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Essential imposition of Neumann condition in Galerkin–Legendre elliptic solvers

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Abstract

A new Galerkin–Legendre direct spectral solver for the Neumann problem associated with Laplace and Helmholtz operators in rectangular domains is presented. The algorithm differs from other Neumann spectral solvers by the high sparsity of the matrices, exploited in conjunction with the direct product structure of the problem. The homogeneous boundary condition is satisfied exactly by expanding the unknown variable into a polynomial basis of functions which are built upon the Legendre polynomials and have a zero slope at the interval extremes. A double diagonalization process is employed pivoting around the eigenstructure of the pentadiagonal mass matrices in both directions, instead of the full stiffness matrices encountered in the classical variational formulation of the problem with a weak natural imposition of the derivative boundary condition. Nonhomogeneous Neumann data are accounted for by means of a lifting. Numerical results are given to illustrate the performance of the proposed spectral elliptic solver. The algorithm extends easily to the three-dimensional problem.

Keywords: Poisson and Helmholtz equations; Neumann boundary condition; Galerkin–Legendre spectral method; Lifting of the nonhomogeneous Neumann datum; Separation of variables; Direct product structure; Diagonalization algorithm; Fast elliptic spectral solver

0. Introduction

Direct spectral elliptic solvers are commonly based on the diagonalization of matrices representing one-dimensional second-order differential operators according to either the Chebyshev-tau method, see e.g. [1,2], or a collocation scheme, see [3,4]. On the contrary, in spectral solvers of the last generation, based on the Galerkin formulation of the elliptic boundary value problem and using Legendre polynomials, the eigendecomposition is applied to the mass matrix associated with the assumed polynomial basis. The new approach has been adopted in the solution of the Dirichlet problem for Poisson and Helmholtz operators over rectangular regions in two dimensions [5–7] and three dimensions [8]. The advantage of the Legendre

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basis considered in these works is that the stiffness matrix is reduced to the identity matrix, but for the first constant mode, while the mass matrix displays a pentadiagonal profile, for which the eigenproblem is most simple.

It is therefore legitimate to ask whether the simplicity of the new fast spectral solvers for the Dirichlet problem can be retained also in the solution of the Neumann boundary value problem. As a matter of fact, owing to the particular structure of the mass and stiffness matrices, the direct product algorithm developed for the Dirichlet problems in 2D and 3D cannot be extended straightforwardly to the Neumann case. Indeed, since the constant mode is uncontrolled by the second-derivative operator in one dimension under conditions on the slope at both interval extremes, it is impossible to perform the eigendecomposition in a direct-product form, i.e., using directional splitting, unless the structure of the eigenvectors is adequately contrived. Such a structure cannot be achieved when the basis developed for solving problems with a nonhomogeneous Dirichlet condition is used to solve the Neumann problem for the Laplace operator.

A convenient basis of polynomials with zero slope at the endpoints was constructed using Legendre polynomials by Shen [5, p. 1492] so as to obtain stiffness and mass matrices with the same profiles as the basis enforcing Dirichlet conditions. The aim of the present work is to show that this basis allows also to preserve the direct-product character of the spectral solver for elliptic equations under a Neumann boundary condition. In particular, we develop a direct spectral solver for two-dimensional Poisson and Helmholtz equations by adopting the aforementioned Shen's basis and thus enforcing condition of zero normal derivative along the entire boundary in an essential way. This is somewhat unusual in the context of a variational formulation of elliptic boundary value problems and leads to an alternative algorithm with respect to existing Neumann spectral solvers where this kind of boundary condition is accounted for through the integration by parts, see [9,10]. The direct solution algorithm here developed for the Neumann problem in two dimensions relies upon a double diagonalization process very similar to that of the Dirichlet spectral solver [7]. This similarity extends also to the accounting of nonzero boundary values by means of a lifting of the Neumann datum which is found to require a two-step procedure much in the same manner of the elliptic solver under nonhomogeneous Dirichlet conditions. The two steps are necessary to exploit first suitable values at the corners and then the values of the Neumann datum along the four sides of the domain. The point values in the corners will be shown to stem from the derivative of the Neumann datum and are associated with the presence of compatibility conditions between the two slopes in each corner of the domain, as contemplated by the analysis of Grisvard [11].

The paper is organized as follows. In Section 1 we start by introducing the basic concepts. In particular, in Section 1.1 the construction of the basis, first proposed by Shen [5], is carried out; in Section 1.2 the spectral mass and stiffness matrices are presented; in Section 1.3 the solution algorithm is described and finally in Section 1.4 some numerical tests are conducted which confirm the spectral accuracy of the 1D solver. In Section 2 the two-dimensional problem is stated and discretized (Sections 2.1–2.3). The diagonalization algorithm proposed for the ordinary differential equation is extended to the partial differential problem in two dimensions by variable separation in Section 2.4. A few numerical tests are conducted in Section 2.5 to evaluate the accuracy of the 2D solver. In Section 3 the spectral algorithm for solving the Neumann problem in a cube is outlined.

1. 1D problem with Neumann conditions

Let us consider an ordinary differential problem defined by a second-order equation in the interval $[-1, 1]$ supplemented by derivative boundary conditions at the extremes of the interval, namely

$$\left(-\frac{d^2}{dx^2}+\gamma\right)u = f(x) \quad \text{and} \quad u'(\pm 1) = b_{\pm 1}, \tag{1.1}$$

where γ is a nonnegative constant. In the special case $\gamma = 0$ the solution u exists only provided that the data of problem (1.1) satisfy the compatibility condition

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = b_{-1} - b_1 \tag{1.2}$$

in which case u is defined up to an arbitrary additive constant. The treatment of nonzero values of the Neumann conditions is included here in view of its extension from 1D to 2D and 3D, to be considered in the next section.

We can now reformulate problem (1.1) in a variational form as follows:

Given $f \in L^2([-1,1])$ *find* $u \in H^1([-1,1])$ *such that*

$$a(v,u) = (v,f) + v(1)b_1 - v(-1)b_{-1} \quad \forall v \in H^1([-1,1]), \tag{1.3}$$

where $a(v,u) = (v',u') + \gamma(v,u)$, *and* $(\cdot,\cdot)$ *denotes the* L^2 *inner product.*

In the present approach, the "Neumann" boundary conditions are enforced in an essential way. This means that the formulation above must be slightly modified by introducing a *lifting* of the slope data b_{-1} and b_1, by splitting the solution u in the sum of two variables, $u = u_0 + u_b$, to be defined precisely below.

1.1. Construction of a basis enforcing derivative conditions

A spectral Galerkin approximation of the variational problem (1.3) is obtained by introducing a finite dimensional polynomial basis to represent the functions of $H^2([-1,1])$. In this section, we derive a basis for an essential treatment of the derivative boundary conditions. This means to find a subspace of $H^2([-1,1])$ of polynomial functions with zero derivative at both interval extremes. Among different possibilities, the basis proposed by Shen [5] allows to minimize the band-width of the stiffness and mass matrices. To help the implementation of the solver, we detail the construction of such a basis and derive the sparsity patterns and the elements of the two matrices explicitly.

We start from the formula proposed by Shen

$$L_k^{(\star)}(x) = L_k(x) + a_k L_{k+1}(x) + b_k L_{k+2}(x), \quad k \geqslant 0, \tag{1.4}$$

where $L_k(x)$ denotes the Legendre polynomial of degree k, $k = 0, 1, \ldots$, while a_k and b_k are coefficients to be determined. A basis of functions $L^{(\star)}(x)$ with zero slope at the extremes of the interval $[-1, 1]$, namely

$$\frac{\mathrm{d}L_k^{(\star)}(\pm 1)}{\mathrm{d}x} = 0 \tag{1.5}$$

is obtained by solving the system of two equations in the unknowns a_k and b_k, for each $k = 0, 1, \ldots$ This leads to the following basis: $L_0^{(\star)}(x) = 1$ and

$$L_k^{(\star)}(x) = L_k(x) - \frac{k(k+1)}{(k+2)(k+3)} L_{k+2}(x), \quad k \geqslant 1. \tag{1.6}$$

1.2. The spectral matrices

The basis $L_k^{(\star)}(x)$ can be now normalized to make the stiffness matrix equal to the identity, but for the first diagonal element which is zero. The stiffness matrix D is defined from the bilinear form $(v',u') = \int_a^b v'u'\,\mathrm{d}x$ and its elements are

$$d_{i,j}^{(\star)} = \left(L_i^{(\star)\prime}, L_j^{(\star)\prime}\right) \quad (i,j) \geqslant 0. \tag{1.7}$$

