Fast direct solvers for Poisson equation on 2D polar and spherical geometries

Ming-Chih Lai*and Wei-Cheng Wang†

Abstract

A simple and efficient class of FFT-based fast direct solvers for Poisson equation on 2D polar and spherical geometries is presented. These solvers rely on the truncated Fourier series expansion, where the differential equations of the Fourier coefficients are solved by the second- and fourth-order finite difference discretizations. Using a grid by shifting half mesh away from the origin/poles, and incorporating with the symmetry constraint of Fourier coefficients, the coordinate singularities can be easily handled without pole condition. By manipulating the radial mesh width, three different boundary conditions for polar geometry including Dirichlet, Neumann and Robin conditions can be treated equally well. The new method only needs $O(MN \log_2 N)$ arithmetic operations for $M \times N$ grid points.

*Corresponding author. Department of Mathematics, Chung Cheng University, Minghsiung, Chiayi 621, Taiwan. E-mail: mclai@math.ccu.edu.tw

†Department of Mathematics, National Tsing Hua University, Hsinchu, Hsinchu 300, Taiwan.

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1 Introduction

Many physical problems involve solving the elliptic-type equation on cylindrical or spherical domains. It is convenient to rewrite the equation in polar or spherical coordinates. The first problem that has to be dealt with is the coordinate singularities caused by the transformation. The singularities occur at the origin of the polar domain, and at the north and south poles of the spherical domain. It is important to note that the occurrence of those singularities is due to the representation of the governing equation in those coordinates, the solution itself is regular if the right-hand side function and boundary value are smooth enough.

In order to have the desired regularity and accuracy, finite difference method [14, 17, 16], finite volume method [1], and pseudospectral method [4, 8, 15] need to impose appropriate conditions for the solution at the coordinate singularities. The accuracy of the numerical methods depend greatly on the choice of those pole conditions. In finite difference approach, the condition provides numerical boundary approximations at the poles. However, these pole conditions are artificial, there is no need to impose these conditions in Cartesian coordinate system.

In this paper, we develop a new class of FFT-based fast direct solvers for Poisson equation on 2D polar and spherical geometries. We use the truncated Fourier series expansion to derive a set of singular ordinary differential equations for the Fourier coefficients. By shifting the uniform grid half mesh off the origin/poles as described in [12, 7], we discretize the singular equations by finite difference methods. Incorporating with the symmetry constraint of Fourier coefficient, the coordinate singularities can be easily handled without imposing any pole condition. For spherical geometry, using centered difference and the symmetry constraint suffice to develop the second- and fourth-order accurate schemes. To implement the fourth-order scheme for polar geometry, additional one-sided difference approximations for derivatives are employed at the boundary. By manipulating the radial mesh width, three different boundary conditions for polar geometry including Dirichlet, Neumann and Robin conditions can be treated equally well. In both cases, the fourth-order scheme does not increase much extra computational costs.

The rest of the paper is organized as follows. In the next section, we derive the symmetry constraint for the Fourier coefficients of a function defined on polar and spherical geometries. In Section 3 and 4, we present the second- and fourth-order numerical schemes for Poisson equation on a disk and on a sphere, respectively. The numerical results are shown in Section 5 followed by some conclusions.

2 Symmetry constraint

Before we discuss how to discretize the governing equation in polar and spherical coordinates, it is interesting to know that the Fourier coefficients of a function in those coordinates satisfy the symmetry constraint [11]. Here, we review the derivation in [11] for polar coordinates, and then extend to the case of the spherical coordinates.

Let us first consider the transformation between Cartesian and polar coordinates as

$$x = r\cos\theta, \qquad y = r\sin\theta. \tag{1}$$

When we replace r by $-r$ and θ by $\theta+\pi$, the Cartesian coordinates of a point remains the same. Therefore, any scalar function $f(r,\theta)$ satisfies $f(-r,\theta) = f(r,\theta+\pi)$. Using this equality, we have

$$f(-r,\theta) = \sum_{n=-\infty}^{\infty} a_n(-r)\, e^{in\theta} = \sum_{n=-\infty}^{\infty} a_n(r)\, e^{in(\theta+\pi)} = \sum_{n=-\infty}^{\infty} (-1)^n\, a_n(r)\, e^{in\theta}.$$

