A Spectral Method for Polar Coordinates

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A new set of polynomial functions that can be used in spectral expansions of C^* functions in polar coordinates (r, ϕ) is defined by a singular Sturm-Liouville equation. With the use of the basis functions, the spectral representations remain analytic at the pole despite the coordinate singularity because the pole condition is exactly satisfied at the origin for all azimuthal modes, not just a few of the gravest modes (which is the usual case). Based on recurrence relations, fast and stable numerical operators for 1/r, r(d/dr), the Laplacian and Helmholtz operators and their inverses are developed. Although the spacings in the azimuthal direction of the collocation points near the origin are small (i.e., α 1/ M^2 , where M is the number of radial modes), the explicit numerical method for Euler's equation is not stiff at the origin. Namely, the CFL number σ is O(1) where the grid size in σ is defined as π/M (i.e., the maximum allowable timestep is proportional to 1/M, not 1/M2). © 1995 Academic Press, Inc.

1. INTRODUCTION

In cylindrical and spherical coordinates the coordinate singularity can decrease the accuracy or computational efficiency of the spectral method. Orszag [1] used Fourier series with the pole conditions imposed at the coordinate singularity. However, a severe time step restriction can occur in this method. Robert [2] and Merilees [3] imposed the exact pole conditions explicitly onto the expansion functions. Although a fast transform can be used for this family of methods [4], their basis functions are nearly linearly dependent [5, pp. 493–496] and the accuracy deteriorates as the number of coefficients becomes large [3].

Recently, Eisen *et al.* [6] mapped the unit disk onto a rectangle and imposed pole conditions. Huang and Sloan [7] used differential equations to construct pole conditions. Although they could solve the Poisson-type problems successfully, we believe that with their expansion functions and pole conditions, the time step restriction problem that arises for advection problems due to the increased resolution near the coordinate singularity [5, pp. 480–482] cannot be avoided. One way to avoid the time step restriction problem is to use a Fourier filter in the azimuthal direction as used by Fornberg and Sloan [8] and Fornberg [9]. They used Chebyshev expansion in the radial direction on [-1, 1] over the coordinate singularity instead of

on [0, 1]. Their method avoids the time step restriction problem and gives a good result for a simple linear advection problem. However it is not clear how much the unsatisfied pole condition will affect the results for more complicated applications.

In spherical coordinates the spherical harmonics are an example of an orthogonal basis set which treats the coordinate singularity correctly. They have been popular in spherical geometry [5, 10]. In polar coordinates Bessel functions act as the analogue of the spherical harmonics. However, although Bessel functions behave correctly near the coordinate singularity, they are not free of the Gibbs phenomena at any finite outer boundary. In this paper we present a family of complete orthogonal sets of polynomials which satisfies the pole condition exactly. The polynomials satisfy a differential equation singular at the outer boundary and converges spectrally on the interval [0, 1]. As an application, we combine these polynomials with the Fourier modes to form a basis set which converges spectrally on the unit disk in polar coordinates.

2. THE POLYNOMIAL SET

We seek a spectrally accurate method for representing a \mathscr{C}^{∞} function $f(r, \phi)$ over the unit disk. When $f(r, \phi)$ is represented as a Fourier series in ϕ ,

$$f(r,\phi) = \sum_{m=-\infty}^{\infty} f_m(r)e^{im\phi}, \qquad (1)$$

the pole condition is that $f_m(r)$ behaves as $O(r^{|m|+2p})$ as $r \to 0$ for an nonnegative integer p [6]. The goal of the paper is to find basis functions for representing $f_m(r)$ so that the pole condition is maintained, the defining differential equation is singular [11] at the outer boundary so that the basis functions are free of the Gibbs phenomena there, and the weight function is suited for cylindrical or spherical geometry. Also orthogonal polynomials are desirable for the basis functions because they satisfy three term recurrence relations and are easy to manipulate.