First, observe that $d_{0,0}^{(\star)} = 0$ since $L_0^{(\star)}$ is constant. Then, let us suppose, without any loss of generality, that $j \geqslant i \geqslant 1$; integrating by parts the second member of (1.17), one obtains

$$d_{i,j}^{(\star)} = -\left(L_i^{(\star)''}, L_j^{(\star)}\right) + \left[L_i^{(\star)'} L_j^{(\star)}\right]_{-1}^{1} = -\left(L_i^{(\star)''}, L_j^{(\star)}\right), \tag{1.8}$$

since $L_i^{(\star)'}(\pm 1) = 0$ by construction. Introducing now the well-known relationship

$$L_i''(x) = \sum_{\substack{k=0 \\ k+i \text{ even}}}^{i-2} \left(k + \frac{1}{2}\right)[i(i+1) - k(k+1)]L_k(x), \tag{1.9}$$

we have

$$\begin{aligned} L_i^{(\star)''}(x) = & \sum_{\substack{k=0 \\ k+i \text{ even}}}^{i-2} \left(k + \frac{1}{2}\right)[i(i+1) - k(k+1)]L_k(x) \\ & - \frac{i(i+1)}{(i+2)(i+3)} \sum_{\substack{k=0 \\ k+i \text{ even}}}^{i} \left(k + \frac{1}{2}\right)[(i+2)(i+3) - k(k+1)]L_k(x). \end{aligned} \tag{1.10}$$

By the orthogonality of the Legendre polynomials and by the definition of $L_k^{(\star)}(x)$ in (1.6) we immediately observe that $d_{i,j}^{(\star)} = 0$, for $j \neq i$, while for $j = i$ a direct calculation gives

$$d_{i,i}^{(\star)} = \frac{2i(i+1)(2i+3)}{(i+2)(i+3)}. \tag{1.11}$$

The normalized basis is therefore defined as follows: $L_0^{\star}(x) = 1$ and, for $k \geqslant 1$,

$$L_k^{\star}(x) = \left[\frac{(k+2)(k+3)}{2k(k+1)(2k+3)}\right]^{1/2} \left[L_k(x) - \frac{k(k+1)}{(k+2)(k+3)} L_{k+2}(x)\right]. \tag{1.12}$$

The first few functions $L_k^{\star}(x)$ of the normalized basis are drawn in Fig. 1. In terms of this basis the stiffness matrix is

$$ {}^{0}D = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ \vdots \\ N \end{array} \!\!\begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & \cdots & N \end{array} \\ \begin{pmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{pmatrix} \end{array}, \tag{1.13}$$

where the prefixed superscript ^{0} reminds that the leading diagonal element $d_{0,0}$ is zero.

Let us now compute the elements of the mass matrix M:

$$\begin{aligned} m_{i,j} = (L_i^{\star}, L_j^{\star}) = & \left[\frac{(i+2)(i+3)}{2i(i+1)(2i+3)}\right]^{1/2} \left[\frac{(j+2)(j+3)}{2j(j+1)(2j+3)}\right]^{1/2} \left\{(L_i, L_j) - \frac{j(j+1)}{(j+2)(j+3)}(L_i, L_{j+2}) \right. \\ & \left. - \frac{i(i+1)}{(i+2)(i+3)}(L_{i+2}, L_j) + \frac{i(i+1)}{(i+2)(i+3)} \frac{j(j+1)}{(j+2)(j+3)}(L_{i+2}, L_{j+2})\right\}. \end{aligned}$$

Owing to the orthogonality of Legendre polynomials, $m_{i,j}$ is different from zero only for $i = j$ or $i = j \pm 2$. For $i = j$ we have: $m_{0,0} = c_0 = 2$ and, for $i \geqslant 1$,

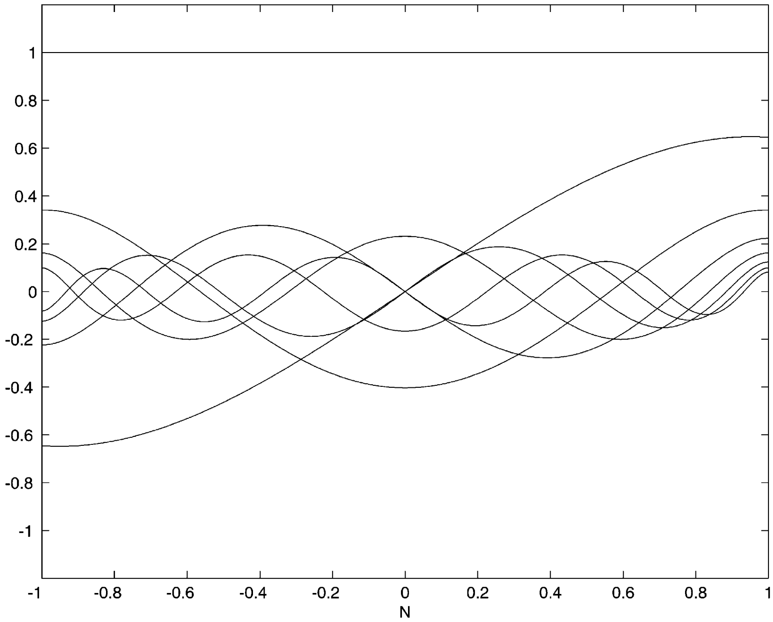

Fig. 1. Functions $L_k^{\star}(x)$ of the basis for 1D boundary value problems with Neumann conditions.

$$m_{i,i} = c_i = \frac{1}{2i-1}\left[\frac{(i+2)(i+3)}{2i(i+1)(2i+3)} + \frac{i(i+1)}{(i+1)(i+3)(2i+5)}\right].$$

For $j = i+2$, $i \geqslant 1$, we have

$$m_{i,i+2} = a_i = -\left[\frac{i(i+1)(i+4)(i+5)}{(2i+3)(2i+7)}\right]^{1/2} \frac{i}{(i+2)(i+3)(2i+5)}.$$

More explicitly, the mass matrix has the following pentadiagonal profile:

$$M = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ \vdots \\ N-2 \\ N-1 \\ N \end{array} \begin{array}{c} \begin{array}{ccccccccc} 0 & 1 & 2 & 3 & 4 & \cdots & N-2 & N-1 & N \end{array} \\ \left(\begin{array}{ccccccccc} c_0 & 0 & 0 & & & & & & \\ 0 & c_1 & 0 & a_1 & & & & & \\ 0 & 0 & c_2 & 0 & a_2 & & & & \\ & a_1 & 0 & c_3 & 0 & \ddots & & & \\ & & a_2 & 0 & c_4 & 0 & \ddots & & \\ & & & \ddots & 0 & \ddots & 0 & a_{N-3} & \\ & & & & \ddots & 0 & c_{N-2} & 0 & a_{N-2} \\ & & & & & a_{N-3} & 0 & c_{N-1} & 0 \\ & & & & & & a_{N-2} & 0 & c_N \end{array}\right) \end{array} \tag{1.14}$$

1.3. Solution algorithm

The chosen basis enforces homogeneous Neumann conditions in an *essential* way. Nonhomogeneous conditions are then imposed by introducing a lifting of the Neumann data b_{-1} and b_1 which will be performed in a fully analytical way in the one-dimensional case. The solution $u(x)$ is split in two components as follows:

$$u(x) = u_0(x) + u_b(x), \tag{1.15}$$

where u_0 is an auxiliary unknown satisfying a modified equation and with zero slope at both interval extremes, while u_b is an arbitrary function whose derivative assumes the prescribed values b_{-1} and b_1 at the endpoints. The modified problem for u_0 is

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \gamma\right)u_0 = \overline{f}(x) \quad \text{and} \quad \frac{\mathrm{d}u_0(\pm 1)}{\mathrm{d}x} = 0, \tag{1.16}$$

where $\overline{f}(x) = f(x) - (-(\mathrm{d}^2/\mathrm{d}x^2) + \gamma)u_b(x)$. In variational terms the problem for the new "lifted" unknown u_0 reads:

Find $u_0(x)$ in $H^2([-1,1])$ such that $u'(\pm 1) = 0$ and

$$a(v, u_0) = F(v) \quad \forall v \in H^2([-1,1]) \text{ with } v'(\pm 1) = 0,$$

where

$$a(v, u) = (v', u') + \gamma(v, u),$$

$$F(v) = (v, f) - (v', u_b') - \gamma(v, u_b) + v(1)b_1 - v(-1)b_{-1}.$$

The function $u_b(x)$ satisfying the original boundary conditions, $u_b(\pm 1) = b_{\pm 1}$, is taken to be the parabola $u_b(x) = \alpha x^2 + \beta x$, so that one obtains immediately: $\alpha = (1/4)(b_1 - b_{-1})$ and $\beta = (1/2)(b_{-1} + b_1)$.