Thus, when the domain of a function is extended to negative values of r, the nth Fourier coefficient of this function satisfies

$$a_n(-r) = (-1)^n a_n(r). \tag{2}$$

Similarly, we can consider the transformation between Cartesian and spherical coordinates as

$$x = \sin\phi\cos\theta, \quad y = \sin\phi\sin\theta, \quad z = \cos\phi. \tag{3}$$

Again, when we replace ϕ by $-\phi$ and θ by $\theta+\pi$, the Cartesian coordinates of a point on a unit sphere is unchanged. So, a scalar function $f(\phi,\theta)$ satisfies $f(-\phi,\theta) = f(\phi,\theta+\pi)$. Using the above equality, we have

$$f(-\phi,\theta) = \sum_{n=-\infty}^{\infty} a_n(-\phi)\, e^{in\theta} = \sum_{n=-\infty}^{\infty} a_n(\phi)\, e^{in(\theta+\pi)} = \sum_{n=-\infty}^{\infty} (-1)^n\, a_n(\phi)\, e^{in\theta}.$$

Thus, if we extend the domain of a function to negative values of ϕ, the nth Fourier coefficient satisfies

$$a_n(-\phi) = (-1)^n a_n(\phi). \tag{4}$$

The above derivation can also be applied to the case of replacing $\pi + \phi$ by $\pi - \phi$ and θ by $\theta + \pi$; thus, we have $f(\pi + \phi, \theta) = f(\pi - \phi, \theta + \pi)$. By extending the value of ϕ beyond π, the nth Fourier coefficient of $f(\pi + \phi, \theta)$ satisfies

$$a_n(\pi + \phi) = (-1)^n \, a_n(\pi - \phi). \tag{5}$$

In the following sections, we shall take advantage of these symmetry constraints to handle the coordinate singularities in numerical discretizations.

3 Fast Poisson solvers in polar coordinates

The Poisson equation on a unit disk can be written as

$$\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = f(r, \theta) \quad 0 < r < 1,\, 0 \le \theta < 2\pi, \tag{6}$$

with the Dirichlet boundary value $u(1, \theta) = g(\theta)$, Neumann boundary value $\frac{\partial u}{\partial r}(1, \theta) = g(\theta)$, or the mixed Robin boundary condition $\frac{\partial u}{\partial r}(1, \theta) + \alpha u(1, \theta) = g(\theta), \alpha > 0$.

For the Neumann problem to have a solution, it is necessary that f satisfies the compatibility condition,

$$\int_0^{2\pi} \int_0^1 f(r, \theta)\, r\, dr\, d\theta = \int_0^{2\pi} g(\theta)\, d\theta. \tag{7}$$

Both finite difference and spectral methods have been proposed in literature to solve Eq. (6) numerically. From the accuracy point of view, spectral methods are in general preferred for linear problems. When the solution is smooth, spectral method can achieve machine precision with relatively few grid points, provided the singularity at the origin is handled properly. However, in practical applications, fourth-order finite difference methods are in general comparable to, and sometimes outperform spectral methods when the solution is less smooth (see Table 4 and 5 below).

Another advantage of finite difference methods is their simplicity. For instance, they can handle various boundary conditions and nonuniform meshes quite easily. In applications such as the computation of Rayleigh-Bénard convection, the heat transfer at the boundary can range from Dirichlet (perfect conducting), Neumann (perfect insulating) to more general Robin type boundary conditions. The finite difference methods can treat all these boundary conditions equally well. In addition, to resolve the boundary layer, we want to place more grid points near the boundary. This is easily achieved by a change of variable in the radial direction. The resulting equation in the stretched variable can be solved with essentially the same cost and complexity in the finite difference setting.

As to the coordinate singularity at the origin, finite difference methods [14, 16, 6] and spectral methods [8, 15] need to to evaluate or to impose some condition of the solution at the origin. In finite difference approach, this pole condition is used to provide a numerical boundary value at the coordinate singularity, while in spectral or pseudospectral method, the pole condition is to capture the solution behavior accurately. Recently, the first author applied the second-order centered difference method to Eq. (6) on a grid which shifts half mesh in radial direction to avoid placing a grid point at the origin [10]. The resulting linear system is solved using the cyclic reduction algorithm [2] directly and there is no need to impose any pole condition in this setting.

