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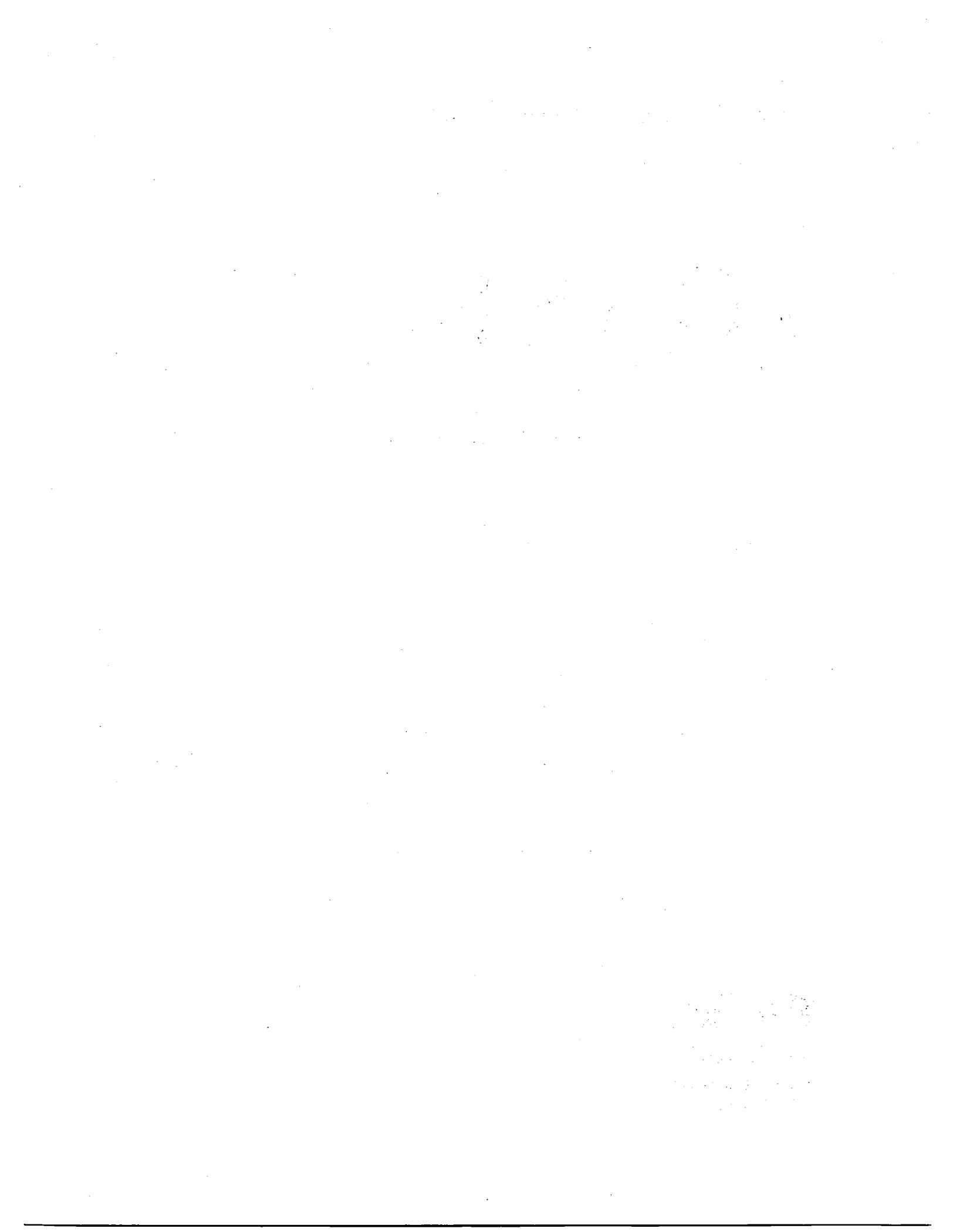Operated by the Universities Space Research Association

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BOUNDARY CONDITIONS IN CHEBYSHEV AND LEGENDRE METHODS

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Abstract

We discuss two different ways of treating non-Dirichlet boundary conditions in Chebyshev and Legendre collocation methods for second order differential problems.

An error analysis is provided. The effect of preconditioning the corresponding spectral operators by finite difference matrices is also investigated.

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1. Introduction

In the analysis of spectral methods, Neumann or third type boundary value problems for second-order elliptic operators have received less attention than Dirichlet boundary value problems. The eigenvalues of a family of Chebyshev collocation operators related to non-Dirichlet boundary conditions were analyzed in [8], while the properties of stability and convergence of such schemes were investigated in [3] using a general variational principle. In both cases, the boundary conditions are satisfied exactly by the spectral solution, while the differential equation is collocated at the interior nodes.

An alternative method of imposing the boundary conditons within a pseudospectral scheme consists of modifying the boundary values of the first derivative according to the Neumann or third type conditions, during the evaluation of the differential operator. The equation is now collocated at the boundary points, too. In this way all the grid-points are treated at the same way by the iterative or time advancing algorithm of solution. We call this method the implicit treatment of the boundary conditions.

In this paper we prove the stability and convergence of both a Legendre and a Chebyshev collocation scheme in which the Neumann boundary conditions are treated implicitly. Global error estimates are derived. Moreoever, it is proved that the spectral solution satisfies the boundary conditions up to an error which decays spectrally. Thus the spectral accuracy of the method is not wasted.

Since the spectral collocation approximations of second order boundary value problems are usually solved by iterative techniques (see, e.g., [13]), we carried out an experimental analysis on the eigenvalues of the corresponding operators, in which the boundary conditions are imposed either

explicitly or implicitly. The results of this investigation are also reported in this paper. It was found that for both the boundary treatments the eigenvalues are real and positive. The matrix arising from an explicit treatment can be preconditioned in a more natural way. However, it is shown in Section 5 how to build-up an effective preconditioner also in the case of implicitly-treated boundary conditions.

Notations: The following notations will be used throughout the paper.

$\mathbb{P}_N$: the space of the algebraic polynomials of degree up to N in the variable x;

$w(x) = (1 - x^2)^{1/2}$: (the Chebyshev weight),

or

$w(x) \equiv 1$: (the Legendre weight);

$L_w^2(-1,1)$: the Hilbert space of the (classes of) Lebesgue integrable functions v such that the norm

$$\|v\|_{0,w} = \left(\int_{-1}^{1} v^2(x)w(x)dx\right)^{1/2}$$

is finite;

$H_w^m(-1,1)$: the Sobolev space of the functions $v \in L_w^2(-1,1)$ such that their distributional derivatives of order up to m are in $L_w^2(-1,1)$, with norm

$$\|v\|_{m,w} = \left(\sum_{k=0}^{m} \int_{-1}^{1} [v^{(k)}(x)]^2 w(x)dx\right)^{1/2};$$

$H_{w,0}^1(-1,1)$:   the subspace of $H_w^1(-1,1)$ of the functions vanishing at the

boundary points $x = \pm 1$;

$L^2(0,T; H_w^m(-1,1))$:   the Hilbert space of the (classes of) functions

$v = v(x,t)$ such that for almost every $t \in (0,T)$ the

function $v(\cdot,t) \in H_w^m(-1,1)$ and the norm

$$\left(\int_0^T \|v(\cdot,t)\|_{m,w}^2 \, dt \right)^{1/2}$$

is finite.