By introducing the finite dimensional space

$$V_N([-1,1]) = \left\{v_N \in \mathbb{P}_N : v_N'(\pm 1) = 0\right\} = \left\{L_k^\star(x),\ k = 0, 1, \ldots, N\right\},$$

the discrete version of the variational problem above reads:

Find $u_{0,N}(x)$ in $V_N([-1,1])$ such that

$$a(v_N, u_{0,N}) = F_N(v_N) \quad \forall v_N \in V_N([-1,1]),$$

where

$$a(v_N, u_N) = \left(v_N', u_N'\right) + \gamma\left(v_N, u_N\right),$$

$$F_N(v_N) = \left(v_N, f\right)_N - \left(v_N', 2\alpha x + \beta\right) - \gamma\left(v_N, \alpha x^2 + \beta x\right) + v(1)b_1 - v(-1)b_{-1},$$

with the integral of the inner product involving f evaluated approximately by means of some formula of numerical quadrature, as indicated by the N subscript in $(\cdot,\cdot)_N$.

By introducing the expansion

$$u_{0,N}(x) = \sum_{i=0}^{N} U_i L_i^\star(x), \tag{1.17}$$

and choosing the test functions $v_N(x)$ equal to the basis functions $L_j^\star(x)$, one obtains the algebraic linear system

$$\left({}^0D + \gamma M\right) U = R, \tag{1.18}$$

where ${}^0D$ and M are the matrices obtained in (1.13) and (1.14), and R is the right-hand side of the "lifted" problem, with components defined by

$$R_j = (L_j^\star(x), f(x))_N + (L_j^{\star\prime}(x), 2\alpha x + \beta) - \gamma(L_j^\star(x), \alpha x^2 + \beta x) + L_j^\star(1) b_1 - L_j^\star(-1) b_{-1},$$
$$j = 0, \ldots, N. \tag{1.19}$$

The linear system (1.18) can be solved by a simple factorization algorithm for a pentadiagonal symmetric matrix (assuming $\gamma > 0$).

However, we describe here a solution method based on the eigendecomposition of the mass matrix M, which will be used in the implementation of the direct solver for the two-dimensional problem and which also allows the proper handling of the singular case $\gamma = 0$. First the pentadiagonal mass M is diagonalized through $W^{\mathrm{T}} M W = \Lambda$, where $\Lambda = \mathrm{diag}(\lambda_0, \lambda_1, \ldots, \lambda_N)$. By virtue of the first row and column of mass matrix (1.14), the eigenvector matrix W has the following block structure:

$$W = \begin{bmatrix} w_{00} & 0 \\ 0 & W_{[N]} \end{bmatrix},$$

where w_{00} is a single element and $W_{[N]}$ is a matrix of order N. Let us multiply system (1.18) by W^{T}, and introduce the transformations $\overline{U} = W^{\mathrm{T}} U$ and $\overline{R} = W^{\mathrm{T}} R$. Using the property

$$W^{\mathrm{T}}\,{}^0D\overline{U} = W^{\mathrm{T}} \begin{bmatrix} 0 & 0 \\ 0 & I_{[N]} \end{bmatrix} \overline{U} = W^{\mathrm{T}} \begin{bmatrix} 0 \\ \overline{U}_{[N]} \end{bmatrix} = {}^0\overline{U}, \tag{1.20}$$

where ${}^0\overline{U} = (0, \overline{U}_1, \overline{U}_2, \ldots, \overline{U}_N)$, the linear system (1.18) becomes

$${}^0\overline{U} + \gamma\Lambda\overline{U} = \overline{R}. \tag{1.21}$$

The transformed system (1.21) can be solved componentwise

$$\begin{cases} \overline{U}_0 = \begin{cases} \text{arbitrary} & \text{if } \gamma = 0, \\ \overline{R}_0/(\gamma\lambda_0) & \text{if } \gamma > 0, \end{cases} \\ \overline{U}_i = \overline{R}_i/(1 + \gamma\lambda_i), \quad i = 1, \ldots, N. \end{cases} \tag{1.22}$$

Of course, when $\gamma = 0$ the solution exists only provided the compatibility condition (1.2) on the data is satisfied; therefore, the fulfillment of such a condition should be checked before assigning an arbitrary value to $\overline{U}_0$.

The antitransformation $U = W\overline{U}$ gives the Legendre expansion coefficients U of $u_{0,N}(x)$ and henceforth the complete solution containing the lifting $u_b(x)$

$$u_N(x) = \sum_{i=0}^{N} U_i L_i^\star(x) + \frac{1}{4}(b_1 - b_{-1})x^2 + \frac{1}{2}(b_{-1} + b_1)x. \tag{1.23}$$

1.4. Numerical tests

The algorithm for the one-dimensional Neumann problem was tested by solving problem (1.1) with $\gamma = 1.5$ and with analytical solution $u(x) = \mathrm{e}^x$. The numerical errors, in the L^∞, L^2 and H^1 norms, are given in Table 1, which shows the spectral accuracy of the method.

Table 1
One-dimensional problem with Neumann conditions, analytical solution $u(x)$, $x \in [-1, 1]$, $\gamma = 1.5$

N	$u(x) = e^x$			$u(x) = \sin x$		
	L^∞ error	L^2 error	H^1 error	L^∞ error	L^2 error	H^1 error
4	1.14×10^{-4}	2.22×10^{-4}	1.88×10^{-3}	5.47×10^{-6}	1.15×10^{-5}	9.78×10^{-5}
6	7.36×10^{-7}	1.59×10^{-6}	2.02×10^{-5}	1.64×10^{-8}	3.76×10^{-8}	4.77×10^{-7}
8	3.21×10^{-9}	7.91×10^{-9}	1.34×10^{-7}	3.26×10^{-11}	8.45×10^{-11}	1.44×10^{-9}
16	2.78×10^{-16}	3.10×10^{-14}	1.25×10^{-13}	8.88×10^{-16}	2.76×10^{-15}	1.06×10^{-14}
32	4.00×10^{-14}	9.63×10^{-14}	1.19×10^{-12}	1.11×10^{-16}	9.78×10^{-15}	9.36×10^{-14}
100	3.73×10^{-14}	1.43×10^{-13}	1.11×10^{-11}	2.22×10^{-15}	1.08×10^{-14}	1.26×10^{-12}

A second test is the same problem above but with the exact solution $u(x) = \sin x$. The corresponding errors are also reported in Table 1 and demonstrate that the expected rate of exponential convergence is achieved.

2. 2D elliptic problem with Neumann condition

Let us now consider the two-dimensional boundary value problem for the Helmholtz operator supplemented by a Neumann condition, namely

$$(-\nabla^2 + \gamma)u = f(x, y) \quad \text{and} \quad \left.\frac{\partial u}{\partial n}\right|_{\partial\Omega} = b(\ell) \tag{2.1}$$

to be solved in the square domain $\Omega = [-1, 1]^2$, where ℓ represents a curvilinear coordinate of $\partial\Omega$. Here, γ is a nonnegative constant and, in the special case $\gamma = 0$, problem (2.1) can have a solution only provided that the data f and b satisfy the compatibility condition

$$\int_{-1}^{1}\int_{-1}^{1} f(x, y)\, dx\, dy = -\oint_{\partial\Omega} b(\ell)\, d\ell \tag{2.2}$$

in which case the solution u is defined up to an arbitrary additive constant.

For the sake of completeness, we consider the general situation of a *nonhomogeneous* Neumann condition and describe a solution algorithm which takes into account a nonzero boundary value b by means of a lifting. The structure of this lifting is very similar to that of the two-step procedure proposed in [7] for the Dirichlet boundary value problem.

As in the one-dimensional problem, the Neumann condition will be enforced according to an *essential* treatment. In a standard variational formulation, this kind of boundary condition is commonly imposed in a *natural* way, which, for $b \neq 0$, amounts to perturb the right-hand side of the weak equation by including a boundary integral involving b. This term results from the integration by parts of the Laplacian term and enforces the nonzero boundary value of the normal derivative of the unknown u in a weak sense.