In this paper, we combine the spectral and finite difference methods to develop a new class of fast direct solvers for Eq. (6). Our approach relies on the truncated Fourier series expansion, where the differential equations of Fourier coefficients are solved by the second- and fourth-order finite difference discretizations.

3.1 Fourier mode equations

Since the solution u on a disk is periodic in θ, we can approximate it by the truncated Fourier series as

$$u(r,\theta) = \sum_{n=-N/2}^{N/2-1} u_n(r)\, e^{in\theta}, \tag{8}$$

where $u_n(r)$ is the complex Fourier coefficient given by

$$u_n(r) = \frac{1}{N} \sum_{j=0}^{N-1} u(r,\theta_j)\, e^{-in\theta_j}, \tag{9}$$

and $\theta_j = 2j\pi/N$, and N is the number of grid points along a circle. The above transformation between the physical space and Fourier space can be efficiently performed using the fast Fourier transform (FFT) with $O(N \log_2 N)$ arithmetic operations.

Substituting those expansions into Eq. (6) and equating the Fourier coefficients, $u_n(r)$ satisfies the ordinary differential equation

$$\frac{d^2 u_n}{dr^2} + \frac{1}{r}\frac{du_n}{dr} - \frac{n^2}{r^2}\, u_n = f_n, \quad 0 < r < 1, \tag{10}$$

with the Dirichlet boundary condition $u_n(1) = g_n$, the Neumann boundary condition $u_n'(1) = g_n$, or the mixed Robin condition $u_n'(1) + \alpha u_n(1) = g_n, \alpha > 0$. Here, the complex Fourier coefficients $f_n(r)$ and g_n are defined in the same manner as Eqs. (8)-(9). Eq. (10) is a singular equation in which the singularity occurs at the origin $r = 0$.

So far, the approach is in common with the spectral or pseudospectral methods. Next, we will introduce both second- and fourth-order finite difference discretizations to solve Eq. (10) without imposing any pole condition. The resulting linear system has a banded diagonal coefficient matrix. The inversion takes only $O(M)$ operations, where M is the number of the discretization points. The implementation of the present scheme is much simpler compared to the spectral methods [4, 8] which involve the fast cosine transform of $O(M \log_2 M)$ operations.

3.2 Second-order method

Using a grid described in [12, 10] to avoid evaluating the value at the origin, we place the grid points at

$$r_i = (i - 1/2)\,\Delta r, \qquad i = 1, 2, \ldots M, M+1, \tag{11}$$

where the mesh width Δr will be specified later. From now on, we denote the discrete values $U_i \approx u_n(r_i)$ and $F_i \approx f_n(r_i)$.

First, we introduce a second-order centered difference scheme for the solution of Eq. (10) with the Dirichlet boundary value $u_n(1) = g_n$. We choose the mesh width $\Delta r = 2/(2M+1)$ so that $r_{M+1} = 1$, and the grid points are defined at the boundary. Applying the centered difference method to Eq. (10), we obtain

$$\frac{U_{i+1} - 2\,U_i + U_{i-1}}{(\Delta r)^2} + \frac{1}{r_i}\frac{U_{i+1} - U_{i-1}}{2\,\Delta r} - \frac{n^2}{{r_i}^2}\,U_i = F_i. \tag{12}$$

This is a tridiagonal linear system of equations for $U_i, i = 1, 2, \ldots M$, which can be solved by $O(M)$ arithmetic operations. In order to complete the linear system, the numerical boundary values U_0 and U_{M+1} should be supplied. When $i = 1$, the coefficient of U_0 in Eq. (12) equals to zero since $r_1 = \Delta r/2$; thus, no approximation for U_0 is needed. The other value U_{M+1} is given by the boundary value g_n. Note that, in [9], the author used the same scheme as (12) on an uniform grid without shifting half mesh so that some approximation at the origin is needed. It turns out that the matrix of the linear system is not as succinct as the one obtained from our approach.

For the Neumann ($\alpha = 0$) or Robin boundary problem, we still use the same grid described in (11) but with different choice of $\Delta r = 1/M$. With the choice of this mesh width, the discrete values of u are defined midway between boundary so that the first derivative can be centered on the grid points. This means, at $r = 1$, we have the approximation

$$\frac{\partial u}{\partial r} + \alpha\, u \approx \frac{U_{M+1} - U_M}{\Delta r} + \alpha\, \frac{U_{M+1} + U_M}{2} = g_n. \tag{13}$$

Therefore, the numerical boundary value U_{M+1} can be obtained in terms of U_M and g_n.