As a defining differential equation which satisfies these requirements, consider the singular Sturm-Liouville equation

$$\frac{(1-r^2)^{1-\alpha}}{r^{\beta}} \frac{d}{dr} \left((1-r^2)^{\alpha} r^{\beta} \frac{dy}{dr} \right) - \frac{|m|(|m|+\beta-1)}{r^2} y + n(n+2\alpha+\beta-1)y = 0,$$
(2)

defined over $0 \le r \le 1$, $0 \le |m| \le n$, where m and n are integers, $0 < \alpha \le 1$, and β is a positive integer. Equation (2) has nth-degree polynomial solution if n + m is even and the Frobenius series about r = 0 can be used to write the solution $y = Q_n^m(\alpha, \beta; r)$ in closed form,

$$Q_{n}^{m}(\alpha, \beta; r) \equiv \sum_{p=0}^{(n-|m|)/2} \Gamma\left(\frac{n+|m|+\gamma-1}{2}+p\right) \\ \frac{\Gamma\left(\frac{2|m|+\beta+1}{2}\right)}{p!\left(\frac{n-|m|}{2}-p\right)!\Gamma\left(\frac{2|m|+\beta+1}{2}+p\right)} r^{|m|+2p},$$

$$\Gamma\left(\frac{2|m|+\beta+1}{2}-p\right) \Gamma\left(\frac{2|m|+\beta+1}{2}+p\right)$$

$$\Gamma\left(\frac{2|m|+\gamma-1}{2}-p\right) \Gamma\left(\frac{2|m|+\gamma-1}{2}-p\right) \Gamma\left(\frac{2|m|+\gamma-1}{2}-p\right)$$

where $\gamma \equiv 2\alpha + \beta$. If m is even, $Q_n^m(\alpha, \beta; r)$ is an even function of r and if m is odd, $Q_n^m(\alpha, \beta; r)$ is an odd function. For $r \to \infty$ 0, $Q_n^m(\alpha, \beta; r)$ behaves as $O(r^{[m]})$ and $Q_n^m(\alpha, \beta; r)e^{im\phi}$ in polar coordinates (r, ϕ) satisfies the pole condition exactly. The $Q_n^m(\alpha, \beta; r)$ are complete and orthogonal with respect to the weight function

$$w(\alpha, \beta; r) \equiv \frac{r^{\beta}}{(1 - r^2)^{1 - \alpha}} \tag{4}$$

so that

$$\int_{0}^{1} Q_{n}^{m}(\alpha, \beta; r) Q_{n}^{m}(\alpha, \beta; r) w(\alpha, \beta; r) dr = I_{n}^{m}(\alpha, \beta) \delta_{nn'}$$
 (5)

where $\delta_{nn'}$ is the Kronecker delta. A recurrence relation for the integration constant $I_n^m(\alpha, \beta)$ will be derived later. Given $I_n^m(\alpha, \beta)$ β), we can form orthonormal functions,

$$\Phi_n^m(\alpha, \beta; r) = (I_n^m(\alpha, \beta))^{-1/2} Q_n^m(\alpha, \beta; r). \tag{6}$$

The $\Phi_n^m(\alpha, \beta; r)$ can be used to expand a scalar function on the unit disk $D \equiv \{(r, \phi) | 0 \le r \le 1, 0 \le \phi < 2\pi\}$ in polar coordinates

$$f(r,\phi) = \sum_{n=0}^{\infty} \sum_{\substack{m=-n\\m+n \text{ even}}}^{n} f_n^m \Phi_n^m(\alpha,\beta;r) e^{im\phi}, \tag{7}$$

where f_n^m are complex expansion coefficients. Note that $f(r, \phi)$ is \mathscr{C}^{∞} on D because of the correct polar behavior of $\Phi_n^m(\alpha, \beta)$; r). The coefficients f_n^m are found by

$$f_n^m = \frac{1}{2\pi} \int_{\phi=0}^{2\pi} \int_{r=0}^{1} f(r,\phi) \Phi_n^m(\alpha,\beta;r) e^{-im\phi} w(\alpha,\beta;r) \, dr \, d\phi. \tag{8}$$

