An error minimized pseudospectral penalty direct Poisson solver

Tzyy-Leng Horng[a], Chun-Hao Teng[b,c,*]

[a]*Department of Applied Mathematics, Feng Chia University, Taichung, Taiwan*
[b]*Department of Applied Mathematics, National Chiao Tung University, 1001 Ta Hsueh Road, Hsinchu, Taiwan 30010.*
[c]*Center of Mathematical Modeling and Scientific Computing, National Chiao Tung University, Hsinchu, Taiwan 30010.*

Abstract

This paper presents a direct Poisson solver based on an error minimized Chebyshev pseudospectral penalty formulation for problems defined on rectangular domains. In this study the penalty parameters are determined analytically such that the discrete L_2 error is minimized. Numerical experiments are conducted and the results show that the penalty scheme computes numerical solutions with better accuracy, compared to the traditional approach with boundary conditions enforced strongly.

Keywords: pseudospectral penalty method, Poisson equations, diagonalization.

1. Introduction

Many physics problems require solving Poisson's equation. For problems defined on domains which are confined with the coordinate systems, there are fast and accurate Poisson and Helmholtz direct solvers based on spectral methods. Here, we give a briefly discussion on a number of direct Poisson solvers based on the modal expansion and the pseudospectral approaches.

Haidvogel and Zang [9] developed an efficient and accurate Poisson solver based on the Chebyshev tau formulation [8, 18] and the eigenvalue-eigenvector matrix diagonalization method [19]. This approach is, indeed, fast and accurate for solving Poisson equations, and has inspired the development of many other direct Poisson solvers. However, as mentioned in [9] this method suffers from the round off error when the discretized system becomes large. To reduce the ill-condition of the Chebyshev tau method, Dang-Vu and Delcarte [2], employed the three-term-recursion formula of Chebyshev polynomials to simplify the spectral differentiation structure. In addition to the Chebyshev tau expansion, Shen [21] developed a Chebyshev Galerkin Poisson solver based on properly choosing the expansion basis, so the resulting discrete system of equations is less ill-condition and can be solved accurately and efficiently by matrix decomposition methods. Recently, advanced developments of spectral-based Poisson and Helmholtz solvers for problems defined on unbounded domains are discussed in [22] and references therein. Generally speaking, due to recursive

*Corresponding author
Email addresses: tlhorng@math.fcu.edu.tw (Tzyy-Leng Horng), tengch@math.nctu.edu.tw (Chun-Hao Teng)

mathematical properties inherited in the Chebyshev polynomials these modal expansion approaches are very efficient in solving linear problems with constant coefficients and with variable coefficients of polynomial type. However, for problems involving general variable coefficients the modal expansion methods become less attractive, because the spectral differentiation structure of a differentiation operator involving variable coefficients can become complicated.

In contrast to the modal expansion approaches, pseudospectral methods have also been used to develop direct and iterative Poisson and Helmholtz solvers. For fluid dynamic simulations, Ku et al. [17] presented a Poisson solver, and Ehrenstein and Peyret [4] presented a Helmholtz solver. Both methods utilize the Chebyshev pseudospectral formulation to discretize the equations in the cartesian coordinate, and the resulting systems of equations are solved by matrix diagonalization techniques. For problems defined on polar/cylindrical and spherical coordinates, pseudospectral formulations and matrix diagonalization techniques can be easily extended. For instance, Chen et al. [1] proposed direct solvers for problems in polar and cylindrical coordinate systems. Navarro et al. [20] employed Chebyshev collocation method and Newton iterative method to study an optimal control problem in a thermoconvective fluid flow. Huang et al. [16] developed an FFT based fast Poisson solver by using spectral-finite difference method and special mapping for problems defined on spherical shells.

Applying pseudospectral methods for partial differentiation equations involves not only discretizing differential equations but also enforcing boundary conditions. This often leads to a discrete system of equations having more equations than unknowns. To resolve this over determined issue, the traditional approach is enforcing the boundary condition strongly via including the boundary conditions and directly discarding the collocation equations at the boundary points. However, as a global approximation method the way of imposing boundary conditions can greatly affect the behavior of numerical solutions over the entire domain. For example, the aforementioned Chebyshev Galerkin method [21] which utilizes basis functions satisfying boundary conditions yield computation solutions with better accuracy compared to those obtained by the Chebyshev-tau method.

Funaro and Gottlieb [5] proposed a penalty approach for imposing boundary condition in pseudospectral approximations for partial differential equations. The penalty approach links boundary conditions and discretization equations through free parameters whose values are determined analytically by satisfying certain constraints. For time dependent problems the penalty parameter is considered as a stabilizer and, thus, the value of the parameter is determined to make the scheme stable. This stabilizing approach has led to successful constructions of pseudospectral schemes for time dependent problems [5, 6, 11–15] since then. In [5] it was also demonstrated that the penalty parameter can be considered as an error minimizer on solving model differential equation $u'(x) = f(x)$ subject to a boundary condition. Indeed, the accuracy of the penalty method is better than that of the traditional pseudospectral discretization with strongly enforced boundary conditions. As mentioned in [5] that a penalty scheme leads to a better approximation is because it takes into account the fact that the solution of a partial differential equation satisfies the equation arbitrary close to the domain boundary. Thus, the traditional approach which discards the discretized equations at the boundaries immediately lose certain level of accuracy of the method. This issue has motivated our study for constructing a scheme for Poisson equations, because the traditional approach leads to discarding two discretization schemes. As a consequence certain level of accuracy of the method is lost.

In this study we adopt the concept illustrated in [5] and present an error minimized pseudospectral penalty formulation for the Poisson equation on a rectangle domain, subject to Dirichlet, Neumann and Robin boundary conditions. The values of the penalty parameters are determined analytically such that the L_2 error of the approximation is minimized from a one dimensional analysis. Numerical validations of the constructed pseudospectral penalty formulation are performed. The results, indeed, show that the present penalty scheme computes more accurate solutions than the traditional pseudospectral formulation does. However, due to the involved mathematical difficulties we are unable to directly conduct an analysis to determine values of the penalty parameters for multidimensional problems. Nevertheless, it is found from extensive numerical experiments that the penalty parameters obtained from one dimensional analysis seem to remain applicable for constant coefficient problems in multidimensional spaces. For more complicated problems such as variable coefficient problems, further investigation on the optimal penalty parameters is worthy to be explored. Comparing our results chiefly with Shen [21], Ehrenstein and Peyret [4] and Haidvogel and Zang [9], we observe that the accuracy of the present method can be as good as the Chebyshev Galerkin method [21], considered as the most accurate method for the problem. Considered as an advantage the scheme is very easy to implement. In the traditional method with boundary conditions enforced strongly, one needs to use the boundary conditions to algebraically eliminate collocated field values at boundary points in the discretized Poisson equations. This can be complicated if Neumann and Robin boundary conditions are involved. In the present method, the boundary conditions is directly appended to the discretized Poisson equations and, thus, makes the present method very easy to implement.

This paper is organized as follows. In Section 2 we present a Chebyshev pseudospectral penalty scheme for solving the model Poisson problem, and special attention is paid upon determining the values of the penalty parameters such that the approximation error is minimized. Section 3 is devoted to the generalization and the numerical validations of the pseudospectral penalty scheme for solving two and three dimensional Poisson equations. Concluding remarks are given in Section 4.