When $w(x) \equiv 1$, we will drop the subscript w in all the previous notations.

2. The Treatment of the Boundary Conditions

We shall base our discussion about different treatments of the boundary conditions upon the following model problems:

$$(2.1) \qquad -u_{xx} + u = f(x), \qquad -1 < x < 1$$

and

$$(2.2) \qquad \begin{cases} u_t - u_{xx} = f(x,t), & -1 < x < 1, \ t > 0 \\ u(x,0) = u_0(x), & -1 < x < 1 \end{cases}$$

In both cases, the solution u is assumed to satisfy the homogeneous boundary conditions:

$$(2.3) \qquad \begin{cases} B_+ \, u \equiv \beta u_x + \alpha u = 0 & \text{at} \quad x = 1 \\ B_- \, u \equiv \delta u_x + \gamma u = 0 & \text{at} \quad x = -1, \end{cases}$$

for real constants α, β, γ and δ such that

$$(2.4) \qquad \begin{cases} \alpha^2 + \beta^2 \neq 0 & \alpha\beta \geq 0 \\ \gamma^2 + \delta^2 \neq 0 & \gamma\delta \leq 0. \end{cases}$$

Under this assumption, one has by partial integration

$$- \int_{-1}^{1} u_{xx} \, u dx \geq \int_{-1}^{1} (u_x)^2 \, dx.$$

Hence, the energy method (see, e.g., [11], Vols. I and II) assures that for all $f \in L^2(-1,1)$ there exists a unique variational solution $u \in H^2(-1,1)$ of the boundary value problem (2.1), (2.3), such that

$$\| u \|_1 \leq \| f \|_0.$$

Similarly, for all $u_0 \in L^2(-1,1)$ and all $f \in L^2(0,T; L^2(-1,1))$ with $T > 0$, there exists a unique variational solution $u \in L^2(0,T; H^1(-1,1)) \cap L^\infty(0,T; L^2(-1,1))$ for the initial-boundary value problem (2.2), (2.3), such that, for all $t \leq T$

$$\| u(t) \|_0^2 + \int_0^t \| u(t) \|_1^2 \, dt \leq \| u_0 \|_0^2 + \exp(t) \int_0^t \| f(\tau) \|_0^2 \, d\tau .$$

Moreover, the regularity of the solution (in the Sobolev scale $H^m(-1,1)$ or $H^m_w(-1,1)$) increases with the regularity of the data.

REMARK 2.1: Weaker assumptions than (2.4) assure the well-posedness of the boundary value problems (2.1)-(2.3) (see, for instance, [8], Theorem 2.1). However, we are not interested here in the minimality of our hypothesis, since we want to focus on the essential aspects of the treatment of the boundary conditions. For the same reason, we confine ourselves to very simple model problems, although the methods we discuss apply to general boundary value problems as well. ∎

We want to discretize (in space) equations (2.1) and (2.2) by a pseudospectral collocation method of Chebyshev or Legendre type. To this end, we look for an approximate solution u^N which is a global algebraic polynomial of degree N in the domain $(-1,1)$. Moreover, we consider the $N + 1$ nodes

$$(2.5) \qquad -1 = x_N < x_{N-1} \cdots < x_1 < x_0 = 1$$

of the Gauss-Lobatto integration rule for the Chebyshev weight $w(x) = (1 - x^2)^{-1/2}$ or for the Legendre weight $w(x) \equiv 1$ in $(-1,1)$, (see [6]). If $w_j, j = 0, \cdots, N$, are the corresponding positive weights, one has the identity

$$(2.6) \qquad \int_{-1}^{1} f(x)w(x)dx = \sum_{j=0}^{N} f(x_j)w_j \qquad \text{for all } f \in \mathbb{P}_{2N-1}.$$

The points w_j, $j = 0, \cdots, N$, are the relative extrema in $[-1,1]$ of the N-th Chebyshev polynomial of first kind or of the N-th Legendre polynomial.

Since a polynomial of degree N is uniquely defined through its values at the nodes (2.5) we shall identify throughout the paper a polynomial of

degree N with the set of its values at the same nodes. Thus, if L is a
matrix of order N + 1 and u ε $\mathbb{P}_N$, Lu will denote the product of the
matrix L by the vector $\{u(x_j) \mid j = 0, \cdots, N\}^T$, i.e.,

$$(2.7) \qquad Lu =: L \begin{pmatrix} u(x_0) \\ \\ u(x_N) \end{pmatrix} \qquad \forall \, u \, \varepsilon \, \mathbb{P}_N.$$

Given a continuous function v in [-1,1], we denote by $I_N v$ the unique
polynomial of degree N, interpolating v at the nodes (2.5), i.e.,

$$(2.8) \qquad I_N v \, \varepsilon \, \mathbb{P}_N, \quad (I_N v)(x_j) = v(x_j), \qquad j = 0, \cdots, N.$$

Some approximation properties of the operator I_N in the Sobolev scale
H_w^m, m ≥ 0, have been analyzed in [1] and will be used hereafter. In
particular, there exists a constant C > 0 independent of N such that if
the Chebyshev points are used, one has

$$(2.9) \qquad \| v - I_N v \|_{0,w} \leq CN^{-m} \| v \|_{m,w}, \quad \forall \, u \, \varepsilon \, H_w^m(-T,T), \quad m > \tfrac{1}{2},$$

while if the Legendre points are used one has

$$(2.9)^{\frown} \qquad \| v - I_N v \|_0 \leq CN^{\tfrac{1}{2} - m} \| v \|_m, \quad \forall \, u \, \varepsilon \, H^m(-1,1), \quad m > \tfrac{1}{2}.$$

Finally, we recall for future reference that the semi-norm

$$\| v \|_{N,w} = \left(\sum_{j=0}^N v^2(x_j) w_j \right)^{1/2}$$

is uniformly equivalent to the norm $\|v\|_{0,w}$ over $\mathbb{P}_N$ (see [1], Sections 3.1, 3.2), i.e., there exist constants $c_1 > 0$, $c_2 > 0$ independent of N such that

$$(2.10) \qquad c_1 \|v\|_{0,w} \leq \|v\|_{N,w} \leq c_2 \|v\|_{0,w}, \qquad \forall u \in \mathbb{P}_N.$$