The spectral convergence (i.e., faster than algebraic) of expansion (7) to a function $f(r, \phi) \in \mathscr{C}^{\infty}$ on D can be shown by using the differential equation (2) with (8). Integrating twice by parts with respect to r, we obtain

$$f_n^m = \frac{1}{2\pi n(n+2\alpha+\beta-1)} \int_{\phi=0}^{2\pi} \int_{r=0}^{1} f_{r=0}$$

$$\times h(r,\phi) \Phi_n^m(\alpha,\beta;r) e^{-im\phi} w(\alpha,\beta;r) dr d\phi,$$
(9)

$$h(r, \phi) = -\frac{(1 - r^2)^{1 - \alpha}}{r^{\beta}} \frac{d}{dr} \left((1 - r^2)^{\alpha} r^{\beta} \frac{df}{dr} \right) + \frac{|m|(|m| + \beta - 1)}{r^2} f.$$
 (10)

Substitution of $r^{|m|}e^{im\phi}$ in $f(r, \phi)$ shows that $h(r, \phi)$ preserves the pole condition if $f(r, \phi)$ satisfies the pole condition exactly. By repeating the integration by parts, we can prove the spectral convergence of the partial sums in Eq. (7) to $f(r, \phi)$.

Within the allowed values of α and β , some particular choices are of interest. If $\alpha = 1$ and $\beta = 1$, the weight function reduce to w(1, 1; r) = r and it agrees with the weight function for the physical integration on the unit disk. In this case, setting m =0 and applying the change of variable $x = 2r^2 - 1$ reduces Eq. (2) to the Legendre equation,

$$\frac{d}{dx}(1-x^2)\frac{dy}{dx} + \frac{n}{2}\left(\frac{n}{2} + 1\right)y = 0.$$
 (11)

Thus $Q_n^0(1, 1; r)$ is related to $P_{n/2}(x)$, the Legendre polynomial of degree n/2, by

$$P_{n/2}(x) \propto Q_n^0(1, 1; \sqrt{(1+x)/2}).$$
 (12)

Also, for arbitrary integer m the $Q_n^m(1, 1; r)$ is related to the shifted Jacobi polynomial $P_n^{(0,m)}(y)$ used by Leonard and Wray [12] by the relation $Q_n^m(1, 1; r) \propto r^{|m|} P_n^{(0,m)} (2r^2 - 1)$. They used $f(r,\phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} f_n^m \Phi_n^m(\alpha,\beta;r) e^{im\phi}, \qquad (7)$ [12] by the relation $Q_n(1,1,r) \propto r^{-n} P_n^{m-n} (2r-1)$. They used $P_n^{(0,m)}(2r^2-1)$ as an element to construct Galerkin type diverging $P_n^{(0,m)}(2r^2-1)$ as an element to construct Galerkin type diverging $P_n^{(0,m)}(2r^2-1)$. gence free vector basis functions.

 $r = r/\sqrt{1-r^2}$. In this case the change of variable

$$x = \sqrt{1 - r^2} \tag{13}$$

transforms (2) to the associated Legendre equation. Thus Q_n^m $(\frac{1}{2}, 1; r)$ is related to $P_n^m(x)$, the associated Legendre function of order m and degree n, by

$$P_n^m(x) \propto Q_n^m(\frac{1}{2}, 1; \sqrt{1 - x^2})$$
 (14)

for $0 \le x \le 1$. Because we have defined $O_n^m(\alpha, \beta; r)$ only for the case where n - |m| is even, only even associated Legendre functions are related to $Q_n^m(\frac{1}{2}, 1; r)$. The odd associated Legendre functions will not have bounded derivatives at r = 1 because dr/dx is zero there. We note that x = 0 is a regular point of the associated Legendre equation while the corresponding point r = 1 is a singular point of (2).

If $\alpha = 1$ and $\beta = 2$, the weight function becomes w(1, 2;r) = r^2 . As we will show in Section 5.1, this choice of α and β is suited for basis functions in the radial direction in spherical coordinates.