2. Model problem and pseudospectral penalty formulation

2.1. Poisson equations and boundary conditions

Consider $u(x)$ satisfying the Poisson equation subject to the boundary conditions of the form,

$$u''(x) = f(x), \quad x \in [-1, 1], \tag{1a}$$

$$\mathcal{B}_\pm u(\pm 1) = g_\pm, \quad \mathcal{B}_\pm = \alpha_\pm \pm \beta_\pm \frac{d}{dx}, \tag{1b}$$

where $\mathcal{B}_\pm$ are the boundary operators, α and β are non-negative real numbers, f is a specified function, and $g_\pm$ are given values.

Employing the pseudospectral Chebyshev method [15], we construct the numerical solution $v(x)$ as

$$v(x) = \sum_{j=0}^{N} l_j(x) v(x_j), \quad l_j(x) = \frac{(-1)^{N+j+1}(1-x^2)T'_N(x)}{c_j N^2 (x - x_j)}, \quad c_j = \begin{cases} 2 & \text{if } j = 0, N \\ 1 & \text{otherwise} \end{cases},$$

where N is a positive integer, $x_j = -\cos(j\pi/N)$ for $0 \leq j \leq N$ are the Gauss-Lobatto-Chebyshev points, $v(x_j)$ are the collocated field values approximating $u(x_j)$, and $l_j(x)$ are the Lagrange interpolating functions associated with the grid points. Notice that since $(1-x^2)T'(x) = C\prod_{i=0}^{N}(x - x_i)$ where C is a constant, the Lagrange interpolating functions satisfy the property $l_j(x_i) = \delta_{ij}$ where δ_{ij} is the usual Kronecker delta function.

To solve Eq. (1) we require $v(x)$ to satisfy the collocation equations

$$v''(x_0) = f(x_0) + \tau_-(\alpha_- v(x_0) - \beta_- v'(x_0) - g_-), \tag{2a}$$

$$v''(x_i) = f(x_i), \quad i = 1, 2, ..., N-1, \tag{2b}$$

$$v''(x_N) = f(x_N) + \tau_+(\alpha_+ v(x_N) + \beta_+ v'(x_N) - g_+), \tag{2c}$$

where $\tau_\pm$ are parameters with values depending the type of the imposed boundary conditions. Notice that for a given N if the values of the penalty parameters approach positive and negative infinity, then Eq. (2a) and Eq. (2c) recover the strongly enforced boundary conditions in the following sense:

$$\alpha_- v(x_0) - \beta_- v'(x_0) - g_- = (v''(x_0) - f(x_0))/\tau_- \to 0,$$

$$\alpha_+ v(x_N) + \beta_+ v'(x_N) - g_+ = (v''(x_N) - f(x_N))/\tau_+ \to 0.$$

An important issue concerning the use of penalty boundary conditions is how to determine the values of these penalty parameters $\tau_\pm$ as the degree of the approximation polynomial N increases. This is the main theme of this study and the details are presented next.

2.2. Error minimizer

Consider the model equation

$$u''(x) = -16\pi^2 \sin(4\pi x) \tag{3}$$

subject to following sets of boundary conditions:

Case (A), Dirichlet boundary conditions at $x = \pm 1$,

$$u(\pm 1) = 0. \tag{4}$$

Case (B), Robin boundary conditions at $x = \pm 1$,

$$u(\pm 1) \pm u'(\pm 1) = 4\pi. \tag{5}$$

Case (C), Dirichlet Boundary condition at $x = -1$ and Neumann boundary condition at $x = 1$

$$u(-1) = 0, \quad u'(1) = 4\pi. \tag{6}$$

Case (D), Neumann boundary condition at $x = -1$ and Robin boundary condition at $x = 1$

$$u'(-1) = 4\pi, \quad u(1) + u'(1) = 4\pi. \tag{7}$$

Case (E), Robin boundary condition at $x = -1$ and Dirichlet boundary condition at $x = 1$

$$u(-1) - u'(-1) = -4\pi, \quad u(1) = 0. \tag{8}$$

The exact solutions to all cases are $u = \sin(4\pi x)$.

We first investigate the error behavior of numerical solutions obtained by the present method as the values of the penalty parameters vary. The model equation subject to boundary conditions Case (A) and Case (B) are solved by the scheme Eq. (2). Since for each case the boundary conditions imposed at $x = \pm 1$ are of the same type, we simply take $\tau_+ = \tau_- = \tau \in (-\infty, 0) \cup (0, \infty)$. We define the approximation error as

$$R(\tau_+, \tau_-) = \left(\frac{\pi}{N} \sum_{i=0}^{N} \frac{(u(x_i) - v(x_i))^2}{c_i} \right)^{1/2}.$$

In Fig. 1 we plot R as a function of τ. It is clearly shown that in each case there exists $\tau = \tau_c$ which minimizes the error. For the Dirichlet case it is found that $\tau_c < 0$ and for the Robin case it is found that $\tau_c > 0$. Depending on the type of the imposed boundary condition, the error behavior is also quite different. For the Dirichlet case the minimum error occurring at τ_c is slightly smaller than the error as $\tau \to \pm\infty$. However, for the Robin case we observe that the error occurring at $\tau = \tau_c$ is less than the error as $\tau \to \pm\infty$, at least by two order in magnitude. This indicates that if the value of τ can be properly chosen then the numerical solution computed by the penalty scheme will have better accuracy than the solution

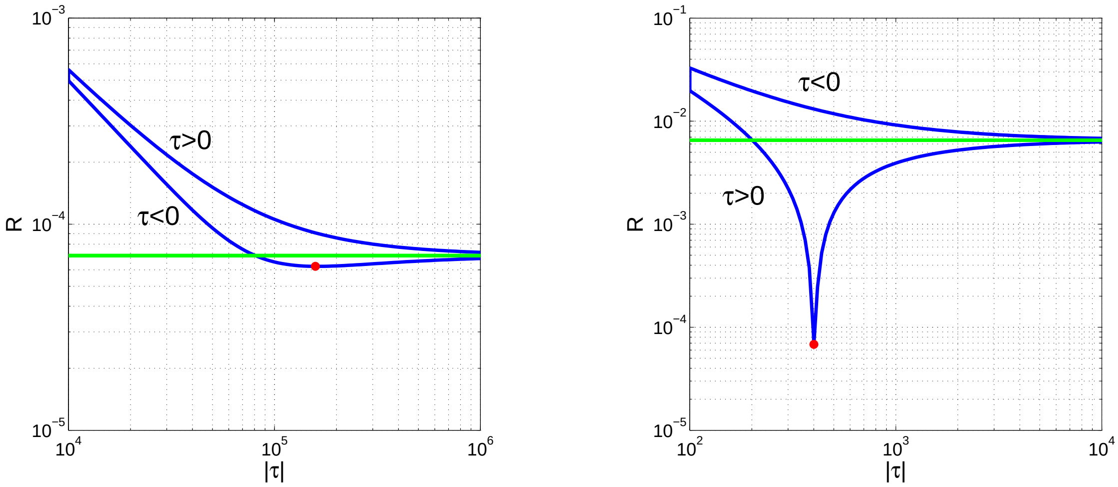

Figure 1: Error as a function of $\tau_- = \tau_+ = \tau$. Left: Eq. (3) subject to boundary conditions Case (A), Eq. (4). Right: Eq. (3) subject to boundary conditions Case (B), Eq. (5). Red dots: errors corresponding to the penalty parameters determined by Eq. (13). Green line: error corresponding to $|\tau| \to \infty$ (boundary conditions enforced strongly). $N = 16$.

obtained by the traditional pseudospectral scheme with boundary conditions enforced strongly. A question is immediately raised. Can we determined the value of τ in the penalty scheme from the prescribed data stated in a Poisson problem, such that the approximation error is minimized? We answer this question in the following analysis.