The classical approach adopted in the context of a Galerkin spectral approximation employs the orthogonal basis built upon ordinary Legendre polynomials. This approach leads to a full stiffness matrix for approximating the two second derivatives with respect to x and y. Alternatively, if one wants the profile of the matrices representing the one-dimensional operators not to be larger than pentadiagonal, the basis of polynomial functions of zero slope at both endpoints, introduced in relation (1.12), should be used. Then, the solution of the elliptic boundary value problem (2.1) is obtained by introducing a lifting of the nonhomogeneous Neumann condition through the definition

$$u = u_0 + u_b, \tag{2.3}$$

where u_0 is an auxiliary unknown satisfying the modified problem

$$(-\nabla^2 + \gamma)u_0 = f - (-\nabla^2 + \gamma)u_b \quad \text{in } \Omega, \quad \text{and} \quad \left.\frac{\partial u_0}{\partial n}\right|_{\partial\Omega} = 0, \tag{2.4}$$

while u_b is an arbitrary function of suitable regularity whose normal derivative on $\partial\Omega$ is equal to the prescribed value b.

2.1. Galerkin–Legendre approximation

The spatial discretization of the two-dimensional elliptic problem (2.1) is obtained by introducing the finite dimensional space built by the direct product of the two bases $\{L_i^\star(x),\ i = 0, 1, \ldots, I\}$ and $\{L_j^\star(y),\ j = 0, 1, \ldots, J\}$. The approximate solution u_N to u is then expressed as the sum of two components:

$$u_N(x, y) = u_{0,N}(x, y) + u_{b,N}(x, y) = \sum_{i=0}^{I} L_i^\star(x)\, u_{i,j}\, L_j^\star(y) \underset{j=0}{\overset{J}{\Sigma}} + u_{b,N}(x, y). \tag{2.5}$$

As in [7], the special symbol Σ (reversed) is used to indicate the summation on the second index. This notation proves helpful in developing the 2D algorithm since it leads quite naturally to matrices pre- and post-multiplying the array of the unknowns to represent the action of the spatial differential operators respectively in the x and y directions. The precise form of the expansion of $u_{b,N}$ in terms of the polynomial basis will be given in Section 2.3.

2.2. Compatibility conditions of the Neumann boundary values

Let $b^{\mathrm{b}}(x)$ and $b^{\mathrm{t}}(x)$, $|x| \leqslant 1$, denote the distribution of the Neumann datum on the bottom and top sides of the domain, and let $b^{\mathrm{l}}(y)$ and $b^{\mathrm{r}}(y)$, $|y| \leqslant 1$, denote its distribution on the left and right sides. Following Grisvard [11], these four functions are not completely independent since they must satisfy the following four compatibility conditions in the corners:

$$\begin{cases} -\dfrac{\mathrm{d}b^{\mathrm{l}}(1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{t}}(-1)}{\mathrm{d}x}, & \dfrac{\mathrm{d}b^{\mathrm{r}}(1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{t}}(1)}{\mathrm{d}x}, \\ \dfrac{\mathrm{d}b^{\mathrm{l}}(-1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{b}}(-1)}{\mathrm{d}x}, & -\dfrac{\mathrm{d}b^{\mathrm{r}}(-1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{b}}(1)}{\mathrm{d}x}. \end{cases} \tag{2.6}$$

These four relations correspond to the conditions of equality of the two mixed second derivatives of the unknown u in the corners. For the development of the solution algorithm, it is convenient to denote explicitly these four corner values (which are deduced from the side distributions of the Neumann data by evaluating their slope at the side extremes) as follows:

$$\begin{cases} c^{\mathrm{lt}} \equiv -\dfrac{\mathrm{d}b^{\mathrm{l}}(1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{t}}(-1)}{\mathrm{d}x}, & c^{\mathrm{rt}} \equiv \dfrac{\mathrm{d}b^{\mathrm{r}}(1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{t}}(1)}{\mathrm{d}x}, \\ c^{\mathrm{lb}} \equiv \dfrac{\mathrm{d}b^{\mathrm{l}}(-1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{b}}(-1)}{\mathrm{d}x}, & c^{\mathrm{rb}} \equiv -\dfrac{\mathrm{d}b^{\mathrm{r}}(-1)}{\mathrm{d}y} = \dfrac{\mathrm{d}b^{\mathrm{b}}(1)}{\mathrm{d}x}. \end{cases} \tag{2.7}$$

2.3. Lifting of nonhomogeneous boundary values

The compatibility conditions (2.6) play a central role in the construction of the lifting for the nonhomogeneous boundary conditions of the two-dimensional problem. In fact, in force of such conditions, the lifting is built in two subsequent steps, much in the same manner as for Dirichlet boundary condition [7]. To this purpose, the function $u_{b,N}(x,y)$ approximating the analytical lifting $u_b(x,y)$ is decomposed in two contributions as follows:

$$u_{b,N} = u_b^{\mathrm{c}} + u_{b,N}^{\mathrm{s}}. \tag{2.8}$$

Here, u_b^{c} is the *corner* component dependent on the four values $c^{\mathrm{lb}}, c^{\mathrm{rb}}, c^{\mathrm{lt}}, c^{\mathrm{rt}}$, defined by (2.7) and associated with the compatibility conditions (2.6), while $u_{b,N}^{\mathrm{s}}$ is the *side* component that accounts for the values of the Neumann datum *inside* each of the sides of the domain.

2.3.1. Corner component of the lifting

The corner component $u_b^{\mathrm{c}}(x,y)$ of the lifting is expressed by means of the polynomial

$$u_b^{\mathrm{c}}(x,y) = r_1 xy + r_2 xy^2 + r_3 x^2 y + r_4 x^2 y^2. \tag{2.9}$$

The coefficients r_1, r_2, r_3 and r_4 are determined by exploiting the compatibility conditions (2.6) and enforcing the following conditions, involving the mixed second derivatives u_{xy} and u_{yx} in each corner, in a pointwise manner

$$\frac{\partial^2 u_b^{\mathrm{c}}(\pm 1, \pm 1)}{\partial x\, \partial y} = c^{\binom{\mathrm{r}}{\mathrm{l}}\binom{\mathrm{t}}{\mathrm{b}}}, \tag{2.10}$$

with the superscripts within parentheses to be selected alternatively according to the signs $\pm$ written on the left. By the expansion (2.9), this is a linear system of four equations in the unknowns (r_1, r_2, r_3, r_4) whose solution is immediately found to be

$$\begin{cases} r_1 = \dfrac{1}{4}\left(c^{\mathrm{lb}} + c^{\mathrm{rb}} + c^{\mathrm{rt}} + c^{\mathrm{lt}}\right), \\ r_2 = \dfrac{1}{8}\left(-c^{\mathrm{lb}} - c^{\mathrm{rb}} + c^{\mathrm{rt}} + c^{\mathrm{lt}}\right), \\ r_3 = \dfrac{1}{8}\left(-c^{\mathrm{lb}} + c^{\mathrm{rb}} + c^{\mathrm{rt}} - c^{\mathrm{lt}}\right), \\ r_4 = \dfrac{1}{16}\left(c^{\mathrm{lb}} - c^{\mathrm{rb}} + c^{\mathrm{rt}} - c^{\mathrm{lt}}\right). \end{cases} \tag{2.11}$$

2.3.2. Side component of the lifting

Once the corner component of the lifting u_b^{c} has been evaluated, the side component $u_{b,N}^{\mathrm{s}}$ is determined so as to satisfy (in a weak sense, see later) a Neumann boundary condition with respect to the perturbed datum

$$\tilde{b} \equiv b - \left.\frac{\partial u_b^{\mathrm{c}}}{\partial n}\right|_{\partial\Omega}, \tag{2.12}$$

obtained by subtracting the normal derivative of the known corner component u_b^{c} from the original Neumann datum. By (2.9), the distribution of this perturbed Neumann condition on the four sides is given explicitly by

$$\begin{aligned} \tilde{b}^{\binom{\mathrm{r}}{\mathrm{l}}}(y) &= b^{\binom{\mathrm{r}}{\mathrm{l}}}(y) - (\pm r_1 + 2r_3)y - (\pm r_2 + 2r_4)y^2, \\ \tilde{b}^{\binom{\mathrm{t}}{\mathrm{b}}}(x) &= b^{\binom{\mathrm{t}}{\mathrm{b}}}(x) - (\pm r_1 + 2r_2)x - (\pm r_3 + 2r_4)x^2. \end{aligned} \tag{2.13}$$