It is worth mentioning that the existence and uniqueness of the solution to Poisson equation with Neumann boundary can be explained by considering the zeroth Fourier mode equation

$$\frac{d^2 u_0}{dr^2} + \frac{1}{r}\frac{du_0}{dr} = f_0, \quad 0 < r < 1, \qquad u_0'(1) = g_0. \tag{14}$$

It is obvious that if the solution of the above equation exists, it is unique up to a constant. The existence of the solution is guaranteed by

$$\int_0^1 f_0(r)\, r\, dr = g_0, \tag{15}$$

which is an equivalent form of Eq. (7). The discrete analogue of (15) can be written as

$$\sum_{i=1}^{M} f_0(r_i)\, r_i\, \Delta r = g_0. \tag{16}$$

One should also note that the tridiagonal linear system resulting from the discretization of the zeroth Fourier mode equation is singular. If the discrete constraint (16) is satisfied, then the right-hand side vector falls into the range of the resulting matrix. Using Gauss elimination with pivoting, a zero pivot element is found for the last entry $i = M$ as well as the corresponding right-hand side of the zero pivot equation. The last element of the solution vector can be assigned to any value. This is the descrete analogue to the nonuniquess of the solution of the Neumann problem.

3.3 Fourth-order method

In this subsection, we use the same grid given in Eq. (11) with the choice of $\Delta r = 2/(2M+1)$. Before introducing the fourth-order scheme, we first write down the fourth-order five point difference operators for the first and second derivatives as

$$u'(r_i) = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\,\Delta r} + O((\Delta r)^4), \tag{17}$$

$$u''(r_i) = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12\,(\Delta r)^2} + O((\Delta r)^4). \tag{18}$$

The above approximations are defined at the interior points. For the boundary points, we use the following one-sided difference formulae given in [5]

$$u'(r_{M+1}) = \frac{3u_{M+2} + 10u_{M+1} - 18u_M + 6u_{M-1} - u_{M-2}}{12\,\Delta r} + O((\Delta r)^4), \tag{19}$$

$$u''(r_{M+1}) = \frac{11u_{M+2} - 20u_{M+1} + 6u_M + 4u_{M-1} - u_{M-2}}{12\,(\Delta r)^2} + O((\Delta r)^4). \tag{20}$$

Now let us discretize Equation (10) using the fourth-order difference operators given in (17)-(18) at the interior points $i = 1, 2, \ldots, M$ as

$$\frac{-U_{i+2} + 16U_{i+1} - 30U_i + 16U_{i-1} - U_{i-2}}{12\,(\Delta r)^2} + \frac{-U_{i+2} + 8U_{i+1} - 8U_{i-1} + U_{i-2}}{12\, r_i\, \Delta r} - \frac{n^2}{r_i^2} U_i = F_i. \quad (21)$$

This is a pentadiagonal system for U_i. Solving (21) is a little more expensive than solving a tridiagonal system, but it still needs only $O(M)$ arithmetic operations.

Again, in order to complete the system, we need to supply numerical boundary values such as U_{-1}, U_0, U_{M+1} and U_{M+2}. The inner numerical boundary values U_0, U_{-1} can be easily found by the symmetry constraint for polar coordinates in Section 2 as

$$U_0 \approx u_n(r_0) = u_n(-\Delta r/2) = (-1)^n\, u_n(\Delta r/2) \approx (-1)^n\, U_1, \quad (22)$$

$$U_{-1} \approx u_n(r_{-1}) = u_n(-3\,\Delta r/2) = (-1)^n\, u_n(3\,\Delta r/2) \approx (-1)^n\, U_2. \quad (23)$$

The outer numerical boundary value U_{M+2} can be obtained as follows. By requiring the equation (10) to be hold at the boundary $r_{M+1} = 1$ as well, we deduce

$$u_n''(r_{M+1}) + u_n'(r_{M+1}) = n^2\, u_n(r_{M+1}) + f_n(r_{M+1}). \quad (24)$$

Substituting the one-sided difference formulae (19)-(20) into the above equation, we obtain a formula for U_{M+2} in terms of $U_{M+1}, U_M, U_{M-1}, U_{M-2}$ and F_{M+1}. For the Dirichlet problem, the value U_{M+1} is known. As to the Neumann or Robin boundary, an approximation of U_{M+1} can be derived using the one-sided difference formula (19).