Following the error minimizing approach shown in [5] we determine the values of the penalty parameters through minimizing the difference between the numerical solution v satisfying Eq. (2) and the exact solution satisfying the interpolated continuous problem on the grid points, i.e.,

$$u''(x_i) = f(x_i), \tag{9a}$$

$$\mathcal{B}_\pm u(\pm 1) = g_\pm \tag{9b}$$

Notice that $u(x)$ in Eq. (9), $v(x)$ in Eq. (2), and $f(x)$ in both equations are polynomials of degree at most N. If the degree of $f(x)$ is at most $N-2$ then $v(x) = u(x)$ though out the whole domain. If the degree of the polynomial f is greater than $N-2$ then f can be expressed as

$$f(x) = A_- f_-(x) + A_+ f_+(x) + P_{N-2}(x), \quad f_\pm(x) = \frac{(1 \pm x)T_N'(x)}{2N^2},$$

where $A_\pm$ are constants and $P_{N-2}(x)$ is a polynomial of degree $N-2$. Therefore, we can consider $u = u_1 + u_2$ where u_1 and u_2 satisfy

$$u_1'' = A_- f_-(x) + A_+ f_+(x), \quad \mathcal{B}_\pm u_1(\pm 1) = 0,$$

$$u_2'' = P_{N-2}, \quad \mathcal{B}_\pm u_2(\pm 1) = g_\pm.$$

Because u_2 can be solved exactly by the pseudospectral penalty formulation, the error function R is attributed to numerically solving u_1. Thus, for error analysis it is sufficient to consider the problem with $f = A_- f_-(x) + A_+ f_+(x)$ in Eq. (9) subject to homogeneous boundary conditions $g_\pm = 0$.

Denote the solutions corresponding to $f = f_+$ and $f = f_-$ by $u = u_+$ and $u = u_-$, respectively. They are

$$\begin{aligned} u_\pm(x) =& \frac{T_{N+1}(x)}{4N^2(N+1)} - \frac{T_{N-1}(x)}{4N^2(N-1)} \pm \frac{T_{N+2}(x)}{8N(N+1)(N+2)} \pm \frac{T_N(x)}{4N^2(N^2-1)} \\ & \mp \frac{T_{N-2}(x)}{8N(N-1)(N-2)} + C_\pm T_1(x) + D_\pm T_0(x), \end{aligned} \tag{10}$$

where C_+, C_-, D_+ and D_- are determined by the boundary conditions, given as

$$C_+ = (\alpha_- G_+ - \alpha_+ H_+)/\gamma, \quad D_+ = ((\alpha_- + \beta_-)G_+ + (\alpha_+ + \beta_+)H_+)/\gamma,$$
$$C_- = (\alpha_- G_- - \alpha_+ H_-)/\gamma, \quad D_- = ((\alpha_- + \beta_-)G_- + (\alpha_+ + \beta_+)H_-)/\gamma,$$

with

$$\gamma = (\alpha_+ + \beta_+)\alpha_- + \alpha_+(\alpha_- + \beta_-),$$
$$G_+ = \frac{\alpha_+}{N^2(N^2-4)} - \frac{\beta_+(2N^2-1)}{2N^2(N^2-1)}, \quad G_- = -\frac{3\alpha_+}{N^2(N^2-1)(N^2-4)} + \frac{\beta_+}{2N^2(N^2-1)}, \tag{11a}$$
$$H_+ = -\frac{(-1)^{N-1}3\alpha_-}{N^2(N^2-1)(N^2-4)} + \frac{(-1)^{N-1}\beta_-}{2N^2(N^2-1)}, \quad H_- = \frac{(-1)^{N-1}\alpha_-}{N^2(N^2-4)} - \frac{(-1)^{N-1}\beta_-(2N^2-1)}{2N^2(N^2-1)}. \tag{11b}$$

For $f = f_\pm$ the corresponding numerical solutions $v = v_\pm(x)$ satisfying Eqs. (2a-c) are linear functions as

$$v_\pm(x;\tau_\pm) = [-\alpha_\mp T_1(x) \mp (\alpha_\mp + \beta_\mp)T_0(x)] \frac{(\pm 1)^N}{\gamma \tau_\pm}. \tag{12}$$

For $f = f_+$ and $f = f_-$ we define the error functions R_+ and R_-, respectively, as

$$R_\pm(\tau_\pm) = \left(\frac{\pi}{N} \sum_{i=0}^{N} \frac{A_\pm^2}{c_i} [u_\pm(x_i) - v_\pm(x_i;\tau_\pm)]^2 \right)^{1/2}.$$

The necessary condition for $\tau_\pm$ to minimize $R_\pm$ is the vanishing of $\partial R_\pm/\partial \tau_\pm$, leading to following equations

$$\sum_{i=0}^{N} \frac{1}{c_i} u_\pm(x_i) v_\pm(x_i;\tau_\pm) = \sum_{i=0}^{N} \frac{1}{c_i} v_\pm^2(x_i;\tau_\pm).$$

Substituting the expressions of $u_\pm$ and $v_\pm$, and employing the discrete orthogonal relationship of Chebyshev polynomials,

$$\sum_{l=0}^{N} \frac{1}{c_l} T_j(x_l) T_k(x_l) = \frac{\delta_{jk} c_j N}{2},$$

we calculate the summations and obtain the parameters $\tau_\pm$ as

$$\tau_+ = \frac{-[\alpha_-^2 + 2(\alpha_- + \beta_-)^2]}{[\alpha_-^2 + 2(\alpha_- + \beta_-)^2]G_+ + [2(\alpha_- + \beta_-)(\alpha_+ + \beta_+) - \alpha_-\alpha_+]H_+}, \tag{13a}$$
$$\tau_- = \frac{(-1)^N[\alpha_+^2 + 2(\alpha_+ + \beta_+)^2]}{[2(\alpha_+ + \beta_+)(\alpha_- + \beta_-) - \alpha_+\alpha_-]G_- + [\alpha_+^2 + 2(\alpha_+ + \beta_+)^2]H_-}, \tag{13b}$$

where $G_\pm$ and $H_\pm$ are provided in Eqs. (11). For the Dirichlet and the Neumann boundary conditions, the penalty parameters can be deduced from Eq. (13) as follows:

Dirichlet boundary condition: $\alpha_\pm = 1$, $\beta_\pm = 0$,

$$\tau_+ = \tau_- = \begin{cases} -(N^2-1)(N^2-4) & \text{for } N \text{ even} \\ -(N^2-1)(N^2-4)(1-2/N^2)^{-1} & \text{for } N \text{ odd} \end{cases}$$

Neumann boundary condition: $\alpha_\pm = 0$, $\beta_\pm = 1$,

$$\tau_+ = \tau_- = \begin{cases} N^2-1 & \text{for } N \text{ even} \\ N^2 & \text{for } N \text{ odd} \end{cases}$$

Notice that in the above analysis the penalty parameters are derived based on minimizing the error functions R_+ and R_- rather than R. This does not cause any problem, because they are related by

$$R^2(\tau_+, \tau_-) \leq 2\left(R_+^2(\tau_+) + R_-^2(\tau_-)\right).$$

This argument is verified by numerical computations. In Fig. 1 the errors corresponding the error minimized penalty parameters are plotted as red dots. It is clearly shown that the penalty parameters provided by Eq. (13), indeed, leads to very accurate computational results.