If the boundary conditions (2.3) are of Dirichlet type (i.e., $\beta = \delta = 0$), the typical spectral collocation scheme consists of collocating the differential equation at the interior nodes (2.5) and setting to zero the solution u^N on the boundary. This procedure, which we shall call the _explicit_ imposition of the boundary conditions, is not restricted to Dirichlet boundary conditions. Thus, the boundary value problem (2.1), (2.3) can be approximated as

$$(2.11) \qquad \begin{cases} u^N \in \mathbb{P}_N \\[2ex] \left(-u^N_{xx} + u^N\right)(x_j) = f(x_j) \qquad j = 1, \cdots, N-1 \\[2ex] \left(B_+ u^N\right)(x_0) = \left(B_- u^N\right)(x_N) = 0, \end{cases}$$

while the initial-boundary value problem (2.2), (2.3) can be discretized in space for all $t > 0$ as

$$(2.12) \qquad \begin{cases} u^N(t) \in \mathbb{P}_N \\[2ex] \left(u^N_t - u^N_{xx}\right)(x_j, t) = f(x_j, t) \qquad j = 1, \cdots, N-1 \\[2ex] \left(B_+ u^N\right)(x_0, t) = \left(B_- u^N\right)(x^N, t) = 0 \end{cases}$$

with the initial condition $u^N(0) = I_N u_0$.

For the Chebyshev collocation points, the convergence of the scheme (2.11) has been proven in [3], where error estimates have also been given. Furthermore, in [8] it has been established that the eigenvalues obtained by replacing f with λu^N in (2.11) are all real, positive and distinct.

The unknowns to be solved for in both (2.11) and (2.12) are the values of u^N at the interior collocation nodes and at the boundary nodes where a non-Dirichlet boundary condition is imposed. The algebraic system (2.11) can be efficiently solved by an iterative method, applied after preconditioning the spectral system (see, e.g., [13], [14]). We shall base our discussion of the computational aspects of the boundary treatment on the Richardson method, which is briefly recalled in Section 5.

The differential system (2.12) can be solved by an implicit or an explicit time-marching method. In the first case, one has to solve at each time step a discrete Helmholtz equation similar to (2.11), for which one can apply one of the iterative procedures proposed for spectral methods. If an explicit scheme is used instead, the solution is advanced only at the interior collocation nodes. The boundary values of u^N at the new time level are subsequently determined in order to satisfy the boundary conditions exactly. Such values are obtained by solving the 2×2 system

$$
\begin{cases}
(\alpha + \beta d_{00})u_0^N + \beta d_{0N}\, u_N^N = -\beta \sum_{j=1}^{N-1} d_{0j}\, u_j^N \\[4mm]
(\gamma + \delta d_{NN})u_N^N + \delta d_{N0}\, u_0^N = -\delta \sum_{j=1}^{N-1} d_{Nj}\, u_j^N
\end{cases}
$$

where $\{d_{ij}\}$ is the matrix representing the spectral derivative at the collocation points (2.5) (an explicit formula for $\{d_{ij}\}$ can be found in [7]).

A completely different strategy can be followed in the process of imposing the boundary conditions: these are taken into account during the spectral evolution of the differential operator, by modifying accordingly the boundary values of the first derivative of the spectral solution. Precisely, assume that both the boundary conditions are of non-Dirichlet type, so that one can set $\beta = \delta = 1$ in (2.3) with no loss of generality. For any $v \in \mathbb{R}_N$ define the polynomial $I_N(Bv_x)$ as follows

$$(2.13) \qquad \begin{cases} I_N(Bv_x) \in \mathbb{R}_N \\[2ex] I_N(Bv_x)(x_0) = -\alpha v(x_0) \\[2ex] I_N(Bv_x)(x_j) = v_x(x_j) \qquad j = 1, \cdots, N-1 \\[2ex] I_N(Bv_x)(x_N) = -\gamma v(x_N). \end{cases}$$

Thus $I_N(Bv_x)$ coincides with v_x at the interior nodes, but it modifies the boundary values of v_x according to (2.3). We consider the following approximation of the boundary value problem (2.1), (2.3):

$$(2.14) \qquad \begin{cases} u^N \in \mathbb{R}_N \\[2ex] -[I_N(Bu_x^N)]_x(x_j) + u^N(x_j) = f(x_j), \qquad j = 0, \cdots, N. \end{cases}$$

Similarly, we discretize the initial-boundary value problem (2.2), (2.3) as follows:

$$(2.15) \quad \begin{cases} u^N(t) \in \mathbb{P}_N \\[2ex] u_t^N(x_j,t) - \left[I_N\left(Bu_x^N\right)\right]_x(x_j,t) = f(x_j,t), \qquad j = 0,\cdots,N \\[2ex] u^N(0) = I_N u_0. \end{cases}$$

Note that the differential equation is now collocated at the boundary points also. On the other hand, the solution is not required to satisfy — and generally it will not satisfy — the boundary conditions exactly. However, it will be proved in the next sections that the boundary conditions are satisfied up to an error which decays spectrally with N.

The procedure now described, first proposed by D. Gottlieb for time dependent problems, will be called the implicit treatment of the boundary conditions. All the iterative or the time-advancing methods proposed for solving the approximation schemes (2.11) or (2.12) respectively, can be applied in computing the solution of (2.14) or (2.15) as well. The computational advantage arising from an implicit treatment of the boundary conditions is that the iterative process of solution acts on all the grid-points in the domain simultaneously. Any distinction between boundary and interior points is avoided.

More complex boundary conditions than (2.3), involving integro-differential or non-linear boundary operators, can be easily implemented in an implicit way, too. For instance, in [5] a far-field radiation condition of the type

$$\frac{\partial u}{\partial r} = K*u,$$

where K*u is a convolution operator on the far-field boundary, was successfully taken into account implicitly within a Fourier-Chebyshev collocation method for an exterior elliptic problem.

3. Theoretical Results for the Legendre Method

Throughout this section we assume that the collocation points (2.5) are the quadrature nodes of a Gass-Lobatto formula for the Legendre weight $w(x) \equiv 1$. The corresponding weights are given by

$$(3.1) \qquad w_j = \frac{2}{N(N + 1)[L_N(x_j)]^2} \, ,$$

(see, e.g., [6]), where $L_N(x)$ denotes the N-th Legendre polynomial such that $L_N(1) = 1$.

We shall carry out an analysis for the implicit treatment of the boundary conditions in the case of Neumann boundary conditions, i.e., we choose $\beta = \delta = 1$ and $\alpha = \gamma = 0$ in (2.3).

The first results concern the stability and convergence properties of the method.