Let us close this section by summarizing the algorithm and the operation counts in the following three steps:

1. Compute the Fourier coefficients for the right-hand side function as in (9) by FFT, which requires $O(MN\log_2 N)$ arithmetic operations.

2. Solve the tridiagonal (2nd-order) or pentadiagonal (4th-order) linear system for each Fourier mode. This requires $O(MN)$ operations.

3. Convert the Fourier coefficients as in (8) by FFT to obtain the solution, which requires $O(MN\log_2 N)$ operations.

The overall operation count is thus $O(MN\log_2 N)$ for $M \times N$ grid points. The method can be easily extended to the Helmholtz-type equation in a straightforward manner.

4 Fast Poisson solvers in spherical coordinates

The solution of elliptic equation on spherical geometry has many applications in the areas of meteorology, geophysics, and astrophysics. The Poisson equation on the surface of a unit sphere can be written as

$$\frac{1}{\sin\phi}\frac{\partial}{\partial\phi}\left(\sin\phi\frac{\partial u}{\partial\phi}\right) + \frac{1}{\sin^2\phi}\frac{\partial^2 u}{\partial\theta^2} = f(\phi,\theta), \tag{25}$$

where $0 \le \phi \le \pi$ represents the colatitude, and $0 \le \theta < 2\pi$ represents the longitude. In order that Eq. (25) has a solution on the sphere, the right-hand side function f must satisfy the compatibility condition,

$$\int_0^{\pi}\int_0^{2\pi} f(\phi,\theta)\,\sin\phi\,d\theta\,d\phi = 0. \tag{26}$$

This can be easily derived by integrating Eq. (25) over the sphere. Moreover, the solution is unique only up to a constant.

It is obvious that Eq. (25) has both singularities at the north ($\phi = 0$) and south poles ($\phi = \pi$). Finite difference method [17] and finite volume method [1] handle those singularities by calculating approximations at poles using the values of f, then solve the resulting linear equations by Fourier method [17] or multigrid method [1]. In [13], Moorthi and Higgins used the second-order centered difference method to solve Eq. (29) below. They imposed pole conditions similar to the ones derived in [1]. Spectral methods [3, 19] solve Eq. (29) using the truncated sine and cosine expansion [18] for u_n, either with [19] or without pole condition [3]. These methods require $O(M \log_2 M)$ operations, where M is the number of the discretization points.

In the following subsections, we shall present the second- and fourth-order centered difference methods for the solution of Eq. (29). The method needs only $O(M)$ operations without imposing any pole condition. The approach is very similar to the finite difference scheme for polar coordinates system introduced in Section 3. Namely, we shift the uniform grid half mesh away from the poles and use the symmetry constraint. The resulting scheme share the same advantages as the polar coordinates case: they are efficient, easy to implement and sufficiently accurate.

4.1 Fourier mode equations

As the polar coordinates case in Section 3, we approximate u by the truncated Fourier series as

$$u(\phi, \theta) = \sum_{n=-N/2}^{N/2-1} u_n(\phi)\, e^{in\theta}, \tag{27}$$

where $u_n(\phi)$ is the complex Fourier coefficient given by

$$u_n(\phi) = \frac{1}{N} \sum_{j=0}^{N-1} u(\phi, \theta_j)\, e^{-in\theta_j}, \tag{28}$$

and $\theta_j = 2j\pi/N$, and N is the number of grid points along a latitude circle. The expansion for the function f can be written in the same way. Substituting these expansions into Eq. (25) and equating the Fourier coefficients, $u_n(\phi)$ satisfies

$$\frac{d^2 u_n}{d\phi^2} + \cot\phi \, \frac{du_n}{d\phi} - \frac{n^2}{\sin^2\phi}\, u_n = f_n(\phi), \quad 0 \le \phi \le \pi. \tag{29}$$

The above equation is a singular ordinary differential equation with singularities at $\phi = 0, \pi$.