To represent the (approximated) side component $u_{b,N}^{\mathrm{s}}(x,y)$ of the lifting we introduce the space

$$\left[\{L_i^{\star}(x), 0 \leqslant i \leqslant I\} \otimes \{y, y^2\}\right] \oplus \left[\{x, x^2\} \otimes \{L_j^{\star}(y), 0 \leqslant j \leqslant J\}\right], \tag{2.14}$$

so that we have the following expansion:

$$u^{s}_{b,N}(x,y)=\left[\sum_{i=0}^{I}L_i^{\star}(x)\left(\alpha_i y+\beta_i y^2\right)\right]+\left[\left(x\gamma_j+x^2\delta_j\right)L_j^{\star}(y)\sum_{j=0}^{J}\right], \tag{2.15}$$

with derivatives

$$\frac{\partial u^{s}_{b,N}(x,y)}{\partial y}=\left[\sum_{i=0}^{I}L_i^{\star}(x)(\alpha_i+2\beta_i y)\right]+\left[\left(x\gamma_j+x^2\delta_j\right)L_j^{\star\prime}(y)\sum_{j=0}^{J}\right], \tag{2.16}$$

$$\frac{\partial u^{s}_{b,N}(x,y)}{\partial x}=\left[\sum_{i=0}^{I}L_i^{\star\prime}(x)\left(\alpha_i y+\beta_i y^2\right)\right]+\left[(\gamma_j+2x\delta_j)L_j^{\star}(y)\sum_{j=0}^{J}\right]. \tag{2.17}$$

We now consider the horizontal sides and impose that the y-derivative expansion (2.16) for $y=\pm 1$ be equal, in the sense of L^2 projection, to $\tilde{b}^{\mathrm{b}}(x)$ and $\tilde{b}^{t}(x)$, that is, we require that

$$\left(L_{i'}^{\star}(x),\frac{\partial u^{s}_{b,N}(x,\pm 1)}{\partial y}\right)=\sum_{i=0}^{I}\left(L_{i'}^{\star},L_i^{\star}\right)(\alpha_i\pm 2\beta_i)=\left(L_{i'}^{\star},\tilde{b}^{\left(\substack{\mathrm{t}\\ \mathrm{b}}\right)}\right).$$

In vector notation, we have a linear system for the two vector unknowns α and β

$$\begin{cases} M(\alpha+2\beta)=B^{\mathrm{t}},\\ M(\alpha-2\beta)=B^{\mathrm{b}},\end{cases}$$

with the right-hand sides defined by $B_i^{\mathrm{t}}=(L_i^{\star},\tilde{b}^{\mathrm{t}})$ and $B_i^{\mathrm{b}}=(L_i^{\star},\tilde{b}^{\mathrm{b}})$ for $0\leqslant i\leqslant I$. The linear system for α and β gives immediately the following two uncoupled linear systems:

$$M\alpha=\frac{1}{2}(B^{\mathrm{t}}-B^{\mathrm{b}})\quad\text{and}\quad M\beta=\frac{1}{4}(B^{\mathrm{b}}+B^{\mathrm{t}}).$$

The integrals defining B^{b} and B^{t} are evaluated by the Gauss–Legendre quadrature formula with $I+1$ points. To this purpose, let $\mathscr{W}\equiv\{w_g,1\leqslant g\leqslant I+1\}$ denote the vector of the Gauss–Legendre weight and $\mathscr{L}\equiv\{\mathscr{L}_{g,i}=L_i^{\star}(x_g),1\leqslant g\leqslant I+1,0\leqslant i\leqslant I\}$ the matrix of the values of the basis functions at the quadrature points. By denoting the values of the perturbed Neumann datum at these points as follows:

$$\tilde{\mathscr{B}}^{\left(\substack{\mathrm{t}\\ \mathrm{b}}\right)}\equiv\left\{\tilde{b}^{\left(\substack{\mathrm{t}\\ \mathrm{b}}\right)}(x_g),\ 1\leqslant g\leqslant I+1\right\} \tag{2.18}$$

and introducing the numerical evaluation of the L^2 integrals on the right sides, the two linear systems above assume the final form

$$M\alpha=\frac{1}{2}\mathscr{L}^{\mathrm{T}}\left\{\mathscr{W}\star\left[\tilde{\mathscr{B}}^{\mathrm{t}}-\tilde{\mathscr{B}}^{\mathrm{b}}\right]\right\}\quad\text{and}\quad M\beta=\frac{1}{4}\mathscr{L}^{\mathrm{T}}\left\{\mathscr{W}\star\left[\tilde{\mathscr{B}}^{\mathrm{b}}+\tilde{\mathscr{B}}^{\mathrm{t}}\right]\right\}, \tag{2.19}$$

where $\star$ denotes the element-by-element multiplication of vectors. The same procedure applied to the two vertical sides leads to other two linear systems, which correspond to the transpose of those obtained for the horizontal sides, namely

$$\gamma^{\mathrm{T}}N=\frac{1}{2}\left\{\left[\tilde{\mathscr{B}}^{\mathrm{r}}-\tilde{\mathscr{B}}^{\mathrm{l}}\right]\star\mathscr{V}\right\}^{\mathrm{T}}\mathscr{K}\quad\text{and}\quad\delta^{\mathrm{T}}N=\frac{1}{4}\left\{\left[\tilde{\mathscr{B}}^{\mathrm{l}}+\tilde{\mathscr{B}}^{\mathrm{r}}\right]\star\mathscr{V}\right\}^{\mathrm{T}}\mathscr{K}, \tag{2.20}$$

with an obvious meaning of the symbols. In conclusion, the determination of the side component of the lifting requires to solve two mass matrix problems of dimension $(I+1)$ and two of dimension $(J+1)$.

The perturbed Neumann datum $\tilde{b}$, which is necessary to determine the side component of the lifting, does not appear anymore in the homogeneous Neumann boundary value problem for the auxiliary unknown u_0, neither in its spectral counterpart for the unknown $u_{0,N}$. In fact, problem (2.4) can be rewritten in the form

$$(-\nabla^2+\gamma)u_0 = f - (-\nabla^2+\gamma)(u_b^{\mathrm{c}}+u_b^{\mathrm{s}}) \quad \text{in } \Omega, \quad \text{and} \quad \left.\frac{\partial u_0}{\partial n}\right|_{\partial\Omega} = 0, \tag{2.21}$$

and its weak variational formulation reads:

Find u_0 in $H^2_{(0)}(\Omega) = \{v \in H^2(\Omega), \partial v/\partial n|_{\partial\Omega} = 0\}$, *such that*

$$a(v,u_0) = F(v) \quad \forall v \in H^2_{(0)}(\Omega),$$

the bilinear form $a(v,u)$ *and the linear functional* $F(v)$ *being defined by*

$$a(v,u) = (\nabla v, \nabla u) + \gamma(v,u),$$
$$F(v) = (v,f) - (\nabla v, \nabla(u_b^{\mathrm{c}}+u_b^{\mathrm{s}})) - \gamma(v, u_b^{\mathrm{c}}+u_b^{\mathrm{s}}) + \oint_{\partial\Omega} vb.$$

2.4. Solution algorithm

The lifted variational problem above, once approximated by expanding u_N by the proposed Legendre basis as in (2.5), leads to the following linear system of algebraic equations (see Fig. 2)

$${}^0DUN + MU\,{}^0E + \gamma MUN = R, \tag{2.22}$$

where the stiffness and mass matrices ${}^0D$ and M have been defined in (1.13) and (1.14), while ${}^0E$ and N are their counterparts in the spatial direction y. Note that the elements of matrix U are the expansion coefficients of the unknown $u_{0,N}$ of the lifted problem. The arrays U and R are in general rectangular matrices, and generalize the vectors occurring in the one-dimensional problem of Section 1.3. The elements $r_{i,j}$, $0 \leqslant (i,j) \leqslant (I,J)$, of matrix R are defined by the right-hand side of the weak equation modified by the lifting

$$\begin{aligned} r_{i,j} = {} & \Big(L_i^\star(x)L_j^\star(y), f(x,y)\Big)_N - \left(L_i^{\star\prime}(x)L_j^\star(y), \frac{\partial u_{b,N}(x,y)}{\partial x}\right) - \left(L_i^\star(x)L_j^{\star\prime}(y), \frac{\partial u_{b,N}(x,y)}{\partial y}\right) \\ & - \gamma\Big(L_i^\star(x)L_j^\star(y), u_{b,N}(x,y)\Big) + \oint_{\partial\Omega} L_i^\star(x) b(\ell) L_j^\star(y), \end{aligned} \tag{2.23}$$

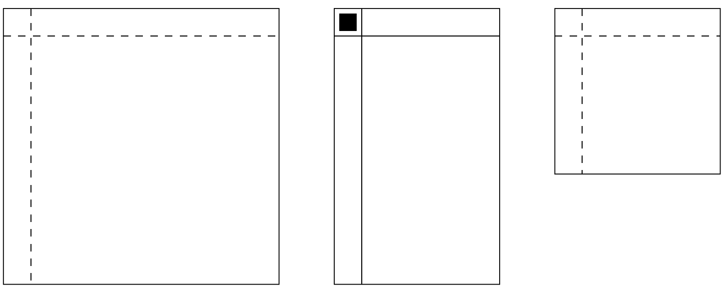

Fig. 2. Matrix structure of the spectral elliptic solver for Neumann boundary condition. Sketch of the role of the constant mode in the two-dimensional Poisson problem.

where $u_{b,N} = u_b^c + u_{b,N}^s$ and the first term involving the integral of f is evaluated numerically by means of a suitable Gauss–Legendre quadrature formula.