Table 1 and Table 2 show the convergence results of the present method on solving Eq. (1) subject to Dirichlet boundary conditions imposed at both end points (Case (A)) and subject to Robin boundary conditions imposed at both end points (Case (B)). The L_2 and L_∞ errors are measured for computations with error minimized τ. For comparison, we also measure the L_2 and L_∞ errors of the solution obtained by the pseudospectral method with strongly enforced boundary conditions. It is shown that the present method is, indeed, better in accuracy. Moreover, we observe that for Robin boundary conditions enforced at the boundaries, the numerical solutions computed by the scheme with error minimized τ are much more accurate than those obtained by the scheme with boundary conditions enforced strongly.

As the penalty parameters vary, the error behavior of numerical solutions obtained by the present method on solving Eq. (1) subject to different types of boundary conditions (Case (C) and (D)) are also conducted. In Fig. 2 and Fig. 3 the L_2 errors are plotted as functions of the parameter τ_+ and τ_- for a fixed N. The L_2 errors corresponding to the error minimized penalty parameters τ_+ and τ_- are marked as red dots. It is shown that these red dots are located at the minimum of the error surfaces.

The convergence studies of the present method on solving Poisson equations involving different types of boundary conditions at boundaries (Case (C) and (D)), are presented in Table 3-5. The results show that for each N the error of the numerical solutions computed by the present error minimized scheme is at least one order of magnitude less than that of the solutions obtained by the scheme with strongly enforced boundary conditions.

Table 1: Convergent tests of the problem, Eq. (3) subject to boundary conditions Case (A), Eq. (6).

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	5.8633e-03	4.8134e-03	6.1393e-03	5.6150e-03
20	6.2430e-05	4.6928e-05	7.0416e-05	6.2465e-05
24	3.2081e-07	2.2365e-07	3.8433e-07	3.4827e-07
28	8.7487e-10	5.9210e-10	1.0927e-09	1.0446e-09
32	1.3760e-12	9.6856e-13	1.7426e-12	1.7695e-12

Table 2: Convergent tests of the problem, Eq. (3) subject to boundary conditions Case (B), Eq. (7).

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	6.1901e-03	5.6880e-03	2.3737e-01	1.9079e-01
20	6.8103e-05	5.9442e-05	6.5479e-03	5.2502e-03
24	3.5437e-07	3.0959e-07	6.1006e-05	4.8855e-05
28	9.6978e-10	8.6371e-10	2.5653e-07	2.0521e-07
32	1.4800e-12	1.3511e-12	5.6771e-10	4.5389e-10

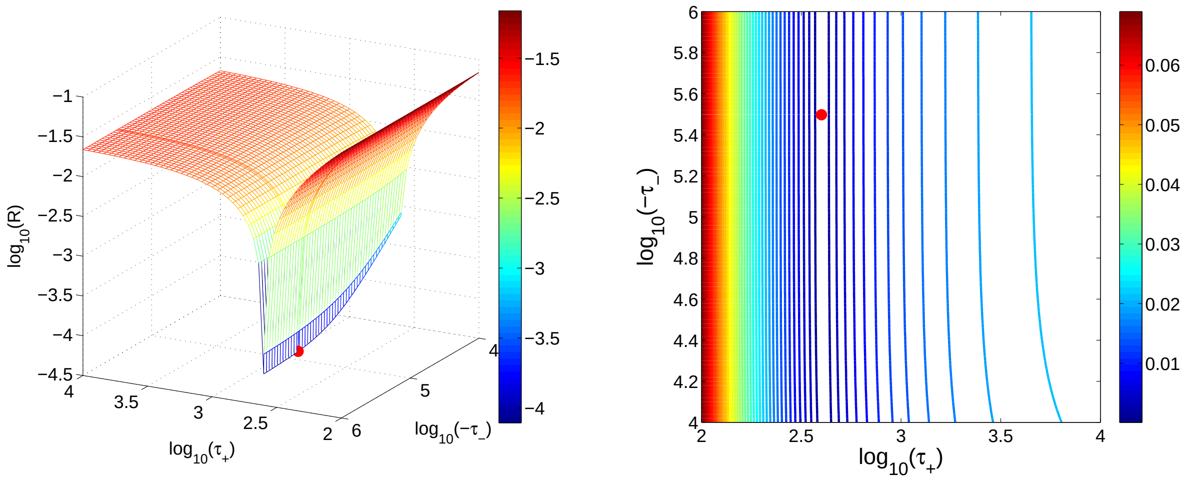

Figure 2: Surface (left) and contour (right) plots of the L_2 error ($R(\tau_+, \tau_-)$) of the numerical solution obtained by the penalty scheme on solving Eq. (3) subject to boundary conditions Case (C). The error corresponding to the error minimized penalty parameters is marked as a red dot. $N = 16$.

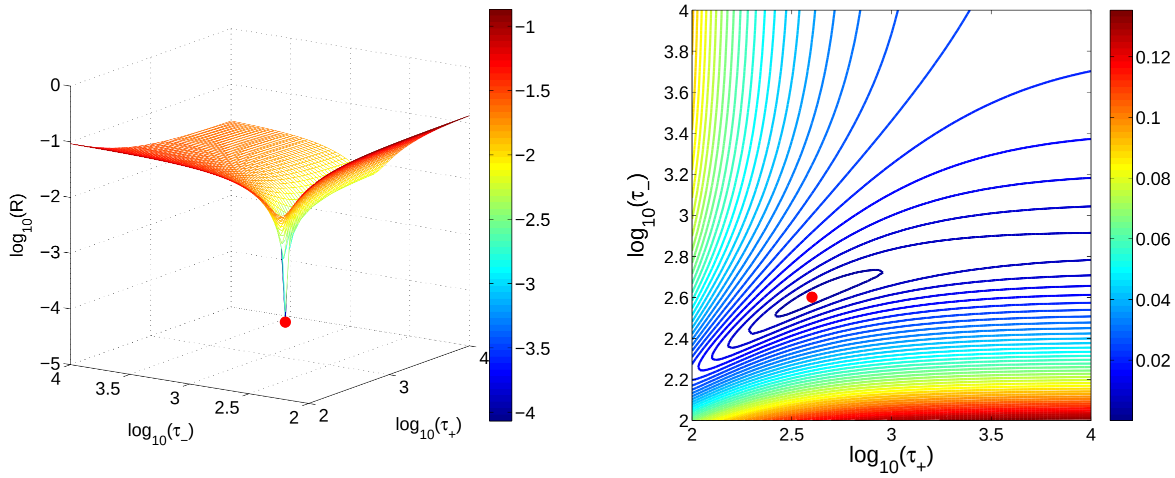

Figure 3: Surface (left) and contour (right) plots of the L_2 error ($R(\tau_+, \tau_-)$) of the numerical solution obtained by the penalty scheme on solving Eq. (3) subject to boundary conditions Case (D). The error corresponding to the error minimized penalty parameters is marked as a red dot. $N = 16$.

3. Generalization of the method

In this section we present a direct Poisson solver based on the pseudospectral penalty and the matrix diagonalization methods for problems defined on a rectangular domain.

3.1. Direct solver for Poisson equations in 3D

Consider the Poisson equation

$$\nabla^2 u(x, y, z) = f(x, y, z), \quad (x, y, z) \in [-1, 1] \times [-1, 1] \times [-1, 1], \tag{14}$$

Table 3: Convergent test of the problem, Eq. (1) subject to boundary conditions Case (C), Eq. (6).

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	7.5861e-03	8.2458e-03	8.2730e-01	7.6315e-01
20	8.4171e-05	8.9049e-05	2.2776e-02	2.1001e-02
24	4.2298e-07	4.4719e-07	2.1196e-04	1.9540e-04
28	1.1169e-09	1.2001e-09	8.9051e-07	8.2080e-07
32	1.5770e-12	1.6215e-12	1.9692e-09	1.8149e-09

Table 4: Convergent test of the problem, Eq. (1) subject to boundary conditions Case (D), Eq. (7).