4.2 Second- and fourth-order numerical methods

Using a grid described in [7] with the grid points

$$\phi_i = (i - 1/2)\, \Delta\phi, \qquad i = 1, \dots M \tag{30}$$

and $\Delta\phi = \pi/M$, we avoid putting grid points directly at the poles; thus, hopefully no pole condition is needed. Let us denote the discrete values by $U_i \approx u_n(\phi_i)$ and $F_i \approx f_n(\phi_i)$. Applying the centered difference method to Eq. (29), we have

$$\frac{U_{i+1} - 2\,U_i + U_{i-1}}{(\Delta\phi)^2} + (\cot\phi_i)\frac{U_{i+1} - U_{i-1}}{2\,\Delta\phi} - \frac{n^2}{\sin^2\phi_i}\, U_i = F_i. \tag{31}$$

This is a tridiagonal linear system for U_i, which can be solved by Gaussian elimination with $O(M)$ arithmetic operations. As before, we should supply the numerical boundary values for U_0 and U_{M+1}. Using the symmetry constraints in Section 2, those values can be obtained by

$$U_0 \approx u_n(\phi_0) = u_n(-\Delta\phi/2) = (-1)^n\, u_n(\Delta\phi/2) \approx (-1)^n\, U_1, \tag{32}$$

$$U_{M+1} \approx u_n(\phi_{M+1}) = u_n(\pi + \Delta\phi/2) = (-1)^n\, u_n(\pi - \Delta\phi/2) \approx (-1)^n\, U_M. \tag{33}$$

Similarly, the fourth-order scheme can be written as

$$\frac{-U_{i+2} + 16U_{i+1} - 30U_i + 16U_{i-1} - U_{i-2}}{12\,(\Delta\phi)^2} + \cot\phi_i\, \frac{-U_{i+2} + 8U_{i+1} - 8U_{i-1} + U_{i-2}}{12\,\Delta\phi} - \frac{n^2}{\sin^2\phi_i} U_i = F_i. \tag{34}$$

This is a pentadiagonal system for U_i. Again, it can be solved directly by $O(M)$ arithmetic operations. To complete this system, the extra numerical boundary values U_{-1} and U_{M+2} need to be supplied. Those values are easily determined by the symmetry constraint as $U_{-1} = (-1)^n\, U_2$ and $U_{M+2} = (-1)^n\, U_{M-1}$.

The above linear system of the zeroth Fourier mode is singular, since the solution to

$$\frac{d^2 u_0}{d\phi^2} + \cot\phi\, \frac{du_0}{d\phi} = f_0(\phi), \quad 0 \le \phi \le \pi, \tag{35}$$

is unique up to a constant. The existence of the solution is guaranteed by

$$\int_0^\pi f_0(\phi)\, \sin\phi\, d\phi = 0, \tag{36}$$

which is an equivalent form of Eq. (26). One can also obtain Eq. (36) by multiplying Eq. (35) by $\sin\phi$, and integrating over the interval $[0, \pi]$. The discrete analogue of (36) reads

$$\sum_{i=1}^{M} f_0(\phi_i)\, \sin\phi_i\, \Delta\phi = 0. \tag{37}$$

A zero pivot element is found at the last entry $i = M$ when solving the above singular system using Gauss elimination. If the discrete constraint Eq. (37) is satisfied, the right-hand side of the zero pivot equation is zero as well. Therefore, the last element of the solution vector can be assigned to any value, in accordance with the fact that the solution of the Poisson equation (25) is not unique.

The operation count is the same as the polar coordinates case; that is, the above method will need just $O(MN\log_2 N)$ arithmetic operations for $M \times N$ grid points. Besides, the present methods can be easily extended to the Helmholtz-type equation on a sphere.

5 Numerical results

In this section, we perform several numerical tests for the second- and fourth-order schemes described in Section 3 and 4. Table 1 shows the maximum errors of the methods for three different solutions of Poisson equation with Dirichlet boundary condition on a disk. In all our tests, we use N grid points in the azimuthal direction and $N/2$ points in the radial direction. The rate of convergence is computed by the formula $\log_2(\frac{E_{N/2}}{E_N})$, where E_N is the maximum error with $N/2 \times N$ grid points. The result shows that the error for the fourth-order scheme is significantly smaller than the error for the second-order scheme (Typically $10^{-3} - 10^{-5}$ smaller in these examples). Super-convergence is observed in the 4th-order scheme for the first example where the exact solution is a cubic polynomial in r.