In Section 5.1, numerical experiments are carried out with parameters $\alpha = 1, \frac{1}{2}$ and $\beta = 1, 2$ for the Bessel and spherical Bessel eigenproblem. Based on the results, the choice $\alpha = 1$, $\beta = 1$ will be used to solve the vorticity equation in Section 5.2.

3. NUMERICAL PROCEDURE

We discuss the procedures to evaluate $\Phi_n^m(r)$ and to find f_n^m in Eq. (7) numerically. We suppress the arguments α and β of $O_n^m(\alpha, \beta; r)$, $\Phi_n^m(\alpha, \beta; r)$, $I_n^m(\alpha, \beta)$, and $w(\alpha, \beta; r)$ and use $\gamma \equiv 2\alpha + \beta$ for brevity. First we derive some useful formulas. The $O_n^m(r)$ satisfy for $n \ge |m|$

$$r\frac{d}{dr}(Q_n^m(r) - Q_{n-2}^m(r)) = nQ_n^m(r) + (n+\gamma-3)Q_{n-2}^m(r), \quad (15)$$

where $Q_{|m|-2}^m(r) \equiv 0$. Equation (15) can be verified easily by the substitution of (3). Using (15) to reduce the order of Eq. (2), we obtain

$$(1 - r^{2})r\frac{d}{dr}Q_{n}^{m}(r)$$

$$= \left(-nr^{2} + \frac{|m|(|m| + \beta - 1) + n(n + \gamma - \beta - 2)}{2n + \gamma - 3}\right)Q_{n}^{m}(r)$$

$$+ \frac{(n - |m| + \gamma - \beta - 2)(n + |m| + \gamma - 3)}{2n + \gamma - 3}Q_{n-2}^{m}(r).$$
(16)

If $\alpha = \frac{1}{2}$ and $\beta = 1$, the weight function becomes $w(\frac{1}{2}, 1)$; Using (15) again we may eliminate the differential term to yield

$$-(n - |m| + 2)(n + |m| + \beta + 1)(2n + \gamma - 3)Q_{n+2}^{m}(r)$$

$$+ (2n + \gamma - 1)\{(2n + \gamma - 3)(2n + \gamma + 1)r^{2}$$

$$- 2n(n + \gamma - 1) - 2|m|(|m| + \beta - 1)$$

$$- (\gamma - 3)(\beta + 1)\}Q_{n}^{m}(r)$$

$$- (n - |m| + \gamma - \beta - 2)(n + |m| + \gamma - 3)$$

$$\times (2n + \gamma + 1)Q_{n-2}^{m}(r) = 0.$$

$$(17)$$

The $Q_n^m(r)$ can be evaluated as follows. By setting n = |m|and n = |m| + 2 in Eq. (3) we obtain

$$Q_{|m|}^{m}(r) = r^{|m|} \tag{18}$$

$$Q_{[m]+2}^{m}(r) = \frac{(2|m|+\gamma-1)}{2} \left(\frac{2|m|+\gamma+1}{2|m|+\beta+1}r^2-1\right) Q_{[m]}^{m}(r). \quad (19)$$

With these starting values, we can stably evaluate $Q_n^m(r)$ for higher values of n by the recurrence relation (17). The recurrence relation for normalization coefficient I_n^m can be obtained by applying (17) to (5) and using the orthogonality of $Q_n^m(r)$,

$$I_n^m = \frac{(2n+\gamma-5)(n-|m|+\gamma-\beta-2)(n+|m|+\gamma-3)}{(n-|m|)(n+|m|+\beta-1)(2n+\gamma-1)} I_{n-2}^m,$$
(20)

where the starting value $I_{[m]}^m$ can be computed by (18) and (5),

$$I_{[m]}^{m} = \Gamma\left(|m| + \frac{\beta+1}{2}\right)\Gamma\left(\frac{\gamma-\beta}{2}\right) / 2\Gamma\left(|m| + \frac{\gamma+1}{2}\right). \quad (21)$$