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	7.7124e-03	8.3458e-03	8.2730e-01	7.6315e-01
20	8.7012e-05	9.1708e-05	2.2776e-02	2.1001e-02
24	4.4364e-07	4.7063e-07	2.1189e-04	1.9534e-04
28	1.1853e-09	1.2869e-09	8.9054e-07	8.2082e-07
32	1.7921e-12	1.9433e-12	1.9697e-09	1.8153e-09

Table 5: Convergent test of the problem, Eq. (1) subject to boundary conditions Case (E), Eq. (8).

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	6.1177e-03	6.0597e-03	2.7512e-01	2.5438e-01
20	6.6056e-05	6.1317e-05	7.5796e-03	7.0003e-03
24	3.3923e-07	3.0780e-07	7.0574e-05	6.5133e-05
28	9.2113e-10	8.3299e-10	2.9660e-07	2.7361e-07
32	1.4328e-12	1.3012e-12	6.5625e-10	6.0519e-10

subject to the boundary conditions

$$\mathcal{B}^x_\pm u(\pm 1, y, z) = g^x_\pm(y, z), \quad \mathcal{B}^x_\pm = \alpha^x_\pm \pm \beta^x_\pm \partial_x, \tag{15a}$$

$$\mathcal{B}^y_\pm u(x, \pm 1, z) = g^y_\pm(x, z), \quad \mathcal{B}^y_\pm = \alpha^y_\pm \pm \beta^y_\pm \partial_y, \tag{15b}$$

$$\mathcal{B}^z_\pm u(x, y, \pm 1) = g^z_\pm(x, y), \quad \mathcal{B}^z_\pm = \alpha^z_\pm \pm \beta^z_\pm \partial_z, \tag{15c}$$

where ∇^2 is the Laplace operators, $\mathcal{B}^x_\pm$, $\mathcal{B}^y_\pm$ and $\mathcal{B}^z_\pm$ are boundary operators acting on the boundary surfaces $x = \pm 1$ $y = \pm 1$ and $z = \pm 1$ respectively, $\alpha^\nu_\pm$ and $\beta^\nu_\pm$ for $\nu = x, y, z$ are parameters characterizing the imposed boundary conditions at the surfaces, and ∂_ν is the partial derivative with respect to the variable ν.

To solve Eq. (14), we introduce the three dimensional grid points

$$(x_i, y_j, z_k) = -\left(\cos\left(\frac{i\pi}{N_x}\right), \cos\left(\frac{j\pi}{N_y}\right), \cos\left(\frac{k\pi}{N_z}\right)\right), \quad 0 \le i/j/k \le N_x/N_y/N_z.$$

The associated three dimensional Lagrange interpolating functions $L_{i,j,k}(x, y, z)$ are constructed as

$$L_{i,j,k}(x, y, z) = l^x_i(x) l^y_j(y) l^z_k(z),$$

where $l_i^x(x)$, $l_j^y(y)$ and $l_k^z(z)$ are the one dimension Lagrange interpolating functions based on the grid points x_i, y_j and z_k, respectively. We construct the numerical solution v as

$$v(x,y,z)=\sum_{k=0}^{N_z}\sum_{j=0}^{N_y}\sum_{i=0}^{N_x}L_{i,j,k}(x,y,z)v_{i,j,k}$$

satisfying the penalty scheme

$$\begin{aligned}\nabla^2 v_{i,j,k}=&f_{i,j,k}+\tau_-^x\delta_{0i}\left(\mathcal{B}_-^x v_{0,j,k}-g_-^x(y_j,z_k)\right)+\tau_+^x\delta_{N_xi}\left(\mathcal{B}_+^x v_{N_x,j,k}-g_+^x(y_j,z_k)\right)\\&+\tau_-^y\delta_{0j}\left(\mathcal{B}_-^y v_{i,0,k}-g_-^y(x_i,z_k)\right)+\tau_+^y\delta_{N_yi}\left(\mathcal{B}_+^y v_{i,Ny,k}-g_+^y(x_i,z_k)\right)\\&+\tau_-^z\delta_{0k}\left(\mathcal{B}_-^z v_{i,j,0}-g_-^z(x_i,y_j)\right)+\tau_+^z\delta_{N_zk}\left(\mathcal{B}_+^z v_{i,j,N_z}-g_+^x(x_i,y_j)\right)\end{aligned}\tag{16}$$

where $f_{i,j,k}=f(x_i,y_j,z_k)$. The scheme can be expressed as

$$\sum_{r=0}^{N_x}A_{i,r}v_{r,j,k}+\sum_{s=0}^{N_y}B_{j,s}v_{i,s,k}+\sum_{t=0}^{N_z}C_{k,t}v_{i,j,t}=F_{i,j,k}\tag{17}$$

where

$$A_{i,r}=\frac{d^2l_r^x(x_i)}{dx^2}-\tau_-^x\delta_{0,i}\left(\alpha_-^x+\beta_-^x\frac{dl_r^x(x_i)}{dx}\right)-\tau_+^x\delta_{N_x,i}\left(\alpha_+^x+\beta_+^x\frac{dl_r^x(x_i)}{dx}\right),\quad 0\le i,r\le N_x,\tag{18a}$$

$$B_{j,s}=\frac{d^2l_s^y(y_j)}{dy^2}-\tau_-^y\delta_{0,j}\left(\alpha_-^y+\beta_-^y\frac{dl_s^y(y_j)}{dy}\right)-\tau_+^y\delta_{N_y,j}\left(\alpha_+^y+\beta_+^y\frac{dl_s^y(y_j)}{dy}\right),\quad 0\le j,s\le N_y,\tag{18b}$$

$$C_{k,t}=\frac{d^2l_t^z(z_k)}{dz^2}-\tau_-^z\delta_{0,k}\left(\alpha_-^z+\beta_-^z\frac{dl_t^z(z_k)}{dz}\right)-\tau_+^z\delta_{N_z,k}\left(\alpha_+^z+\beta_+^z\frac{dl_t^z(z_k)}{dz}\right),\quad 0\le k,t\le N_z,\tag{18c}$$

$$\begin{aligned}F_{i,j,k}=&f_{i,j,k}-\tau_-^x\delta_{0,i}g_-^x(y_j,z_k)-\tau_+^x\delta_{N_x,i}g_+^x(y_j,z_k)-\tau_-^y\delta_{0,j}g_-^y(x_i,z_k)-\tau_+^y\delta_{N_y,j}g_+^y(x_i,z_k)\\&-\tau_-^z\delta_{0k}g_-^z(x_i,y_j)-\tau_+^z\delta_{N_zk}g_+^x(x_i,y_j).\end{aligned}\tag{18d}$$