Table 2 and 3 show the maximum errors of the two methods for different solutions to Poisson equation with Neumann and Robin boundary conditions, respectively. We see that the schemes indeed have the desired order of accuracy for the Neumann and Robin boundary problems.

Table 4 shows the error comparison between the present fourth-order scheme with the spectral collocation method described in [4]. Here, we choose the same exact solutions to Dirichlet problem and quote the numerical results from Table VI in [4]. (Note that, in their table, the number N has a different meaning from the one used in this paper. They use N as the number of points in radial direction, but we use $N/2$ instead.) As expected, the error of the spectral method reaches machine precision with relatively few grid points for smooth solutions. However, when the solution is less regular, our fourth-order finite difference result has smaller errors than the result obtained by the method in [4].

Table 5 shows another error comparison of the solutions to Helmholtz equation $\Delta u - \lambda u = f$ with various parameter λ. The exact solution is $u = \cos(3r\cos\theta + 4r\sin\theta + 0.7)$, and the number of grid points used is $N = 16$. One can see the present fourth-order numerical errors are comparable with the errors obtained by the pseudospectral method [8], but are smaller than the ones obtained by [4], especially, when λ becomes larger.

Table 6 shows the maximum errors of the second- and fourth-order methods for different solutions of Poisson equation on a sphere. The number N is the number of grid points used in the longitude, while $N/2$ points used in the colatitude. Again, the results show that the error for fourth-order scheme is significantly smaller than the error for the second-order scheme.

Table 7 shows the maximum errors of the two methods for different solutions of a simple Helmholtz equation $\Delta u - u = f$ on a sphere. One can see second- and fourth-order convergence respectively in both Table 6 and 7.

6 Conclusions

In this paper, we have combined the spectral and finite difference methods to develop FFT-based fast direct solvers for Poisson equation on 2D polar and spherical geometries. The method first uses the truncated Fourier series expansion to derive a set of singular ODEs for the Fourier coefficients, then solves those singular equations by second- and fourth-order finite difference discretizations. Using an uniform grid by shifting half mesh away from the origin/poles, and incorporating with the derived symmetry constraint of Fourier coefficients, the coordinate singularities can be easily handled without pole condition. By manipulating the radial mesh width, three different boundary conditions for polar geometry including Dirichlet, Neumann and Robin conditions can be treated equally well. Both second- and fourth-order schemes only need $O(MN \log_2 N)$ arithmetic operations for $M \times N$ mesh points. Furthermore, the extension of the method to Helmholtz-type equation is straightforward.

It is also worth noting that the methods presented here is highly parallelizable. A fast Fourier transform is performed in the azimuthal direction on each concentric grid circle (the disk case) or colatitude (the sphere case). These transformations can be processed in parallel. The resulting banded diagonal system associated with different Fourier modes are decoupled from each other, thus can be inverted in parallel as well. The present method is also very easy to implement since many FFT subroutines are available. In forthcoming papers, we shall extend these schemes to three-dimensional geometries and apply them to the computation of Boussinesq equations and other fluid dynamical problems.

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$u = 1 + 3/4\, r\cos\theta + 1/4\, r^3\cos 3\theta$	N=32	64	128	256
2nd-order	4.416E-05	1.138E-05	2.891E-06	7.284E-07
rate	-	1.96	1.98	1.99
4th-order	2.220E-15	4.774E-15	1.688E-14	6.217E-14
$u = \sin(r\cos\theta)$				
2nd-order	7.501E-05	1.930E-05	4.896E-06	1.234E-06
rate	-	1.96	1.98	1.99
4th-order	4.807E-08	3.218E-09	2.085E-10	1.327E-11
rate	-	3.90	3.95	3.98
$u = e^{r(\cos\theta+\sin\theta)}$				
2nd-order	7.849E-04	2.024E-04	5.140E-05	1.295E-05
rate	-	1.96	1.98	1.99
4th-order	8.702E-07	5.948E-08	3.886E-09	2.485E-10
rate	-	3.87	3.94	3.97

Table 1: The maximum errors of different solutions to Poisson equation with Dirichlet boundary condition.