The solution of linear system (2.22) is obtained by diagonalizing the mass matrices M and N. First we solve the symmetric eigenvalue problems

$$Mw^{(i)} = \lambda_i w^{(i)}, \quad 0 \leqslant i \leqslant I \qquad \text{and} \qquad Nv^{(j)} = \sigma_j v^{(j)}, \quad 0 \leqslant j \leqslant J.$$

By introducing the eigenvector matrices $W \equiv [w^{(0)}, \ldots, w^{(I)}]$ and $V \equiv [v^{(0)}, \ldots, v^{(J)}]$, one has $W^{\mathrm{T}}MW = \Lambda = \mathrm{diag}(\lambda_0, \lambda_1, \ldots, \lambda_I)$ and $V^{\mathrm{T}}NV = \Sigma = \mathrm{diag}(\sigma_0, \sigma_1, \ldots, \sigma_J)$, respectively.

Then, by means of the double transformations $\overline{R} = W^{\mathrm{T}}RV$ and $\overline{U} = W^{\mathrm{T}}UV$, the linear system (2.22) becomes

$$W^{\mathrm{T}}\,{}^0DW\overline{U}\Sigma + \Lambda\overline{U}V^{\mathrm{T}}\,{}^0EV + \gamma\Lambda\overline{U}\Sigma = \overline{R}. \tag{2.24}$$

We recall now from Section 1.2 that, in the assumed spectral basis, the stiffness matrices ${}^0D$ and ${}^0E$ are identity matrices but for their first leading element which is zero, cf. Eq. (1.13) and that the mass matrices M and N have a zero first row and a zero first column but for the leading diagonal entry c_0, cf. (1.14). As a consequence, the matrices W and V have the following block structure

$$W = \begin{bmatrix} w_{00} & 0 \\ 0 & W_{[I]} \end{bmatrix}, \quad V = \begin{bmatrix} v_{00} & 0 \\ 0 & V_{[J]} \end{bmatrix}.$$

It follows that we have the relation

$$W^{\mathrm{T}}\,{}^0DW = \begin{bmatrix} w_{00} & 0 \\ 0 & W_{[I]}^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & I_{[I]} \end{bmatrix} \begin{bmatrix} w_{00} & 0 \\ 0 & W_{[I]} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & I_{[I]} \end{bmatrix} = {}^0D,$$

and the analogous result $V^{\mathrm{T}}\,{}^0EV = {}^0E$. Thus, the transformed linear system simplifies to

$${}^0D\overline{U}\Sigma + \Lambda\overline{U}\,{}^0E + \gamma\Lambda\overline{U}\Sigma = \overline{R} \tag{2.25}$$

and it can be solved componentwise as follows:

$$\begin{cases} \overline{u}_{0,0} = \begin{cases} \text{arbitrary} & \text{if } \gamma = 0, \\ \overline{r}_{0,0}/(\gamma\lambda_0\sigma_0) & \text{if } \gamma > 0, \end{cases} \\ \overline{u}_{0,j} = \overline{r}_{0,j}/(\lambda_0(1+\gamma\sigma_j)), & 1 \leqslant j \leqslant J, \\ \overline{u}_{i,0} = \overline{r}_{i,0}/((1+\gamma\lambda_i)\sigma_0), & 1 \leqslant i \leqslant I, \\ \overline{u}_{i,j} = \overline{r}_{i,j}/(\sigma_j + \lambda_i + \gamma\lambda_i\sigma_j), & 1 \leqslant (i,j) \leqslant (I,J). \end{cases} \tag{2.26}$$

Note that, when $\gamma = 0$, the fulfillment of the compatibility condition (2.2) must be checked before assigning to $\overline{u}_{0,0}$ an arbitrary value.

By performing the double back transformation $U = W\overline{U}V^{\mathrm{T}}$, the matrix of Legendre coefficients U of the solution component $u_{0,N}(x,y)$ is obtained, and from that the complete solution to the original nonhomogeneous Neumann boundary value problem is finally obtained

$$u_N(x,y) = \sum_{i=0}^{I} L_i^{\star}(x)\, u_{i,j}\, L_j^{\star}(y) \sum_{j=0}^{J} + u_{b,N}^{s}(x,y) + u_b^{c}(x,y). \tag{2.27}$$

2.5. Numerical results

The double diagonalization algorithm is tested by solving the Helmholtz equation with $\gamma = 1$ and the Laplace equation in the domain $\Omega = (-1,1)^2$. The L^∞, L^2 and H^1 errors of the spectral solution to

Table 2
Comparison of essential and natural treatment of Neumann condition for Helmholtz equation with exact solution $u = x^2 + e^{x+2y}$, $\Omega = (-1,1)^2$, $\gamma = 1$

$I = J$	Essential treatment			Natural treatment		
	L^∞ error	L^2 error	H^1 error	L^∞ error	L^2 error	H^1 error
8	3.1×10^{-5}	3.0×10^{-5}	1.7×10^{-4}	1.7×10^{-5}	1.2×10^{-5}	1.8×10^{-4}
12	4.3×10^{-9}	3.8×10^{-9}	2.7×10^{-8}	9.3×10^{-10}	6.3×10^{-10}	1.5×10^{-8}
16	2.0×10^{-13}	1.3×10^{-13}	9.2×10^{-13}	3.7×10^{-13}	2.2×10^{-13}	8.5×10^{-13}
32	1.0×10^{-13}	5.5×10^{-14}	5.1×10^{-13}	5.5×10^{-12}	3.3×10^{-12}	1.1×10^{-11}
100	1.2×10^{-12}	7.3×10^{-13}	1.4×10^{-11}	1.4×10^{-10}	8.7×10^{-11}	4.2×10^{-10}

Table 3
Poisson–Neumann problem with exact solution $u = x^2 + e^{x+2y}$, $\Omega = (-1,1)^2$

$I = J$	L^∞ error	L^2 error	H^1 error	Time (ms)
8	4.1×10^{-5}	3.6×10^{-5}	1.8×10^{-4}	34
12	5.3×10^{-9}	4.3×10^{-9}	2.7×10^{-8}	41
16	1.7×10^{-13}	1.2×10^{-13}	9.3×10^{-13}	41
32	1.0×10^{-13}	5.0×10^{-14}	5.1×10^{-13}	77
100	1.2×10^{-12}	7.1×10^{-13}	1.4×10^{-11}	585

Table 4
Helmholtz–Neumann problem with exact solution $u = \cos(\pi x)\cos(\pi y)$, $\Omega = (-1,1)^2$, $\gamma = 1$

$I = J$	L^∞ error	L^2 error	H^1 error	Time (ms)
8	1.75×10^{-4}	1.56×10^{-4}	1.01×10^{-3}	30
12	5.19×10^{-8}	4.62×10^{-8}	3.51×10^{-7}	36
16	4.69×10^{-12}	4.17×10^{-12}	3.57×10^{-11}	43
32	7.77×10^{-15}	2.56×10^{-15}	1.35×10^{-14}	110
100	7.89×10^{-14}	3.29×10^{-14}	1.50×10^{-13}	1703

Helmholtz problem with exact solution $u(x,y) = x^2 + e^{x+2y}$ for different values of N are given in Table 2. The spectral convergence of the method is clearly recognized. For comparison, we report also results obtained by a spectral solver based on the natural treatment of the Neumann condition and on the diagonalization of the stiffness matrix. This solver displays a slightly better accuracy at low spatial resolution, while at higher resolutions the proposed method is found to be more accurate. This behaviour is due to a better conditioning of the mass matrix of the proposed algorithm with respect to the (full) stiffness matrix in the standard approach.