Let $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ be the matrices with entries as $A_{i,r}$, $B_{j,s}$ and $C_{k,t}$, respectively. Assume that the matrices $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ have the following transformation

$$\boldsymbol{A}=\boldsymbol{X}^{-1}\boldsymbol{\Lambda}^x\boldsymbol{X},\quad \boldsymbol{\Lambda}^x=\mathrm{diag}(\lambda_0^x,\lambda_1^x,...,\lambda_{N_x}^x),\tag{19a}$$

$$\boldsymbol{B}=\boldsymbol{Y}^{-1}\boldsymbol{\Lambda}^y\boldsymbol{Y},\quad \boldsymbol{\Lambda}^y=\mathrm{diag}(\lambda_0^y,\lambda_1^y,...,\lambda_{N_y}^y),\tag{19b}$$

$$\boldsymbol{C}=\boldsymbol{Z}^{-1}\boldsymbol{\Lambda}^z\boldsymbol{Z},\quad \boldsymbol{\Lambda}^z=\mathrm{diag}(\lambda_0^z,\lambda_1^z,...,\lambda_{N_z}^z),\tag{19c}$$

where λ_i^x, λ_j^y and λ_k^z are the eigenvalues of the matrices $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$, and $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{Z}$ are the eigenvector matrices of $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$, respectively. Then, we can first compute

$$\widetilde{F}_{r,s,t}=\frac{1}{\lambda_r^x+\lambda_s^y+\lambda_t^z}\sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\sum_{k=0}^{N_z}X_{r,i}^{-1}Y_{s,j}^{-1}Z_{t,k}^{-1}F_{i,j,k},\tag{20}$$

in which $X_{r,i}^{-1}$, $Y_{s,j}^{-1}$ and $Z_{t,k}^{-1}$ are matrix elements of $\boldsymbol{X}^{-1}$, $\boldsymbol{Y}^{-1}$ and $\boldsymbol{Z}^{-1}$, respectively. Then, numerical solution is computed as

$$v_{i,j,k}=\sum_{r=0}^{N_x}\sum_{s=0}^{N_y}\sum_{t=0}^{N_z}X_{i,r}Y_{j,s}Z_{k,t}\widetilde{F}_{r,s,t},\tag{21}$$

with $X_{i,r}$, $Y_{j,s}$ and $Z_{k,t}$ being the matrix elements of $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{Z}$.

For the two dimensional problems

$$\nabla^2 u(x,y) = f(x,y), \quad (x,y) \in [-1,1]\times[-1,1],$$
$$\mathcal{B}^x_{\pm} u(\pm 1, y) = g^x_{\pm}(y), \quad \mathcal{B}^x_{\pm} = \alpha^x_{\pm} \pm \beta^x_{\pm}\partial_x,$$
$$\mathcal{B}^y_{\pm} u(x, \pm 1) = g^y_{\pm}(x), \quad \mathcal{B}^y_{\pm} = \alpha^y_{\pm} \pm \beta^y_{\pm}\partial_y,$$

the scheme can be deduced from the above formulation as

$$F_{i,j} = f_{i,j} - \tau^x_{-}\delta_{0,i} g^x_{-}(y_j) - \tau^x_{+}\delta_{N_x,i} g^x_{+}(y_j) - \tau^y_{-}\delta_{0,j} g^y_{-}(x_i) - \tau^y_{+}\delta_{N_y,j} g^y_{+}(x_i),$$
$$\widetilde{F}_{r,s} = \frac{1}{\lambda^x_r + \lambda^y_s}\sum_{i=0}^{N_x}\sum_{j=0}^{N_y} X^{-1}_{r,i} Y^{-1}_{s,j} F_{i,j}, \quad v_{i,j} = \sum_{r=0}^{N_x}\sum_{s=0}^{N_y} X_{i,r} Y_{j,s} \widetilde{F}_{r,s}.$$

Unlike the one dimensional problem, we are unable to conduct a multidimensional analysis to determine the values of the penalty parameters. However, as we shall see later from the numerical results, adopting the penalty parameters obtained from the one dimensional analysis in the multidimensional schemes also computes error minimized results. This may be due to the fact that the 2D and 3D schemes are based on tensor product formulation which possibly preserve the error minimized property of the one-dimensional scheme. The theoretical issue may be worth to be analyzed in the future.

The matrix diagonalization method relies on the eigenvalue-eigenvector decomposition of the matrices $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ (see Eqs. (19a-c)). In this study we assume that the these matrices can be diagonalized based on the following results obtained by others. The eigenvalue spectra of these matrices, depending on the values of the penalty parameters and the imposed boundary conditions, have been investigated theoretically and numerically in several studies. For $|\tau_+| = |\tau_-| \to \infty$ the present formulation recovers the traditional method with boundary conditions enforced strongly. Gottlieb and Lustman [7] proved that the eigenvalues of the traditional method are distinct and negative, indicating that the matrices $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ can be diagonalized. For sufficiently large values of the penalty parameters, Funaro and Gottlieb [5] showed analytically that the non vanishing eigenvalues of these matrices, resulting from the penalty formulation with Neumann boundary conditions, are distinct and negative. Hesthaven and Gottlieb [11] mentioned that the eigenvalue spectra of these matrixes resulting from the penalty formulation remain distinct for a wide positive value range of these penalty parameters by numerical computations. In addition to these known results, we have also verified the assumption by conducting extensive computations of the eigenvalue spectra of these matrices for a wide value range of these penalty parameters, including negative values of the parameters. Our computations indicate that the eigenvalue spectra remain distinct. Thus, we are confident that this assumption is reasonable.

3.2. Numerical validations

We have conducted a series of numerical experiments to validate the present method. The results are present next.

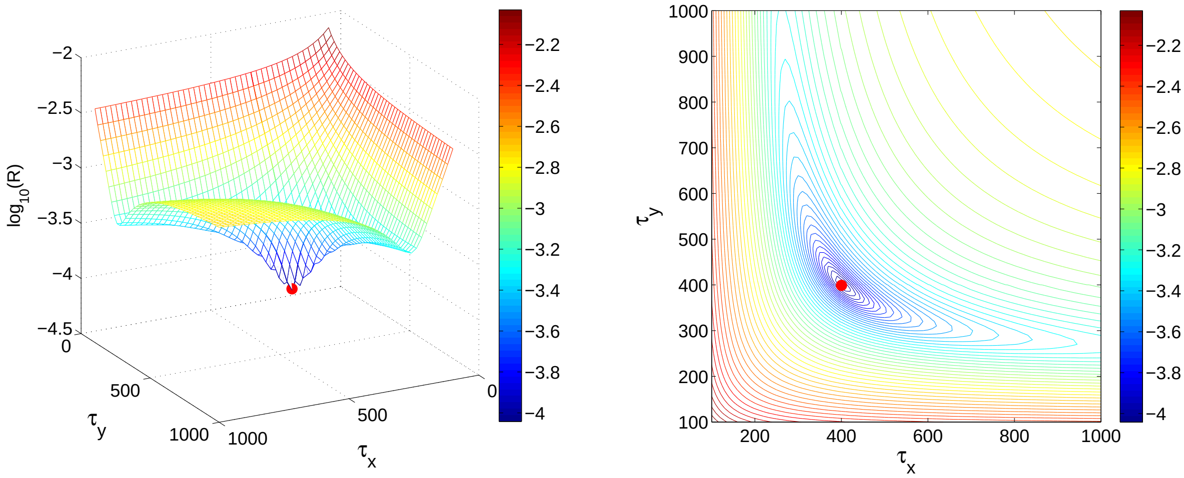

Figure 4: Surface and contour plots of $\log_{10}(L_2 \text{ error})$ as a function of the penalty parameters τ_x and τ_y for $N_x = N_y = 20$. Test problem: $u_{xx} + u_{yy} = -32\pi^2 \sin(4\pi x)\sin(4\pi y)$ subject to boundary conditions Case (A), Eq. (23).

