumes the parabolic profile $V(x) \equiv 1 - x^2$. If the eigenvalue problem (4.5.1)–(4.5.2) is solved as a fourth-order problem, the boundary conditions (4.5.2) can be imposed without difficulties. Such an approach has been followed, for instance, using a finite element method with Hermite local basis [40] and using a spectral approximation with Chebyshev polynomials [41, 42]. Another method of solution is to transform the fourth-order equation into a system of two second-order equations by introducing the *vorticity* variable $\zeta = v_x - u_y$ in conjunc-

TABLE IV.2

Sixth-Order Linear Equation

N	Maximum absolute error	L^2 error	Convergence order
200	0.59(−5)	0.28(−5)	
400	0.37(−6)	0.17(−6)	4.00
800	0.23(−7)	0.11(−7)	4.01

tion with the *stream function* ψ. The conditions supplementing such an equation system can be found following the analysis given in [28]. The present work being devoted to a first-order formulation, the Orr–Sommerfeld problem will be reformulated by introducing the additional variables $\xi = \zeta'$ and $\phi = \psi'$. The complete set of conditions for the variables (ξ, ζ, ϕ, ψ) is determined by a reasoning similar to that followed in Section 3.1 where the integral conditions appropriate to a fourth-order boundary value problem have been obtained. There is, however, a slight difference due to the fact that the variables with missing boundary conditions are defined here in terms of ψ through the relationships

$$\zeta = (-D^2 + \alpha^2)\psi \qquad \text{and} \qquad \xi = D(-D^2 + \alpha^2)\psi,$$

so that the Green identities for the operators $(-D^2 + \alpha^2)$ and $D(-D^2 + \alpha^2)$ are necessary to determine the integral conditions for ζ and ξ, respectively. The full set of first-order equations with the corresponding conditions is found to be

$$\begin{aligned}
&\xi' = W(x, \alpha)\zeta + i\alpha R V''(x)\psi, && \int_{-1}^{+1} \xi[\cosh(\alpha x) - \cosh\alpha]\, dx = 0,\\
&\zeta' = \xi, && \int_{-1}^{+1} \zeta \cosh(\alpha x)\, dx = 0,\\
&\phi' = -\zeta + \alpha^2\psi, && \phi(-1) = 0 \text{ or } \phi(+1) = 0,\\
&\psi' = \phi, && \psi(-1) = 0 \text{ or } \psi(+1) = 0,
\end{aligned} \tag{4.5.3}$$

where $W(x, \alpha) \equiv \alpha^2 + i\alpha R[V(x) - c]$. By introducing the quantities

$$y = \begin{bmatrix} \xi \\ \zeta \\ \phi \\ \psi \end{bmatrix}, \qquad A(x) = \begin{bmatrix} 0 & W(x, \alpha) & 0 & i\alpha R V''(x) \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & \alpha^2 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \tag{4.5.4}$$

the differential system can be written in the notation of Section 1 as $y' = A(x)\, y$. The discretization over a grid with N points provides the generalized eigenvalue problem $(\mathbf{A} - c\mathbf{B})\mathbf{y} = 0$, where $\mathbf{y}$ is a $4N$-vector, whereas $\mathbf{A}$ and $\mathbf{B}$ are $4N \times 4N$ matrices. A single eigenvalue and the associated eigenfunction can be evaluated using the standard shifted-inverse-power iterative method. For high values of the Reynolds number, the solution provided by the backward and forward substitutions can be, however, so inaccurate that the iterative method may fail to converge. In order to guarantee the converge also in these difficult situations, it is possible to resort to the Wilkinson refinement procedure (see section 2.4). For computational efficiency, the solution of the linear system will be refined only when the error due to the ill-posedness of the system is greater than the relative error in the inverse power iteration.

TABLE V.1

Eigenvalue of the Orr–Sommerfeld Problem for Plane Poiseuille Flow at $R = 10^4$ and $\alpha = 1$

N	c
100	0.23752 89394 + i0.00373 95295
200	0.23752 66440 + i0.00373 96594
400	0.23752 64984 + i0.00373 96698
800	0.23752 64894 + i0.00373 96705
[41, 42]	0.23752 649 + i0.00373 967

Note. Coordinate transformation parameter $a = 1.4$. Initial eigenvalue for the shifted-inverse-power method $\hat{c} = 0.24 + i0.0038$.