A second numerical test is for the Poisson equation with the same exact solution $u = x^2 + e^{x+2y}$. The numerical errors are reported in Table 3 with the CPU times obtained on a Digital 433au workstation. The last test is the Helmholtz equation with $\gamma = 1$ and with exact solution $u(x,y) = \cos(\pi x)\cos(\pi y)$. The errors and CPU times obtained on the same machine are reported in Table 4. The exponential rate of convergence is achieved also in this case.

3. The lifting for the 3D Neumann problem

In this section, we outline the extension of the 2D solution algorithm to the 3D Neumann problem in the cube $[-1,1]^3$. We focus on the analysis of the compatibility conditions existing among the Neumann boundary data prescribed on the six faces of the domain. To this aim, we first observe that these data are specified by giving the following six functions of two variables:

$$b^{\binom{\mathrm{r}}{\mathrm{l}}}(y,z), \quad b^{\binom{\mathrm{t}}{\mathrm{b}}}(x,z), \quad b^{\binom{\mathrm{n}}{\mathrm{f}}}(x,y) \tag{3.1}$$

for $|x| \leqslant 1,\ |y| \leqslant 1$ and $|z| \leqslant 1$. These functions represent the distribution of the normal derivative of the unknown u respectively on the "right" and "left" faces, $x = \pm 1$, on the 'top" and "bottom" faces, $y = \pm 1$, and the "near" and "far" faces, $z = \pm 1$, of the cube, in a right-handed Cartesian system.

3.1. Compatibility conditions

According to the analysis of Grisvard [11], to have solutions with a $H^2(\Omega)$ regularity these functions cannot be specified independently from each other and must satisfy two sets of compatibility conditions. The first set of conditions consists in equalities of the mixed second derivatives of the functions (3.1). More precisely, for each triplet of functions sharing a vertex in their definition domain, the three mixed second derivatives must coincide at this common point. For instance, considering the vertex in the left–bottom–near corner of the cube, we have the conditions

$$\frac{\partial^2 b^{\mathrm{l}}(-1,-1)}{\partial y\, \partial z} = \frac{\partial^2 b^{\mathrm{b}}(-1,-1)}{\partial x\, \partial z} = \frac{\partial^2 b^{\mathrm{n}}(-1,-1)}{\partial x\, \partial y}. \tag{3.2}$$

It can be noted that the value of the mixed second derivatives of the three functions of the Neumann datum in their common vertex is nothing but the value of the *third-order* mixed derivative of the unknown u in the considered vertex, namely

$$\frac{\partial^3 u(-1,-1,-1)}{\partial x\, \partial y\, \partial z}. \tag{3.3}$$

We can therefore introduce such a corner value from the functions of the Neumann conditions and consider this value as a definite distinct datum of the elliptic problem as follows:

$$d^{\mathrm{lbn}} \equiv \frac{\partial^2 b^{\mathrm{l}}(-1,-1)}{\partial y\, \partial z} = \frac{\partial^2 b^{\mathrm{b}}(-1,-1)}{\partial x\, \partial z} = \frac{\partial^2 b^{\mathrm{n}}(-1,-1)}{\partial x\, \partial y} = \frac{\partial^3 u(-1,-1,-1)}{\partial x\, \partial y\, \partial z}. \tag{3.4}$$

Of course, similar definitions hold for the other seven vertices, and we collect them in the following formal definition:

$$d^{\binom{\mathrm{r}}{\mathrm{l}}\binom{\mathrm{t}}{\mathrm{b}}\binom{\mathrm{f}}{\mathrm{n}}} \equiv \frac{\partial^3 u(\pm 1, \pm 1, \pm 1)}{\partial x\, \partial y\, \partial z}. \tag{3.5}$$

The second set of compatibility conditions among the six functions in (3.1) consists in a constraint involving two functions of each pair associated with two intersecting faces of the cube. More precisely, for each edge the two functions specifying the normal derivative of the unknown on the two faces must have their first derivative in direction perpendicular to the edge to be coincident, *modulo* the sign. Considering for instance the edge $|x| \leqslant 1,\ y = -1,\ z = -1$, the first derivative of $b^{\mathrm{b}}(x,z)$ with respect to z must coincide with the first derivative of $b^{\mathrm{n}}(x,y)$ with respect to y. We can therefore define the following function of x:

$$c^{xe_1}(x) \equiv \frac{\partial b^{\mathrm{b}}(x,-1)}{\partial z} = \frac{\partial b^{\mathrm{n}}(x,-1)}{\partial y} = -\frac{\partial^2 u(x,-1,-1)}{\partial y\, \partial z} \tag{3.6}$$

for $|x| \leqslant 1$, a function which can be computed in any case from either $b^{\mathrm{b}}(x,y)$ or $b^{\mathrm{n}}(x,y)$. Similar definitions hold for the other three edges parallel to the x axis, $|x| \leqslant 1,\ y = \pm 1,\ z = \pm 1$, so that the definition of the corresponding four functions is synthesized formally as follows:

$$c^{xe_\ell}(x) \equiv -\frac{\partial^2 u(x, \pm 1, \pm 1)}{\partial y\, \partial z}, \quad \ell = 1, 2, 3, 4. \tag{3.7}$$

Analogous definitions are valid for the four edges parallel to the y axis and for those parallel to the z axis.

3.2. The three-step lifting

The spectral solution of the 3D Neumann problem is expressed in the standard lifted form

$$u_N(x, y, z) = u_{0,N}(x, y, z) + u_{b,N}(x, y, z), \tag{3.8}$$

where the function to perform the lifting of the nonhomogeneous Neumann datum b is decomposed in the three parts

$$u_{b,N}(x, y, z) = u_b^{\mathrm{v}}(x, y, z) + u_{b,N}^{\mathrm{e}}(x, y, z) + u_{b,N}^{\mathrm{f}}(x, y, z) \tag{3.9}$$

associated respectively with the vertices, the edges and the faces of the cubic domain. These three components are evaluated in a cascadic manner, by an extension of the method for the two-dimensional equation described in Section 2.3.

First, the vertex component of the lifting is expressed as the polynomial

$$u_b^{\mathrm{v}}(x, y, z) = r_1 xyz + r_2 xyz^2 + r_3 xy^2 z + r_4 x^2 yz + r_5 x^2 y^2 z + r_6 x^2 yz^2 + r_7 xy^2 z^2 + r_8 x^2 y^2 z^2 \tag{3.10}$$

whose coefficients are determined by imposing the eight conditions at the vertices

$$\frac{\partial^3 u_b^{\mathrm{v}}(\pm 1, \pm 1, \pm 1)}{\partial x\, \partial y\, \partial z} = d^{\binom{\mathrm{r}}{\mathrm{l}}\binom{\mathrm{t}}{\mathrm{b}}\binom{\mathrm{n}}{\mathrm{f}}}. \tag{3.11}$$

Once the vertex component of the lifting $u_b^{\mathrm{v}}(x, y, z)$ has been determined, the edge component $u_{b,N}^{\mathrm{e}}(x, y, z)$ is evaluated by expanding it in the space

$$\begin{aligned} &\big[\{L_i^\star(x), 0 \leqslant i \leqslant I\} \otimes \{y, y^2\} \otimes \{z, z^2\}\big] \oplus [\{x, x^2\}. \otimes \{L_j^\star(y), 0 \leqslant j \leqslant J\} \otimes \{z, z^2\}] \\ &\quad \oplus \big[\{x, x^2\} \otimes \{y, y^2\} \otimes \{L_k^\star(z), 0 \leqslant k \leqslant K\}\big], \end{aligned} \tag{3.12}$$

namely, by introducing the representation

$$\begin{aligned} u_{b,N}^{\mathrm{e}}(x, y, z) = \sum_{i=0}^{I} L_i^\star(x)\big(\alpha_i yz + \beta_i yz^2 + \delta_i y^2 z + \gamma_i y^2 z^2\big) &+ \big(xza_j + xz^2 b_j + x^2 zc_j \\ &+ x^2 z^2 d_j\big) L_j^\star(y) \sum_{j=0}^{J} + \big(xyA_k + xy^2 B_k + x^2 yC_k + x^2 y^2 D_k\big) L_k^\star(z) \sum_{k=0}^{K}. \end{aligned} \tag{3.13}$$