3.2.1. 2D problem

Consider $u = \sin(4\pi x)\sin(4\pi y)$ satisfying the 2D Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -32\pi^2 \sin(4\pi x)\sin(4\pi y), \quad (x, y) \in [-1, 1] \times [-1, 1] \tag{22}$$

subject to the following boundary conditions:

Case (A),

$$u(\pm 1, y) \pm \frac{\partial u(\pm 1, y)}{\partial x} = \pm 4\pi \sin(4\pi y), \quad \frac{\partial u(x, \pm 1)}{\partial y} = 4\pi \sin(4\pi x) \tag{23}$$

Case (B),

$$u(\pm 1, y) = 0, \quad u(x, \pm 1) = 0, \tag{24}$$

Case (C),

$$u(-1, y) = 0, \quad \frac{\partial u(1, y)}{\partial x} = 4\pi \sin(4\pi y), \quad u(x, -1) = 0, \quad u(x, 1) + \frac{\partial u(x, 1)}{\partial y} = 4\pi \sin(4\pi x) \tag{25}$$

To investigate the error behavior as the penalty parameters vary, Eq. (22) subject to boundary conditions Case (A), is solved by the penalty scheme. Since along each coordinate direction the boundary conditions imposed at the two ends are of the same kind, we take $\tau^x_\pm = \tau_x$ and $\tau^y_\pm = \tau_y$. The error as function of τ_x and τ_y is demonstrated in Fig. 4, for $N = 20$. It is shown clearly that the error surface has a dip minimum, and the error corresponding to the error minimized penalty parameters τ_x and τ_y is at the dip. The results indicates that the error minimizing penalty parameter obtained from the 1D analysis remain valid for 2D problems.

Table 6: Convergence test of the 2D Poisson equation, Eq. (22), subject to boundary condition Case (A), Eq. (23).

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	7.7325e-03	5.2042e-03	1.0911e-01	9.3090e-02
20	9.1325e-05	6.8995e-05	3.0619e-03	2.5662e-03
24	4.9615e-07	3.8162e-07	2.8567e-05	2.3930e-05
28	2.2247e-12	1.9539e-12	2.6613e-10	2.2226e-10
32	7.3045e-14	9.4147e-14	1.9322e-14	2.3648e-14
48	4.0532e-14	5.5681e-14	5.9653e-14	7.2664e-14
64	8.7292e-14	6.6391e-14	1.0678e-13	1.2695e-13

Table 6 present the convergence studies of the error minimized scheme on solving the 2D Poisson equation subject to boundary conditions Case (A) as N increases. It is shown that the penalty scheme with error minimized penalty parameters indeed computes solutions with better accuracy before the error is driven down to the numerical noise level.

Table 7 presents the convergence study of the method on solving Eq. (22) subject to boundary conditions Case (B). This test problem has been used in many research works, and our results are compared to those obtained by other methods [4, 9, 21]. It is shown that the solution computed by the method is more accurate than that computed by the Chebyshev tau method [9]. Compared to the pseudospectral approximation with boundary conditions enforced strongly [4], we see that the present penalty scheme computes solutions with better accuracy, even at the numerical noise level. In addition, our results are as accurate as those obtained by the most accurate Chebyshev Galerkin method [21], for $N = 16$ and $N = 32$. For higher values of N it is observed that the present solution accuracy is limited to $\mathcal{O}(10^{-14})$ and can not be further improved by increasing N, indicating that the round-off error has affected the accuracy of the solution. On the other hand, the Chebyshev Galerkin method [21] which uses specially constructed bases, has better round-off error performance. This may be due to the boundary conditions are exactly satisfied in Galerkin method, while the boundary conditions are only approximately satisfied in current method.

Table 8 presents the convergence study of the method on solving Eq. (22) subject to boundary conditions Case (C). For this case the boundary conditions imposed at parallel sides are of different kinds. Compared to the traditional approach it is shown that the penalty scheme computes solutions with better accuracy.

Table 7: Convergence test of 2D Poisson equation, Eq. (22), subject to boundary conditions Case (B), Eq. (24). CT: Chebyshev Tau method [9]; CC: Chebyshev collocation method [4]; CG: Chebyshev Galerkin [21].

	present method		CT	CC	CG
N	L_2 error	L_∞ error	L_∞ error	L_∞ error	L_∞ error
16	6.89e-03	5.25e-03	3.33e-02	5.25e-03	5.22e-03
20	8.54e-05	6.26e-05		7.52e-05	
24	4.75e-07	3.76e-07	6.89e-06	4.05e-07	
32	2.17e-12	1.78e-12	4.77e-11	2.87e-12	2.17e-12
40	1.24e-14	2.05e-14		1.47e-12	
48	9.40e-15	1.03e-14	1.90e-12	3.63e-12	
64	3.15e-14	5.05e-14	8.67e-13	3.90e-12	6.11e-15

3.2.2. 3D problem

We give our final test example. Consider $u = \sin(4\pi x)\sin(4\pi y)\sin(4\pi z)$ satisfying the 3D Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = -48\pi^2 \sin(4\pi x)\sin(4\pi y)\sin(4\pi z), \quad (x, y) \in [-1, 1] \times [-1, 1] \times [-1, 1] \tag{26}$$

subject to the following boundary conditions:

$$u(\pm 1, y, z) = 0, \quad \frac{\partial u(1, y, z)}{\partial x} = 4\pi \sin(4\pi y)\sin(4\pi z) \tag{27a}$$

$$\frac{\partial u(x, -1, z)}{\partial y} = 4\pi \sin(4\pi x)\sin(4\pi z), \quad u(x, 1, z) + \frac{\partial u(x, 1, z)}{\partial y} = 4\pi \sin(4\pi x)\sin(4\pi z) \tag{27b}$$

$$u(x, y, -1) - \frac{\partial u(x, y, -1)}{\partial z} = -4\pi \sin(4\pi x)\sin(4\pi y), \quad \frac{\partial u(x, y, 1)}{\partial z} = 4\pi \sin(4\pi x)\sin(4\pi y) \tag{27c}$$

The problem is solved by the penalty scheme and the pseudospectral formulation with boundary condition enforced strongly. The convergence study is presented in Table 9. It is shown that the penalty scheme with the error minimized τ indeed computes more accurate approximations for $N < 32$. However, as $N \geq 32$ the system of equations becomes large we observe that the error can not be driven down due to the round off error.

3.3. Computational issues

As to computing efficiency, the asymptotic operation count for current method in 3D case based on Eqs. (20) and (21) is $2N_xN_yN_z(N_x + N_y + N_z)$, and its counterpart for 2D case is $2N_xN_y(N_x + N_y)$ [10]. Obviously, it is far superior to method expressing Laplace operator in tensor product. For an FFT-based method the asymptotic operation count is basically $2N_xN_yN_z(\log(N_x) + \log(N_y) + \log(N_z))$ for 3D

Table 8: Convergent test of 2D Poisson equation, Eq. (22) subject to boundary conditions Case (C), Eq. (25).

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	7.30e-03	5.28e-03	6.75e-02	1.00e-01
20	8.84e-05	6.75e-05	1.87e-03	2.75e-03
24	4.87e-07	3.80e-07	1.74e-05	2.57e-05
28	2.21e-12	1.93e-12	1.68e-10	2.43e-10
32	1.59e-14	1.94e-14	1.94e-11	2.25e-11
48	2.08e-14	2.74e-14	6.12e-11	8.92e-11
64	3.75e-14	4.24e-14	1.43e-11	3.31e-11

Table 9: Convergence test of the 3D problem, Eq. (26) subject to the boundary conditions Eq. (27)

	present method		strongly enforced BC	
N	L_2 error	L_∞ error	L_2 error	L_∞ error
16	9.0627e-03	5.4835e-03	4.5057e-02	5.6987e-02
20	1.1572e-04	8.7926e-05	1.3111e-03	1.6651e-03
24	6.5795e-07	5.0986e-07	1.2725e-05	1.5583e-05
28	3.0727e-12	2.6552e-12	1.2452e-10	1.4530e-10
32	2.0128e-14	2.8533e-14	1.1011e-14	1.3784e-14
48	2.5304e-14	3.2713e-14	1.5377e-14	1.5321e-14
64	8.4110e-14	1.1653e-13	3.0008e-14	3.7415e-14

case, and $2N_xN_y(\log(N_x) + \log(N_y))$ for 2D case. Indeed, our method which relies on extensive matrix-matrix multiplications is inferior to FFT-based methods in theory. However, this inferiority also depends on hardware. For moderate N_x, N_y, and N_z, it is not necessarily inferior in computers nowadays [3]. Of course, for large grid resolution, FFT-based methods remain the the best choice.