THEOREM 3.1: Let u^N be the solution of (2.12). The following estimate holds:

$$(3.2) \qquad \int_{-1}^{1} [u^N(x)]^2 \, dx + 2 \sum_{j=1}^{N-1} [u_x^N(x_j)]^2 \, w_j \leq \int_{-1}^{1} [I_N f(x)]^2 \, dx.$$

PROOF: Equation (2.12) can be equivalently written as

(3.3)
$$-[I_N(Bu_x^N)]_x + u^N = I_N f, \qquad -1 < x < 1,$$

since both sides are polynomials of degree N which match at $N + 1$ distinct points. Multiply by u^N and integrate over $(-1,1)$. Since $I_N(Bu_x^N)$ vanishes at the end points (see (2.11)), we have by partial integration

(3.4)
$$\int_{-1}^{1} I_N(Bu_x^N)u_x^N \, dx + \int_{-1}^{1} [u^N(x)]^2 \, dx = \int_{-1}^{1} I_N f(x)u^N(x)dx.$$

On the other hand, by (2.6)

$$\int_{-1}^{1} I_N(Bu_x^N)u_x^N \, dx = \sum_{j=1}^{N-1} [u_x^N(x_j)]^2 w_j ,$$

whence (3.3) follows by applying the Cauchy-Schwarz inequality to the right-hand side of (3.4). ■

THEOREM 3.2: Let u be the solution of the boundary value problem (2.1), (2.3), and u^N the solution of (2.12). Assume the $u \in H^m(-1,1)$ with $m > 5/2$. There exist two constants $C' > 0$, $C'' > 0$ independent of N, u and u^N such that

(3.5)
$$\|u - u^N\|_0 + \left(\sum_{j=1}^{N-1} [u_x - u_x^N]^2(x_j)w_j \right)^{1/2}$$
$$\leq C'N^{2-m}\|u\|_m + C''N^{\frac{5}{2}-m}\|f\|_{m-2}$$

PROOF: Set $V = \{v \in H^2(-1,1) \mid v_x(\pm 1) = 0\}$ and
$V_N = \{v \in \mathbb{P}_N \mid v_x(\pm 1) = 0\}$. Let us define first a projection operator

$$R_N: V \longrightarrow V_N$$

in the following way. Given $v \in V$, denote by w^N the orthogonal projection of v_x upon $\mathbb{P}_{N-1} \cap H_0^1(-1,1)$ in the inner product of $H^1(-1,1)$. According to [12], Theorem 1.6, we have

$$\|v_x - w^N\|_k \leq CN^{k+1-m}\|v\|_m, \qquad k = 0,1.$$

If we set

$$(R_N v)(x) = \mu + \int_{-1}^{x} w(s)ds,$$

where μ is such that

$$\int_{-1}^{1} R_N v(x)dx = \int_{-1}^{1} v(x)dx,$$

it is not difficult to check by a duality argument that

$$(3.6) \qquad \|v - R_N v\|_k \leq CN^{k-m}\|v\|_m, \qquad k = 0,1,2.$$

By definition, $\tilde{u} = R_N u$ satisfies the equation

$$-\left[I_N(B\tilde{u}_x)\right]_x + \tilde{u} = \left(-\tilde{u}_{xx} + u_{xx}\right) + \left(\tilde{u} - u\right) + f.$$

It follows from Theorem 3.1 that the difference $e^N = \tilde{u} - u^N$ satisfies the inequality

$$\int_{-1}^{1} [e^N(x)]^2 \, dx + 2 \sum_{j=1}^{N-1} [e_x^N(x_j)]^2 \, w_j \leq \int_{-1}^{1} [f - I_N f]^2 \, dx$$

$$+ \int_{-1}^{1} [u_{xx} - \tilde{u}_{xx}]^2 \, dx + \int_{-1}^{1} [u - \tilde{u}]^2 \, dx.$$

According to (3.6) and (2.9) one has

(3.7)

$$\int_{-1}^{1} [e^N(x)]^2 \, dx + 2 \sum_{j=1}^{N-1} [e_x^N(x_j)]^2 \, w_j \leq \tilde{C} N^{4-2m} \|u\|_m^2 + \tilde{C}'' N^{5-2m} \|f\|_{m-2}^2 .$$

On the other hand, we have by (2.10)

$$\sum_{j=1}^{N-1} [u_x - \tilde{u}_x]^2(x_j)w_j = \sum_{j=0}^{N} [u_x - \tilde{u}_x]^2(x_j)w_j \leq C \| I_N(u_x - \tilde{u}_x) \|_0^2$$

$$\leq C \{ \| u_x - \tilde{u}_x \|_0^2 + \| (I - I_N)(u_x - \tilde{u}_x) \|_0^2 \}$$

$$\leq C \{ \| u_x - \tilde{u}_x \|_0^2 + C N^{-1} \| u_x - \tilde{u}_x \|_1^2 \}$$

$$\leq C N^{3-2m} \|u\|_m^2 .$$

Then (3.5) follows from (3.6)-(3.7), using the triangle inequality for $u - u^N = (u - \tilde{u}) + e^N$. ∎

REMARK 3.1: Theorem 3.2 can also be proved by a different proof, similar to the one which will be given in the next section for establishing Theorem 4.2. ■

The previous theorems guarantee the stability and convergence of the approximation (2.14) in the norm

$$(3.8) \qquad \|v\|_* = \Big(\int_{-1}^{1} v^2(x)dx + \sum_{j=1}^{N-1} v_x^2(x_j)w_j \Big)^{1/2}.$$

Therefore, we are led to investigate the relationship between this norm and the usual energy norm

$$\|v\|_1 = \Big(\int_{-1}^{1} v^2(x)dx + \int_{-1}^{1} v_x^2(x)dx \Big)^{1/2}.$$

The two norms are clearly equivalent for polynomials of degree up to N, in the sense that

$$(3.9) \qquad \|v\|_* \leq \|v\|_1 \leq C(N)\|v\|_*, \qquad \forall \ v \ \varepsilon \ \mathbb{P}_N,$$

where C(N) is a function of N. However, the two norms are not uniformly equivalent, i.e., C(N) cannot be bounded independently of N. For instance, take $v = L_N$, the N-th Legendre polynomial. One has $\|L_N\|_*^2 = \|L_N\|_0^2 = 2/(1 + 2N)$, but $\|L_N\|_1^2 = 2 + 2/(1 + 2N)$. The numerical evaluation of C(N) shows that

$$(3.10) \qquad C(N) \simeq N^{3/2} \quad \text{as} \quad N \to \infty$$

Table 1. The constant C(N)

N	C(N)	$C(N)/N^{3/2}$
2	4.	1.42
4	9.6	1.19
6	16.6	1.13
8	24.8	1.10
10	34.0	1.08
12	44.2	1.06
14	55.2	1.05
16	67.0	1.05
18	79.6	1.04
20	93.0	1.04

The asymptotic behavior of C(N) observed experimentally can be mathematically proved as follows.