The eigenvalue associated with the most unstable mode for Poiseuille plane flow has been calculated using a uniform grid over the entire interval $[-1, 1]$ for moderately large values of R. For $R = 10^4$ and $R = 10^6$ and a wavenumber $\alpha = 1$, the agreement of the present results with the values published in the literature [41, 42, 15] is fully satisfactory. The eigenfunction of the considered mode being symmetric, the eigenproblem can be solved on the half interval $[0, 1]$, using the conditions appropriate to the even subproblem, namely,

$$\xi(0) = 0,$$

$$\int_0^1 \zeta \cosh(\alpha x)\, dx = 0,$$

$$\phi(0) = 0 \qquad \text{or} \qquad \phi(1) = 0,$$

$$\psi(1) = 0.$$

Numerically identical results have been obtained on the two intervals. At larger values of the Reynolds number a great reduction of the number of grid points to

TABLE V.2

Eigenvalue c and Transformation Parameter a in the Orr–Sommerfeld Problem for Plane Poiseuille Flow, $\alpha = 1$

$\log_{10} R$	c	a
4	0.23752 64894 + i0.00373 96705	1.4
5	0.14592 47902 − i0.01504 20430	2.0
6	0.06659 25239 − i0.01398 32675	2.5
7	0.03064 12978 − i0.00726 04873	3.0
8	0.01471 134 − i0.00351 239	3.5
9	0.00656 63030 − i0.00166 00213	4.0

be used for a fixed accuracy is afforded by introducing the stretching of the variable x suggested in [43] as

$$x = x(X) = \frac{\tanh(aX)}{\tanh(a)},$$

where a is an adjustable parameter. For example, using the stretching $a = 1.4$ for $R = 10^4$, the value of c converges to the very accurate estimate given in [41, 42] in the manner shown in Table V.1. The fourth-order accurate scheme with 400 points has the same accuracy of a spectral calculation with 25 Chebyshev modes.

When R is higher, the value of the stretching parameter a must be increased. The values of c and a for R in the range $10^4 \leqslant R \leqslant 10^9$ are given in Table V.2. The accuracy of the eigenvalues calculated on a mesh of 800 points is greater than in the orthonormalization method on finer grids.

The convergence of the eigenfunctions for the cases $R = 10^6$ and $R = 10^9$ to the reference solutions provided by Davey [15] is shown in Tables V.3 and V.4, by comparing the values of the real and imaginary parts of ψ at some selected points.

TABLE V.3

Selected Values of the Eigenfunction of the Orr–Sommerfeld Problem for Plane Poiseuille Flow with $R = 10^6$ and $\alpha = 1$

	Linear multipoint method				[14]	
	$N = 400$		$N = 800$		$N = 700$	
x	ψ_r	ψ_i	ψ_r	ψ_i	ψ_r	ψ_i
0	1	0	1	0	1	0
0.10	0.994272	0.000161	0.994274	0.000161	0.994275	0.000161
0.20	0.976933	0.000646	0.976934	0.000646	0.976935	0.000646
0.30	0.947462	0.001467	0.947466	0.001467	0.947467	0.001467
0.40	0.904969	0.002640	0.904972	0.002640	0.904973	0.002640
0.50	0.848079	0.004196	0.848081	0.004196	0.848082	0.004196
0.60	0.774779	0.006182	0.774782	0.006182	0.774783	0.006182
0.70	0.682077	0.008679	0.682079	0.008679	0.682080	0.008679
0.80	0.565123	0.011865	0.565125	0.011864	0.565125	0.011864
0.90	0.414020	0.016380	0.414021	0.016380	0.414021	0.016380
0.91	0.396177	0.017003	0.396177	0.017002	0.396177	0.017002
0.92	0.377634	0.017708	0.377636	0.017708	0.377635	0.017708
0.93	0.358173	0.018515	0.358173	0.018515	0.358173	0.018515
0.94	0.338029	0.018894	0.338028	0.018894	0.338027	0.018894
0.95	0.319253	0.021545	0.319256	0.021544	0.319256	0.021543
0.96	0.292479	0.034693	0.292486	0.034693	0.292490	0.034694
0.97	0.235163	0.043859	0.235170	0.043868	0.235171	0.043870
0.98	0.152351	0.022454	0.152351	0.022454	0.152351	0.022455
0.99	0.059842	−0.006412	0.059840	−0.006417	0.059840	−0.006417
1	0	0	0	0	0	0