Not only the present penalty formulation has an advantage over the traditional pseudospectral method [4] in accuracy, it is also very easy to implement. In the traditional approach one needs to use the boundary conditions to algebraically eliminate the collocated field values at the boundary points in the discretized partial differential equations. For Dirichlet boundary conditions, the tradition approach can still be implemented easily. However, if Neumann or Robin boundary condition is involved, the eliminating procedure increases the complexity in coding. As we have seen the expression of the scheme in this section, the boundary conditions are directly appended to the discretized partial differential equations. This straightforward approach, thus, makes the penalty scheme very easy in coding.

We end this section by a brief discussion on applying the present formulation for discretizing the Laplace operator in heat equations. We want to emphasis that the proposed penalty formulation for the Laplace operator is for elliptic problems, not for parabolic ones. In fact, applying the present pseudospectral penalty Laplace operator for heat equations involving Dirichlet boundary conditions, will leads to unstable computations, because the matrix resulting from the present pseudospectral penalty discretization is not semi-negative definite. When Dirichlet boundary condition is involved it is found from numerical computations that all the eigenvalues of the discretized Laplace operator are distinct. However, there are two positive eigenvalues approaching positive infinity as N increases, and this is the origin of the instability. We have devised method to overcome this issue and will present it elsewhere due to the scope of this study.

4. Concluding remarks

We have presented a pseudospectral penalty direct solver for Poisson equations subject to general boundary conditions defined on rectangular domain. In the present formulation the values of the penalty parameter are chosen analytically such that the error is minimized. From numerical experiments the present method with error minimized parameters, indeed, computes solutions with better accuracy compared to those obtained by the traditional approach which strongly enforces boundary conditions. Since the present and the traditional pseudospectral methods are only different by the imposition of boundary conditions, the present formulation can be adopted easily into the traditional solver to improve the accuracy of Poisson solvers.

Compared to the modal expansion spectral methods, the pseudospectral method based on Lagrange interpolation basis offers more flexibility on solving partial differential equations with variable coefficients. With the use of the penalty methodology of imposing boundary conditions as shown in the present study, it is also possible to improve the accuracy of other pseudospectral direct Poisson solvers in polar and cylindrical coordinates with boundary conditions enforced strongly.

As mentioned in [5] the solution of a partial differential equation satisfies the equation arbitrary close to the boundary. Taking this argument into account, the penalty formulation which includes the discretized equations at the boundaries instead of discarding them, thus, yield numerical solutions with better accuracy, also as observed in the present results. This implicates that the penalty methodology can be a very promising approach to construct pseudospectral schemes with better accuracy for fourth order elliptic partial differential equations. For this type of equations four boundary conditions are specified. As a consequence, the traditional pseudospectral formulation with strongly enforced boundary conditions discards four discretized equations to make into a well determined system. With the use of the error minimized penalty method, these discarded equations can be included in the formulation to improve the accuracy of solutions. We hope to report this development in the near future.

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References

[1] H. Chen, Y. Su and B. D. Shizgal, A direct spectral collocation Poisson solver in polar and cylinder coordinates. J. Comput. Phys., 160 (2000) 453-469.

[2] H. Dang-Vu and C. Delcarte, An accurate solution of the Poisson equation by the Chebyshev Collocation method. J. Comput. Phys., 104 (1993) 211-220.

[3] W. S. Don and A. Solomonoff, Accuracy and speed in computing the Chebyshev collocation derivatives, SIAM J. Sci. Comput., 16 (1995) 1253-1268.

[4] U. Ehrenstein and R. Peyret, A Chebyshev Collocation method for the Navier-Stokes equations with application to double-diffusive convection, International Journal for numerical methods in fluids, 9 (1989) 427-452.

[5] D. Funaro and D. Gottlieb, A new method of imposing boundary conditions in pseudospectral approximations of hyperbolic equations, Math. Comp., 51 (1988) 599-613.

[6] D. Funaro and D. Gottlieb, Convergence results for pseudospectral approximations of hyperbolic systems by a penalty-type boundary treatment, Math. Comp. 57 (1991) 585-596.

[7] D. Gottlieb and L. Lustman, The spectrum of the Chebyshev collocation operator for the heat equation, SIAM J. Numer. Anal., 20 (1983) 909-921.

[8] D. Gottlieb and S. Orszag, Numerical Analysis of Spectral Methods: Theory and Applications, SIAM, Philadelphia, 1977.

[9] D. B. Haidvogel and T. Zang, The accurate solution of Poisson's equation by expansion in Chebyshev polynomials, J. Comput. Phys., 30 (1979) 167-180.

[10] P. Havdenwang, G. Labrosse and S. Abboudi, Chebyshev 3-D spectral and 2-D pseudospectral solvers for the Helmholtz equation, J. Comput. Phys., 55 (1984) 115-128.

[11] J. S. Hesthaven and D. Gottlieb, A stable penalty method for the compressible Navier–Stokes equations: I. open boundary contitions, SIAM J. Sci. Comput., 17 (1996) 579-612.

[12] J. S. Hesthaven, A stable penalty method for the compressible Navier–Stokes equations: III. multidimensional domain decomposition schemes, SIAM J. Sci. Comput., 20 (1999) 62-93.

[13] J. S. Hesthaven, Spectral penalty methods, Appl. Numer. Math., 33 (2000) 23-41.

[14] J. S. Hesthaven and T. Warburton, Nodal high-order methods on unstructured grids: I. time-domain solution of Maxwell's equations, J. Comput. Phys., 181 (2002) 186-221.

[15] J. S. Hesthaven, S. Gottlieb and D. Gottlieb, Spectral Methods for Time-Dependent Problems, Cambridge University Press, Cambridge UK, 2007.

[16] Y.-L. Huang, J.-G. Liu and W.-C. Wang, An FFT based fast Poisson solver on spherical shells, Commun. Comput. Phys., 9 (2011), 649-667.

[17] H. C. Ku, R. S. Hirsh and T. Taylor, A pseudospectral method for solution of the three-dimensional incompressible Navier-Stokes equations. J. Comput. Phys., 70 (1987) 493-462.

[18] C. Lanczos, Applied Analysis, Prentice-Hall, Englewood Cliffs, N.J., 1956.

[19] R. E. Lynch, J. R. Rice and D. H. Thomas, Direct solution of partial difference equations by tensor product methods, Numer: Math. 6 (1964) 185-199.

[20] M. C. Navarro, H. Herrero and S. Hoyas, Chebyshev collocation for optimal control in a thermoconvective flow, Commun. Comput. Phys., 5 (2009), 649-666.

[21] J. Shen, Efficient spectral-Galerkin method II. Direct solvers of second and fourth order equations by using Chebyshev polynomials. SIAM J. Sci. Comput., 16 (1995) 74-87.

[22] J. Shen and L.-L. Wang, Some recent advances on spectral methods for unbounded domains, Commun. Comput. Phys., 5 (2009), 195-241.