$u=\sin(r\cos\theta)$	N=32	64	128	256
2nd-order	1.087E-04	2.714E-05	6.782E-06	1.695E-06
rate	-	2.00	2.00	2.00
4th-order	1.999E-07	1.346E-08	8.724E-10	5.556E-11
rate	-	3.89	3.95	3.97
$u=\sin(r\cos\theta)\cos(r\sin\theta)$				
2nd-order	1.403E-04	3.497E-05	8.738E-06	2.184E-06
rate	-	2.00	2.00	2.00
4th-order	3.847E-07	2.460E-08	1.553E-09	9.746E-11
rate	-	3.97	3.98	3.99

Table 2: The maximum errors of different solutions to Poisson equation with Neumann boundary condition.

$u = \sin(r\cos\theta)$	N=32	64	128	256
2nd-order	1.359E-04	3.535E-05	9.010E-06	2.274E-06
rate	-	1.94	1.97	1.99
4th-order	1.062E-07	7.098E-09	4.586E-10	2.914E-11
rate	-	3.90	3.95	3.98
$u = e^{r(\cos\theta + \sin\theta)}$				
2nd-order	9.175E-04	2.476E-04	6.422E-05	1.635E-05
rate	-	1.89	1.95	1.97
4th-order	4.072E-06	2.885E-07	1.923E-08	1.242E-09
rate	-	3.82	3.91	3.95

Table 3: The maximum errors of different solutions to Poisson equation with Robin boundary condition $\frac{\partial u}{\partial n} + u = g$.

$u = \cos(7r\cos\theta + 8r\sin\theta + 0.7)$	N=16	32	64
4th-order	0.395	4.352E-03	2.901E-04
[4]	1.474	4.873E-04	7.994E-15
$u = r^3$	N=16	32	64
4th-order	1.096E-03	1.869E-04	2.941E-05
[4]	2.922E-02	4.223E-03	6.045E-04
$u = r^{2.5}$	N=16	32	64
4th-order	1.352E-02	3.195E-04	7.030E-05
[4]	7.677E-02	1.647E-02	3.438E-03

Table 4: Comparison of the present fourth-order method to Poisson equation with the spectral method in [4].

λ	4th-order	[4]	[8]
0	2.491E-03	2.457E-03	1.115E-03
1	2.266E-03	2.143E-03	1.106E-03
5	1.755E-03	4.497E-03	1.073E-03
10	1.446E-03	8.368E-03	1.034E-03
30	9.731E-04	2.139E-02	9.029E-04
100	6.725E-04	5.294E-02	6.284E-04

Table 5: Comparison of the present fourth-order method with the pseudospectral methods in [4, 8] for $\Delta u - \lambda u = f$ with of the exact solution $u = \cos(3r\cos\theta + 4r\sin\theta + 0.7)$ and $N = 16$.

$u = \sin\phi\,\cos\theta$	N=32	64	128	256
2nd-order	9.355E-04	2.256E-04	5.642E-05	1.410E-05
rate	-	2.05	2.00	2.00
4th-order	8.377E-06	5.213E-07	3.251E-08	2.029E-09
rate	-	4.01	4.00	4.00
$u = \sin^4\phi\,(0.5\sin 2\theta - \sin\theta - \cos\theta)$				
2nd-order	1.385E-02	3.594E-03	9.064E-04	2.271E-04
rate	-	1.95	1.99	2.00
4th-order	9.124E-04	5.568E-05	3.554E-06	2.213E-07
rate	-	4.01	4.00	4.01
$u = \cos\phi\sin^2\phi\,\cos(2(\theta - 1.5))$				
2nd-order	4.106E-03	1.031E-03	2.573E-04	6.438E-05
rate	-	1.99	2.00	2.00
4th-order	1.586E-04	1.054E-05	6.654E-07	4.164E-08
rate	-	3.91	3.99	4.00

Table 6: The maximum errors for different solutions of Poisson equation on a sphere.

$u = e^{\cos\phi}$	N=32	64	128	256
2nd-order	1.840E-02	4.605E-03	1.152E-03	2.879E-04
rate	-	2.00	2.00	2.00
4th-order	7.648E-04	4.974E-05	3.141E-06	1.968E-07
rate	-	3.95	3.99	4.00
$u = e^{\sin\phi\,\cos\theta}$				
2nd-order	5.772E-03	1.450E-03	3.625E-04	9.060E-05
rate	-	2.00	2.00	2.00
4th-order	1.692E-04	1.068E-05	6.726E-07	4.211E-08
rate	-	3.99	3.99	4.00

Table 7: The maximum errors for different solutions of Helmholtz equation on a sphere.