TABLE V.4

Selected Values of the Eigenfunction of the Orr–Sommerfeld Problem for Plane Poiseuille Flow with $R = 10^9$ and $\alpha = 1$

	Linear multipoint method				[14]	
	$N = 400$		$N = 800$		$N = 24000$	
x	ψ_r	ψ_i	ψ_r	ψ_i	ψ_r	ψ_i
0	1	0	1	0	1	0
0.900	0.479059	0.001682	0.479061	0.001682	0.479061	0.001682
0.910	0.463504	0.001738	0.463504	0.001738	0.463504	0.001738
0.920	0.447431	0.001798	0.447432	0.001798	0.447432	0.001798
0.930	0.430794	0.001862	0.430794	0.001862	0.430795	0.001862
0.940	0.413527	0.001933	0.413528	0.001933	0.413527	0.001933
0.950	0.395547	0.002012	0,395547	0.002012	0.395547	0.002012
0.960	0.376731	0.002102	0.376731	0.002102	0.376731	0.002102
0.970	0.356894	0.002212	0.356894	0.002212	0.356894	0.002212
0.980	0.335708	0.002360	0.335708	0.002360	0.335708	0.002360
0.990	0.312405	0.002616	0.312405	0.002616	0.312404	0.002616
0.991	0.309884	0.002658	0.309884	0.002658	0.309883	0.002658
0.992	0.307325	0.002710	0.307326	0.002710	0.307325	0.002710
0.993	0.304603	0.002861	0.304604	0.002863	0.304604	0.002864
0.994	0.301615	0.002168	0.301609	0.002170	0.301606	0.002171
0.995	0.302998	0.001796	0.302995	0.001773	0.302993	0.001767
0.996	0.302919	0.018106	0.302941	0.018100	0.302941	0.018100
0.997	0.261235	0.043246	0.261251	0.043261	0.261255	0.043265
0.998	0.171739	0.029029	0.171740	0.029030	0.171740	0.029031
0.999	0.066752	−0.005564	0.066749	−0.005571	0.066749	−0.005572
1	0	0	0	0	0	0

The values of the present solutions at these points have been obtained by means of a linear interpolation.

The great accuracy of the results provided by the proposed scheme using the integral conditions jointly with the variable stretching is not surprising when one considers that an integrally conditioned vorticity equation was at the heart of the asymptotic stability analysis for plane Couette flow undertaken by Davey [44].

5. Conclusion

In this paper linear multipoint methods with an even order of accuracy for the solution of boundary value problems for ordinary differential equations have been presented. The key point which has made it possible to establish the new class of numerical schemes is the recognition that the systems of first-order equations stemming from two-point boundary value problems constitute a category of ordinary differential problems quite distinct from that one associated with initial value

problems. As a consequence, conditions of an integral (nonlocal) type, instead of the usual boundary value (local) type, have been found to supplement the system of first-order equations, so that the idea of marching in time or using a step-by-step integration procedure has been dismissed. The introduction of the concept of nonlocal conditions led to outline a simple and unitary numerical framework for the solution of practically any kind of boundary value problems. With respect to initial value methods, the new formulation presents the advantage that the number of independent or dependent variables is not increased and that no orthogonalization procedure is required.

The linear multipoint schemes have then been applied to solve a wide spectrum of linear and nonlinear test problems. Satisfactory results have been obtained without encountering the numerical difficulties faced by simple superposition methods provided that the Wilkinson refinement procedure is employed in the case of stiff equations. The fourth-order accurate multipoint method has also been used in conjunction with the shifted-inverse-power iteration method to compute eigenvalues and eigenfunctions of an Orr–Sommerfeld problem when the Reynolds number is large. Although the method has proven to be successful in refining the eigenvalue associated with the most unstable mode for plane Poiseuille flow, the significance of the proposed formulation for the solution of the general eigenvalue problem remains to be investigated.

It can be concluded by emphasizing once more the extreme simplicity, efficiency, and reliability of the proposed method, all properties resulting from the fact that it is based on an algebraically exact representation of the original boundary value problem.

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