The three sets of unknown coefficients in expansion (3.13) are found by equating the L^2 projection of the "trace" of $u_{b,N}^{\mathrm{e}}(x, y, z)$ along the edges to the projection of the edge functions in (3.7) and the similar ones for the other eight edges, suitably perturbed to include the effect of the (previously computed) vertex component $u_b^{\mathrm{v}}(x, y, z)$ of the lifting. Considering for instance the unknowns $(\alpha_i, \beta_i, \gamma_i, \delta_i)$, $0 \leqslant i \leqslant I$, the four edge functions $c^{xe_\ell}(x)$ are replaced by the functions $\tilde{c}^{xe_\ell}(x)$ defined by

$$\tilde{c}^{xe_\ell}(x) = c^{xe_\ell}(x) - u_b^{\mathrm{v}}(x, \pm 1, \pm 1), \quad \ell = 1, 2, 3, 4. \tag{3.14}$$

Now, the L^2 projection along the four edges gives the linear systems of equations

$$\left(L_{i'}^{\star}(x), \frac{\partial^2 u_{b,N}^{\mathrm{e}}(x, \pm 1, \pm 1)}{\partial y\, \partial z}\right) = -\left(L_{i'}^{\star}, \tilde{c}^{xe_\ell}\right), \quad \ell = 1, 2, 3, 4. \tag{3.15}$$

The full system for the unknowns $(\alpha_i, \beta_i, \gamma_i, \delta_i)$, $0 \leqslant i \leqslant I$, decomposes into four independent linear systems, each involving the mass matrix M in the x direction.

The other unknowns (a_j, b_j, c_j, d_j), $0 \leqslant j \leqslant J$, and (A_k, B_k, C_k, D_k), $0 \leqslant k \leqslant K$, of the expansion (3.13) are determined similarly.

Finally, the face component $u_{b,N}^{\mathrm{f}}(x, y, z)$ of the lifting is sought in the space

$$\begin{aligned}&[\{L_i^{\star}(x), 0. \leqslant i \leqslant I\} \otimes \{L_j^{\star}(y), 0 \leqslant j \leqslant J\} \otimes \{z, z^2\}] \oplus [\{x, x^2\}. \otimes \{L_j^{\star}(y), 0 \leqslant j \leqslant J\} \\ &\quad \otimes \{L_k^{\star}(z), 0 \leqslant k \leqslant K\}] \oplus \left[\{L_i^{\star}(x), 0 \leqslant i \leqslant I\} \otimes \{y, y^2\} \otimes \{L_k^{\star}(z), 0 \leqslant k \leqslant K\}\right]\end{aligned} \tag{3.16}$$

so that we have the expansion

$$\begin{aligned}u_{b,N}^{\mathrm{f}}(x, y, z) = &\sum_{i=0}^{I} L_i^{\star}(x)\left(\alpha_{i,j} z + \beta_{i,j} z^2\right) L_j^{\star}(y) \sum_{j=0}^{J} + \sum_{j=0}^{J} L_j^{\star}(y)\left(x a_{j,k} + x^2 b_{j,k}\right) L_k^{\star}(z) \sum_{k=0}^{K} \\ &+ \sum_{i=0}^{I} L_i^{\star}(x)\left(A_{i,k} y + B_{i,k} y^2\right) L_k^{\star}(z) \sum_{k=0}^{K}.\end{aligned} \tag{3.17}$$

The unknown coefficients in (3.17) are determined by equating the L^2 projection of $u_{b,N}^{\mathrm{f}}(x, y, z)$ to Neumann boundary datum b suitably modified for accounting the effect of the previously computed vertex and edge components of the lifting. In other words, we introduce the modified Neumann boundary datum $\tilde{b}$ by the following definition:

$$\tilde{b}^{\binom{\mathrm{r}}{\mathrm{l}}}(y, z) = b^{\binom{\mathrm{r}}{\mathrm{l}}}(y, z) - u_b^{\mathrm{v}}(\pm 1, y, z) - u_{b,N}^{\mathrm{e}}(\pm 1, y, z). \tag{3.18}$$

The weak equations that determine the unknowns $(a_{j,k}, b_{j,k})$, $0 \leqslant j \leqslant J$, $0 \leqslant k \leqslant K$, are

$$\left(L_{j'}^{\star}(y) L_{k'}^{\star}(z), \frac{\partial u_{b,N}^{\mathrm{f}}(\pm 1, y, z)}{\partial x}\right) = -\left(L_{j'}^{\star} L_{k'}^{\star}, \tilde{b}^{\binom{\mathrm{r}}{\mathrm{l}}}\right), \tag{3.19}$$

with similar equations holding for the unknowns $(\alpha_{i,j}, \beta_{i,j})$, $0 \leqslant i \leqslant I$, $0 \leqslant j \leqslant J$, and $(A_{i,k}, B_{i,k})$, $0 \leqslant i \leqslant I$, $0 \leqslant k \leqslant K$.

4. Conclusions

A direct Galerkin–Legendre spectral method for the efficient solution of the Neumann problem for Laplace and Helmholtz operators in two dimensions has been presented. The proposed method exploits the eigenstructure of the mass matrix for the diagonalization process instead of the stiffness matrix as in fast spectral solvers for elliptic problems based on the *tau* method or a collocative approach. The method relies upon a particular Legendre basis proposed by Shen [5] and imposes the Neumann boundary condition in an essential way in order to apply the double diagonalization procedure in both spatial directions, by implementing variable separation and reducing the discrete solution to a sequence of only one-dimensional problems. The matrix elements of the discrete operators are provided explicitly in the paper: the mass matrix is pentadiagonal with only three nonzero diagonals, while the stiffness matrix is simply the identity *modulo* the first diagonal element associated with the constant mode, which is zero.

The discrete lifting for taking into account nonhomogeneous Neumann data in problems in two and three dimensions has been described. In particular, the lifting for the 2D problem has been implemented to obtain a general and efficient algorithm which represents an alternative to other elliptic spectral solvers characterized by a natural treatment of the Neumann condition. The proposed new basis for the Neumann problem has been used in spectral calculations of natural convection instabilities [12].

We can conclude by observing that the idea of using a lifting for Neumann boundary data is original and has been found necessary to exploit the direct product structure of the 2D and 3D problems in conjunction with sparse matrix patterns.

References

[1] D. Gottlieb, S.A. Orszag, Numerical Analysis of Spectral Methods: Theory and Applications, SIAM, Philadelphia, 1977.
[2] D.B. Haidvogel, T.A. Zang, The accurate solution of Poisson's equation by expansion in Chebyshev polynomials, J. Comput. Phys. 30 (1979) 167–180.
[3] C. Canuto, M.Y. Hussaini, A. Quarteroni, T.A. Zang, Spectral Methods in Fluid Mechanics, Springer, New York, 1988.
[4] J.P. Boyd, Chebyshev and Fourier Spectral Methods, second ed., Dover Publications, Mineola, 2001.
[5] J. Shen, Efficient spectral-Galerkin method. I. Direct solvers of second- and fourth-order equations using Legendre polynomials, SIAM J. Sci. Comput. 15 (1994) 1489–1505.
[6] J. Shen, Efficient spectral-Galerkin method. II. Direct solvers of second- and fourth-order equations using Chebyshev polynomials, SIAM J. Sci. Comput. 16 (1995) 74–87.
[7] F. Auteri, L. Quartapelle, Galerkin spectral method for the vorticity and stream function equations, J. Comput. Phys. 149 (1999) 306–332.
[8] F. Auteri, L. Quartapelle, Galerkin–Legendre spectral method for the 3D Helmholtz equation, J. Comput. Phys. 161 (2000) 454–483.
[9] C. Bernardi, Y. Maday, Approximations spectrales des problèmes aux limites elliptiques, Springer, Paris, 1992.
[10] A. Quarteroni, A. Valli, Numerical Approximation of Partial Differential Equations, second printing, Springer, Berlin, 1997.
[11] P. Grisvard, Elliptic Problems in Nonsmooth Domains, Pitman, London, 1985.
[12] F. Auteri, N. Parolini, Simulation of the differentially heated 8:1 rectangular cavity by a Galerkin–Legendre spectral projection method, in: K.J. Bathe (Ed.), Proceedings of the First MIT Conference on Computational Fluid and Solid Mechanics, Elsevier, Amsterdam, 2001, pp. 1451–1455.