THEOREM 3.3: Let C(N) be defined by (3.9). Then

$$(3.11) \qquad\qquad C(N) \leq CN^{3/2}$$

PROOF: By (2.6),

$$\|v\|_1^2 = \|v\|_*^2 - v_x^2(1)w_0 - v_x^2(-1)w_N \qquad \forall\ v \in \mathbb{P}_N,$$

where w_0, w_N are given in (3.1). Then the theorem follows immediately from the next lemma. ∎

LEMMA 3.1: There exist two positive constrants C_1 and C_2 such that for all $v \in \mathbb{P}_N$

$$(3.12) \qquad |v_x(\pm 1)| \leq C_1 N^{5/2} \|v\|_0 + C_2 N^{3/2} \left(\sum_{j=1}^{N-1} [v_x(x_j)]^2 w_j \right)^{1/2}$$

PROOF: Recalling the expansion of v_x in terms of Legendre polynomials (see, e.g., [9], Appendix) one has

$$\int_{-1}^{1} v_x(x) L_N(x) dx = 0$$

$$\int_{-1}^{1} v_x(x) L_{N-1}(x) dx = (2N + 1) \int_{-1}^{1} v(x) L_N(x) dx$$

or equivalently

$$(3.13) \qquad v_x(1) w_0 + (-1)^N v_x(-1) w_N = - \sum_{j=1}^{N-1} v_x(x_j) L_N(x_j) w_j$$

$$v_x(1) w_0 - (-1)^N v_x(-1) w_N = - \sum_{j=1}^{N-1} v_x(x_j) L_{N-1}(x_j) w_j$$

$$(3.14) \qquad \qquad \qquad + (2N + 1) \int_{-1}^{1} v(x) L_N(x) dx.$$

Then (3.12) follows using (3.1) and the Cauchy-Schwarz inequality on the right-hand side. ∎

The spectral solution u^N of problem (2.12) is not required to satisfy (and generally it will not satisfy exactly) the boundary conditions (2.3).

However, since these are taken into account in the collocation process, one expects u^N to satisfy approximate boundary conditions very close to the exact ones. Lemma 3.1 yields an estimate for the values of u_x^N on the boundary. Actually, define $\tilde{u} = R_N u$ as in the proof of Theorem 3.2 and set again $e^N = \tilde{u} - u^N$, so that $|e_x^N(\pm 1)| = |u_x^N(\pm 1)|$. Using (3.12) for $v = e^N$ and (3.7), one obtains the following result.

THEOREM 3.4: Under the hypothesis of Theorem 3.2, the following estimate holds:

$$(3.15) \qquad |u_x^N(\pm 1)| \leq c^\frown N^{9/2-m} \| u \|_m + c^{\frown\frown} N^{5-m} \| f \|_{m-2}.$$

■

Estimate (3.15) shows in particular that the boundary conditions are satisfied with spectral accuracy when they are imposed implicitly in a collocation scheme.

The analysis of stability and convergence for the discrete initial boundary value problem (2.13) can be carried out by the same technique used in the proofs of Theorems 3.1 and 3.2. We omit the details of the analysis and we report hereafter the final result.

THEOREM 3.5: Let the solution u of the initial-Neumann boundary value problem (2.2)-(2.3) satisfy the following regularity assumptions:

$$u \in L^2(0,T; H^m(-1,1)), \quad u_t \in L^2(0,T; H^{m-2}(-1,1))$$

for a fixed $T > 0$ and $m > 5/2$. If u^N denotes the solution of the approximation scheme (2.13), then for all $t \leq T$

$$\|u(t) - u^N(t)\|_0 + (\int_0^t \sum_{j=1}^{N-1} [u_x - u_x^N]^2(x_j,t)w_j)^{1/2} \leq C'N^{2-m} \|u_0\|_{m-2}$$

$$(3.16) \qquad + \exp(\tfrac{t}{2})\{C''N^{2-m} [\int_0^t \|u(\tau)\|_m^2 d\tau + \int_0^t \|u_t(\tau)\|^2 d\tau]^{1/2}$$

$$+ C'''N^{5/2-m} (\int_0^t \|f(\tau)\|_{m-2}^2 d\tau)^{1/2}\},$$

for suitable constants C', C'', C''' independent of u, u^N and N. ∎

4. Theoretical Results for the Chebyshev Method

The most popular family of collocation points is the family of the Chebyshev points, which we consider in this section. The nodes (2.5) are given by

$$(4.1) \qquad x_j = \cos \frac{j\pi}{N} \qquad j = 0,\cdots,N,$$

while the corresponding weights are

$$(4.2) \qquad \begin{cases} w_j = \dfrac{\pi}{N} & j = 1,\cdots,N-1 \\[2mm] w_0 = w_N = \dfrac{\pi}{2N}. \end{cases}$$

Hereafter, we shall discuss some theoretical properties of the implicit treatment of the Neumann boundary conditions. From now on we assume that $\beta = \delta = 1$ and $\alpha = \gamma = 0$ in (2.3).

First, we prove the stability and the convergence of the time-independent scheme (2.14).

THEOREM 4.1: Let u^N be the solution of (2.14). There exists a constant $C > 0$ independent of N and u^N such that

$$(4.3) \quad \int_{-1}^{1} [u^N(x)]^2 \, w(x)dx + \sum_{j=1}^{N-1} [u_x^N(x_j)]^2 \, w_j \leq C \int_{-1}^{1} [I_N f(x)]^2 \, w(x)dx.$$

PROOF: Equation (2.14) can be equivalently written as

$$(4.4) \quad -I_N(Bu_x^N)_x + u^N = I_N f, \quad -1 < x < 1$$

since both sides of (4.4) are polynomials of degree N which match at $N + 1$ distinct points. Following an idea due to D. Gottlieb, let us differentiate (4.4) with respect to x. If we set $U^N(x) = I_N(Bu_x^N)(x)$, then U^N is a polynomial of degree N which vanishes at the boundary points and satisfies the collocation equation

$$(4.5) \quad -U_{xx}^N(x_j) + U^N(x_j) = (I_N f)(x_j), \quad j = 1, \cdots, N-1.$$

The stability analysis for the Chebyshev collocation approximation of the Dirichlet boundary value problem (see [2]) yields the estimate

$$(4.6) \quad \|U^N\|_{0,w} + \|U_x^N\|_{0,w} \leq C\|I_N f\|_{0,w}$$

for a constant $C > 0$ independent of N. Using this estimate and equation (4.4) we obtain the further inequality

$$(4.7) \qquad \|u^N\|_{0,w} \leq C\|I_N f\|_{0,w}.$$

This proves (4.3). ∎

THEOREM 4.2: Let u be the solution of the boundary value problem (2.1), (2.3) and u^N the solution of (2.14). Assume that $u \in H^m_w(-1,1)$ with $m > 5/2$. There exists a constant $C > 0$ independent of N, u and u^N such that

$$(4.8) \qquad \|u - u^N\|_{0,w} + \left(\sum_{j=1}^{N-1} [u_x - u^N_x](x_j)w_j \right)^{1/2} \leq CN^{2-m} \|u\|_{m,w}.$$