Next, we consider the numerical evaluation of f_n^m defined by Eq. (7). Consider the partial sum approximation $f_M(r, \phi)$ to $f(r, \phi)$ for an even integer M,

$$f_m(r) \equiv \sum_{\substack{n=|m|\\ n+m \text{ order}}}^{\dot{M}} f_n^m \Phi_n^m(r) \tag{22}$$

$$f_M(r, \phi) \equiv \sum_{m=-M+1}^{M-1} f_m(r)e^{im\phi} \simeq f(r, \phi),$$
 (23)

where $\hat{M} \equiv M - 1$ if m is odd and $\hat{M} \equiv M - 2$ if m is even. If we choose $M \equiv 2^p$, where p is a positive integer, the standard fast Fourier transform can be used with (23) to find $f_m(r)$. The inverse transform of Eq. (22) is

$$f_n^m = \int_0^1 f_m(r) \Phi_n^m(r) w(r) \, dr. \tag{24}$$

We now derive a Gaussian quadrature formula for (24) to compute f_n^m efficiently. First, note that the product $f_n(r)\Phi_n^m(r)$ is an even polynomial whose degree is at most 2M-2. The Lagrange quadrature formula [13, p. 402] for (24) is

$$\int_{0}^{1} f_{m}(r) \Phi_{n}^{m}(r) w(r) dr = \sum_{i=1}^{M/2} f_{m}(r_{i}) \Phi_{n}^{m}(r_{i}) w_{i} + E, \qquad (25)$$

where r_i are the abscissas of the quadrature, E is the error of the formula. Here we assume that $0 \le r_1 < r_2 ... < r_{M/2} \le 1$. The weight w_i is

$$w_{i} = \left(1 / \left(\frac{\pi'(r)}{2r} \bigg|_{r_{i}}\right)\right) \int_{0}^{1} \frac{\pi(r)}{r^{2} - r_{i}^{2}} w(r) dr, \qquad (26)$$

where

$$\pi(r) \equiv \prod_{i=1}^{M/2} (r^2 - r_j^2). \tag{27}$$

By construction, the formula (25) is exact or E=0 if the degree of the product $f_m(r)\Phi_n^m(r)$ is less than or equal to M-2. Now dividing $f_m(r)\Phi_n^m(r)$ by $\pi(r)$, we can write $f_m(r)\Phi_n^m(r)=s(r)+\pi(r)q(r)$, where s(r) and q(r) are even polynomials of degree at most M-2. Substituting this expression into (25) and observing that $s(r_i)=f_m(r_i)\Phi_n^m(r_i)$ for $1 \le i \le M/2$, we obtain

$$E = \int_0^1 \pi(r)q(r)w(r) dr.$$
 (28)

Thus if we choose $\pi(r) = Q_M^0(r)$, by orthogonality E vanishes identically and the coefficients f_n^m can be computed exactly by (24) and (25) when $f_M(r, \phi)$ is equal to $f(r, \phi)$. Thus the abscissas of the Gaussian quadrature correspond to the positive zeros of $Q_M^0(r)$. The zeros of $Q_M^0(r)$ need to be computed numerically.

The weight coefficients w_i of Gaussian quadrature can be evaluated as follows. First we write (17) with m = 0 as

$$\frac{r^2 Q_n^0(r)}{I_n^0} = \frac{C_n}{I_n^0} Q_{n+2}^0(r) + D_n Q_n^0(r) + \frac{C_{n-2}}{I_{n-2}^0} Q_{n-2}^0(r), \quad (29)$$

where

$$C_n = \frac{(n+2)(n+\beta+1)}{(2n+\gamma-1)(2n+\gamma+1)}. (30)$$

The D_n is not important here and the definition is not given. Multiplying (29) by $Q_n^0(\rho)$, subtracting the same equation with r and ρ exchanged and summing over n=0 to n=M for even n, we obtain the Christoffel-Darboux formula [13]

$$\sum_{\substack{p=0\\p \text{ even}}}^{M} \frac{Q_p^0(r)Q_p^0(\rho)}{I_p^0} = \frac{C_M}{I_M^0} \left(\frac{Q_{M+2}^0(r)Q_M^0(\rho) - Q_M^0(r)Q_{M+2}^0(\rho)}{r^2 - \rho^2} \right). \tag{31}$$