PROOF: The convergence analysis for the approximation (4.5) gives the estimate ([2])

$$\|u_{xx} - U^N_x\|_{0,w} + \|u_x - U^N\|_{0,w} \leq C_1 N^{2-m} \|u\|_{m,w} + C_2 N^{2-m} \|f\|_{m-2,w}$$

$$(4.9)$$

$$\leq C_3 N^{2-m} \|u\|_{m,w},$$

where we have used (2.1) in order to bound the norm $\|f\|_{m-2,w}$ by the norm $\|u\|_{m,w}$. By equations (2.1) and (4.4) we get

$$\|u - u^N\|_{0,w} \leq C_4 N^{2-m} \|u\|_{m,w}.$$

On the other hand, the equivalence of norms (2.10) and the triangle inequality yields the inequality

$$\sum_{j=1}^{N-1} [u_x - u_x^N]^2 (x_j) w_j \le C_5 \{ \|u_x - I_N u_x\|_{0,w}^2 + \|u_x - U^N\|_{0,w}^2 \},$$

whence the result, using (4.9) and (2.9). ∎

As for the Legendre method discussed in the previous section, it is possible to estimate the error on the boundary conditions produced by the spectral solution. We have the following result.

THEOREM 4.3: Under the hypothesis of Theorem 4.2, there exists a constant $C > 0$ independent of N and u^N such that

$$(4.10) \qquad\qquad |u_x^N(\pm 1)| \le CN^{4-m} \|u\|_{m,w}$$

PROOF: For any polynomial $v \in \mathbb{P}_N$, one has (see, e.g., [9])

$$\int_{-1}^{1} v_x(x) T_N(x) w(x) dx = 0$$

$$\int_{-1}^{1} v_x(x) T_{N-1}(x) w(x) dx = N \int_{-1}^{1} v(x) T_N(x) w(x) dx,$$

whence

$$(4.11) \qquad \frac{\pi}{2N} [v_x(1) + (-1)^N v_x(-1)] = -\sum_{j=1}^{N-1} v_x(x_j) T_N(x_j) w_j$$

$$\frac{\pi}{2N}\left[v_x(1) - (-1)^N v_x(-1)\right] = -\sum_{j=1}^{N-1} v_x(x_j)T_{N-1}(x_j)w_j$$

(4.12)

$$+ N \int_{-1}^{1} v(x)T_N(x)w(x)dx.$$

Let $\tilde{u} \in \mathbb{P}_N$ be a primitive of the H_w^1-projection of u_x upon the space $\{v \in \mathbb{P}_{N-1} \mid v(\pm 1) = 0\}$. Then (4.10) follows from (4.11) and (4.12), choosing here $v = u^N - \tilde{u}$ and using Theorem 4.2 in order to estimate the right-hand sides. ∎

As far as the evolution scheme (2.15) is concerned, the following convergence estimate holds.

THEOREM 4.4: Let the solution u of the initial-Neumann boundary value problem (2.2), (2.3) satisfy the following regularity assumptions:

$$u \in L^2(0,T; H_w^m(-1,1)), \quad u_t \in L^2(0,T; H_w^{m-1}(-1,1))$$

for a fixed $T > 0$ and $m > 5/2$. Moreover, let $u_0 \in H_w^m(-1,1)$. If u^N denotes the solution of the approximation (2.15), one has for all $t \leq T$

$$\|u(t) - u^N(t)\|_{0,w} + \left(\sum_{j=1}^{N-1} [u_x - u_x^N]^2(x_j,t)w_j\right)^{1/2}$$

(4.13)

$$\leq CN^{2-m}\left\{\|u_0\|_{m,w} + \exp\left(\frac{t}{2}\right)\left[\int_0^t \|u(\tau)\|_m^2 \, d\tau\right.\right.$$

$$\left.\left. + \int_0^t \|u_t(\tau)\|_{m-1}^2 \, dt\right]\right\}$$

PROOF: As in the proofs of Theorems 4.1 and 4.2 we set

$$U^N(x,t) = I_N(Bu_x^N)(x,t)$$

and we x- differentiate the equation

$$u_t^N - I_N(Bu_x^N)_x = I_N f,$$

which is equivalent to (2.15). Estimate (4.13) is then a consequence of the convergence analysis for the Chebyshev approximation to an initial-Dirichlet boundary value problem (see [2], Theorem 3.3). The error on the initial data is

$$u_{0,x} - U^N(0) = u_{0,x} - I_N(Bu_x^N(0)) = u_{0,x} - I_N(B(I_N u_0)_x).$$

The L_w^2- norm of this term can be estimated as follows:

$$\|u_{0,x} - U^N(0)\|_{0,w} \leq \|u_{0,x} - I_N u_{0,x}\|_{0,w} + \|I_N[u_{0,x} - B(I_N u_0)_x]\|_{0,w}$$

$$(\text{by } (2.10)) \quad \leq \|u_{0,x} - I_N u_{0,x}\|_{0,w} + C\|u_{0,x} - B(I_N u_0)_x\|_{N,w} .$$

Since both $u_{0,x}$ and $B(I_N u_0)_x$ are zero at the boundary, one has

$$\|u_{0,x} - B(I_N u_0)_x\|_{N,w}^2 \leq \sum_{j=0}^{N} [u_{0,x} - (I_N u_0)_x]^2(x_j)w_j$$

$$\leq C\|I_N u_{0,x} - (I_N u_0)_x\|_{0,w}^2$$

$$\leq C\{\|u_{0,x} - I_N(u_{0,x})\|_{0,w} + \|u_{0,x} - (I_N u_0)_x\|_{0,w}\}^2 .$$

By the estimate (3.7) in [1] we conclude that

$$\|u_{0,x} - U^N(0)\|_{0,w} \leq CN^{2-m} \|u_0\|_m.$$

The remaining part of the proof is straightforward. ■

5.   Computational Aspects of the Methods

5.1   The Richardson Iterations

The Richardson method with a finite difference preconditioning (see [13]) is certainly the simplest and most popular iterative method for solving spectral systems. We shall briefly discuss the use of this method in the solution of the linear systems (2.11) and (2.14). Hereafter we assume again that $\beta = \delta = 1$ in (2.3).

The system (2.11) can be written as

$$(5.1) \qquad\qquad L_E u^N = F_E,$$

where L_E is the matrix of order $N + 1$ defined by the relation (recall (2.7)):

$$(5.2) \quad L_E v = \begin{pmatrix} (-B_+v)(x_0) \\ \vdots \\ (-v_{xx} + v)(x_j) \\ \vdots \\ (B_-v)(x_N) \end{pmatrix} \qquad j = 1, \cdots, N-1, \quad \text{for all } v \in \mathbb{R}_N,$$

and $F_E = \left(0, f(x_1), \cdots, f(x_{N-1}), 0\right)^T$. An approximate inverse A_E of L_E, to be used as a preconditioner, can be built up by low order finite differences at the nodes (2.5) as follows:

$$(5.3) \quad A_E v = \begin{pmatrix} \dfrac{v_1 - v_0}{h_0} - \alpha v_0 \\ \vdots \\ -\dfrac{2}{h_{j-1}[h_j + h_{j-1}]} v_{j-1} + [\dfrac{2}{h_j h_{j-1}} - 1]v_j - \dfrac{2}{h_j[h_j + h_{j-1}]} v_{j+1} \\ \vdots \\ \dfrac{v_{N-1} - v_N}{h_{N-1}} + \gamma v_N \end{pmatrix}$$

for all $v \in \mathbb{P}_N$, where $h_j = x_j - x_{j+1}$. Thus, a one-sided finite difference approximation of the boundry conditon is imposed at the boundary nodes, while centered differences are used at the interior.

The system (2.14) is represented as

$$(5.4) \quad L_I u^N = F_I,$$

where L_I is the matrix of order $N+1$ defined by the relation

$$(5.5) \quad L_I v = \{[-I_N(Bv_x)_x + v](x_j)\}_{0 \leq j \leq N}^T \quad \text{for all } v \in \mathbb{P}_N$$

and $F_I = \{f(x_j)\}_{0 \leq j \leq N}^T$. Preconditioning this matrix is a more delicate matter than preconditioning the matrix (5.2). In analogy with (5.3), one could consider the matrix A_I defined as

$$(5.6) \qquad A_I v = \begin{pmatrix} \dfrac{2(1 + \alpha h_0)v_0 - 2v_1}{h_0^2} + v_0 \\[2mm] \vdots \\[2mm] \dfrac{-2}{h_{j-1}[h_j + h_{j-1}]} v_{j-1} + \Big[\dfrac{2}{h_j \, h_{j-1}} - 1\Big]v_j + \dfrac{-2}{h_j[h_j + h_{j-1}]} v_{j+1} \\[2mm] \vdots \\[2mm] \dfrac{2(1 - \gamma h_{N-1})v_N - 2v_{N-1}}{h_{N-1}^2} + v_N \end{pmatrix} \quad ;$$

namely, the differential operator is discretized also at the boundary nodes by a centered difference formula, and the boundary conditions are used in eliminating the auxiliary nodes outside the domain. Such a matrix exhibits very poor preconditioning properties for the matrix (5.5). This can be explained by considering the structure of the spectrum of L_I in the case of Neumann boundary conditions. The eigenvalue 1 has double multiplicity, the corresponding eigenfunctions being $v \equiv 1$ and $v = \phi_N$ (the N-th Chebyshev or Legendre orthogonal polynomial). Actually, the Gauss-Lobatto quadrature nodes are such that $\phi_{N,x}(x_j) = 0$ for $j = 1, \cdots, N-1$. Hence

$$I_N(B\phi_{N,x}) \equiv 0.$$

On the contrary, ϕ_N is not an eigenfunction for the matrix (5.6) and 1 is a simple eigenvalue.

However, it is easy to build up a finite difference approximation of the operator (2.1) which for the Neumann boundary conditions has 1 as a double eigenvalue with eigenfunctions $v \equiv 1$ and $v = \phi_N$. At each interior node $x_j (j-1, \cdots, N-1)$, define the differentiation formula

$$(5.7) \qquad a_j u(x_{j-1}) + b_j u(x_j) + c_j u(x_{j+1}) \approx u_x(x_j)$$

by the conditions of being first order accurate and of satisfying the identity

$$a_j \phi_N(x_{j-1}) + b_j \phi_N(x_j) + c_j \phi_N(x_{j+1}) = 0.$$

If the Chebyshev points (4.1) are used, then $\phi_N(x_j) = T_N(x_j) = (-1)^j$, hence $b_j = 0$ and (5.7) is the centered difference approximation of the first derivative.

After computing the numbers a_j, b_j and c_j we define the matrix A_I as follows

$$(5.8) \qquad A_I = - \begin{pmatrix} \dfrac{1}{h_0} & \dfrac{-1}{h_0} & & 0 \\ & a_j & b_j & c_j \\ 0 & & \dfrac{1}{h_N} & \dfrac{-1}{h_N} \end{pmatrix} \begin{pmatrix} -\alpha & 0 & & 0 \\ & a_j & b_j & c_j \\ 0 & & 0 & \beta \end{pmatrix} + \begin{pmatrix} 1 & & & 0 \\ & & 1 & \\ 0 & & & 1 \end{pmatrix}$$

The matrix A_I is a five-diagonal approximation of the operator L_I, which has the required spectral properties.

The Richardson method is applied in solving (5.1) and (5.4) in the following form:

$$(5.9) \qquad u^{N,k+1} = u^{N,k} + \alpha^k A^{-1}(F - L u^{N,k}) \qquad k \geq 0,$$

where $\alpha^k > 0$ is an acceleration parameter. In (5.9), A, F and L stand for A_E, F_E, L_E if the system (5.1) is to be solved, and for A_I, F_I, L_I if the system (5.4) is considered instead. Under the assumption that the matrix $A^{-1}L$ is diagonalizable, the method is convergent (with a proper choice of the acceleration parameter) provided all the eigenvalues of $A^{-1}L$ have strictly positive real parts. For the pure Dirichlet boundary value problem this is true since it has been proven ([10]) that the eigenvalues of $A^{-1}L$ lie in the interval $[1, \pi^2/4]$. For the general boundary conditions (2.3), the behavior of the eigenvalues has been investigated numerically and will be discussed hereafter.

The convergence of the Richardson method is crucially influenced by the choice of the parameter α^k. Several strategies have been proposed ([13], [14], [10]). The simplest and most effective one consists of computing α^k by minimizing some Hilbertian norm of the residual $r^{k+1} = F - Lu^{N,k+1}$. Assume that the Hilbertian norm is defined by the inner product

$$((u,v)) = \sum_{ij} h_{ij} u_i v_j ,$$

where $H = \{h_{ij}\}$ is a symmetric positive definite matrix. Then, the resulting expression for α^k is

$$(5.10) \qquad \alpha^k = \frac{((r^k, LA^{-1} r^k))}{((LA^{-1} r^k, LA^{-1} r^k))} .$$

The iterative procedure (5.9)-(5.10) (called the Minimal Residual Richardson Method) will not break down if α^k remains bounded away from 0. This occurs if the symmetric part of the matrix HLA^{-1} is positive definite.

Unfortunately, the numerical computations described in the next subsection show that whenever the boundary conditions are not of Dirichlet type few eigenvalues of $HLA^{-1} + (HLA^{-1})^T$ are of negative sign.

Thus one has to resort to iterative methods which converge even if the symmetric part of the matrix of the system is indefinite. Among them, the algorithm Orthodir (see [15]) seems particularly apt to be used with spectral methods. Setting $B = A^{-1} L$, the algorithm is defined as

$$u^{N,k+1} = u^{N,k} + \alpha^k p^k$$

where the descent direction p^k is given by

$$p^k = Bp^{k-1} - \sum_{j=0}^{k-1} \beta_{kj} p^j, \qquad \beta_{kj} = - \frac{(B^2 p^{k-1}, Bp^j)}{(Bp^j, Bp^j)} , \qquad .$$

and α^k is chosen by the minimal residual strategy.

A truncated version, consisting of setting $\beta_{kj} = 0$ if $j < k-1$, is generally preferred, although the convergence is not assured in this case. Since one step of Orthodir requires twice as many operations as one step of Richardson's method, it is convenient to execute a few Orthodir iterations only when the Richardson method breaks down, then going back to the original method. See [5] for a successful application of this strategy.

5.2 The Behavior of the Eigenvalues

The eigenvalues of the spectral matrices L, $HL + (HL)^T$ and the preconditioned matrices $A^{-1}L$, $HLA^{-1} + (HLA^{-1})^T$ were computed by EISPACK routines. The computation was carried out for $N = 2^k$, $k = 2, \cdots, 6$ and for

the boundary conditions $\alpha = \gamma = 0$ (pure Neumann) $\alpha = 1, \gamma = 0$ (mixed Neumann-Robin) and $\alpha = \gamma = 5$ (pure Robin). The eigenvalues were found scarcely sensitive to the kind of boundary conditions, the qualitative behavior being the same for the three conditions considered. The following discussion refers to the pure Neumann problem.

a) Chebyshev explicit method ((5.1), (4.1))

The eigenvalues of the matrix L_E defined in (5.2) are real, positive, distinct and bounded from below by 1. The eigenvalues of the preconditioned matrix $A_E^{-1} L_E$, with A_E defined in (5.3), are also real positive and distinct. Moreover, they lie in the interval $[1, \pi^2/4]$, as shown in Table 2.

Table 2. Largest eigenvalues for the
Chebyshev "explicit" method

N	L_E	$A_E^{-1} L_E$
4	24.	1.75
8	231.	2.10
16	3242.	2.29
32	50,208.	2.38
64	701,902.	2.44

Let H be the matrix associated with the Chebyshev discrete inner product, i.e., $H = \text{diag}\{w_0, \cdots, w_N\}$ where the w_j's are defined in (4.2). The symmetric part of the matrices HL_E and $HL_E A_E^{-1}$ is indefinite. In both cases two eigenvalues are negative and their largest modulus is of the order of the largest positive eigenvalues. Unlike $A_E^{-1} L_E$, the eigenvalues of

$HL_E \ A_E^{-1} + \left(HL_E \ A_E^{-1}\right)^T$ are not bounded independently of N, the largest eigenvalue growing like $O(N^4)$. A similar behavior occurs if H is the identity matrix.

b) Chebyshev implicit method ((5.4), (4.2))

The eigenvalues of the matrix L_I defined in (5.5) are real and positive, as it easily follows from (4.5). Moreover, they are all simple, except the smallest eigenvalues 1 which is double, as already pointed out. If the matrix (5.6) is used as a preconditioner, the largest eigenvalues of the matrix $A_I^{-1} L_I$ remains bounded, but the smallest eigenvalue tends to zero as $O(N^{-3})$.

If the matrix (5.8) is used instead, the smallest eigenvalue of the matrix $A_I^{-1} L_I$ is 1 with double multiplicity, while the modulus of the largest eigenvalue, although not bounded independently of N, grows like $O(N^{3/2})$.

Table 3. Largest modulus of the eigenvalues
for the Chebyshev "implicit" method.
The matrix A_I is defined in (5.8).

N	C(N)	$A_I^{-1} L_I$
4	19.	5.
8	214.	14.6
16	3174.	38.
32	49,938.	107.
64	700,893.	342.

The eigenvalues of $A_I^{-1} L_I$ are all real and positive, except the two largest eigenvalues which for $N \geq 32$ are complex conjugate (with positive real parts).

The symmetric part of the matrices HL_I and $HL_I A_I^{-1}$ are indefinite. The number of negative eigenvalues for $HL_I + (HL_I)^T$ is 2 in all the cases under investigation, while for $HL_I A_I^{-1} + (HL_I A_I^{-1})^T$ this number grows slowly with N (it is 6 for $N = 64$).

c) Legendre explicit method ((5.1), (3.1))

The eigenvalues of L_E and $A_E^{-1} L_E$ behave qualitatively as the eigenvalues of the corresponding matrices for the Chebyshev method. Table 4 contains the largest eigenvalues for the two matrices, the smallest eigenvalue being 1 in all cases.

Table 4. Largest eigenvalues for the Legendre "explicit" method

N	L_E	$A_E^{-1} L_E$
4	22.	1.6
8	162.	1.9
16	1978.	2.17
32	28,639.	2.31
64	432,449.	2.41

For the Legendre method too, the symmetric parts of HL_E and $HL_E A_E^{-1}$ (where $H = \text{diag}\{w_0, \cdots, w_N\}$, w_j being defined in (3.1)), are indefinite.

d) <u>Legendre implicit method ((5.4), (3.1))</u>

The eigenvalues of the matrix L_I are real, positive and bounded from below by 1. Such properties can be easily proved using the identity (3.4). The same properties are shared by the eigenvalues of the preconditioned matrix $A_I^{-1} L_I$, with A_I defined in (5.8); in this case the largest eigenvalue grows like $O(N^{3/2})$.

Table 5. Largest eigenvalues for the
Legendre "implicit" method

N	L_E	$A_I^{-1} L_I$
4	17.	5.6
8	146.	18.7
16	1921.	55.
32	28,424.	148.
64	431,676.	384.

The symmetric parts of the matrices HL_I and $HL_I A_I^{-1}$ are indefinite.

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16. Abstract

We discuss two different ways of treating non-Dirichlet boundary conditions in Chebyshev and Legendre collocation methods for second order differential problems.

An error analysis is provided. The effect of preconditioning the corresponding spectral operators by finite difference matrices is also investigated.

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