Replacing ρ by r_i , using $Q_M^0(r_i) = 0$, multiplying both sides of (31) by $Q_0^0(r)w(r)$, integrating from zero to one with respect to r, and using (29) with $r = r_i$, we obtain

$$\int_{0}^{1} \frac{Q_{M}^{0}(r)}{r^{2} - r_{i}^{2}} w(r) dr = \frac{I_{M-2}^{0}}{C_{M-2}Q_{M-2}^{0}(r_{i})}.$$
 (32)

Combining (32) and (26) with $\pi(r) = Q_M^0(r)$ and using (16), we obtain the formula for w_i ,

$$w_i = \frac{2(2M + \gamma - 3)r_i^2(1 - r_i^2)}{(M + \gamma - \beta - 2)(M + \gamma - 3)C_{M-2}(\Phi_{M-2}^0(r_i))^2}.$$
 (33)

In the collocation method, a quadrature point is desirable at the boundary to impose the boundary condition. In this case, the Gauss-Radau quadrature can be used [13]. The appropriate choice of $\pi(r)$ is

$$\pi(r) = Q_M^0(r) - \frac{(M+\gamma-\beta-2)(M+\gamma-3)}{M(M+\beta-1)} Q_{M-2}^0(r), \quad (34)$$

where $\pi(r)$ is designed to satisfy $\pi(1) = 0$. The weight coefficients for $1 \le i \le M/2 - 1$ are given by

$$w_i = \frac{2(2M + \gamma - 5)r_i^2}{(M + \gamma - \beta - 2)(M + \gamma - 3)(\Phi_{M-2}^0(r_i))^2}$$
 (35)

which can be obtained in a similar way as (33) was obtained by using (31) and $\pi(r_i) = 0$. The weight coefficient $w_{M/2}$ corresponding to $r_{M/2} = 1$ can be computed by the relation

$$w_{M/2} = I_0^0 - \sum_{i=1}^{M/2-1} w_i. (36)$$

Because the degree of $f_m(r)\Phi_n^m(r)$ is the same as the degree of $\pi(r)q(r)$ in (28), it is seen by the form of (34) that the Gauss-Radau quadrature is exact only if the degree of $f_m(r)\Phi_n^m(r)$ is equal to or less than 2M-4. To obtain the desired degree of precision 2M-2, the number of abscissas is increased by one. Then the degree of precision of the quadrature becomes 2M.

Products of two functions can be computed efficiently by using the M/2 abscissas of the Gaussian quadrature or the M/2 + 1 abscissas of the Gauss-Radau quadrature as collocation points. Dealiasing can be done by the usual 3/2's rule [5, pp. 268-276].

To perform the numerical integrations, we need to store the values of $Q_n^m(r)$ at each collocation point. This requires $O(M^3)$ words of memory and this is the largest memory requirement for a typical two-dimensional calculation. However, we note that the same situation occurs when one uses the associated Legendre functions for spherical harmonics. Transforms (22) and (25) are essentially matrix multiplications and are not as efficient as the fast Fourier transform. However, fast transform [15] can be applied to our basis functions if the matrices are sufficiently large. The application of multipole expansions [16] is an alternative for the pseudospectral method.

4. OPERATORS

In order to compute derivatives and other operations in expensively, recurrence relations are desirable. We present recurrence relations for the elementary operators r^2 , r(d/dr), and their inverses. Then we show the recurrence relation for the Helmholtz operator and a procedure to solve for its inverse. Let

$$g_m(r) \equiv \sum_{\substack{n=|m|\\ n+m \text{ even}}}^{\infty} a_n^m Q_n^m(r) \tag{37}$$

and for some linear operator L,

$$Lg_m(r) \equiv \sum_{\substack{n=|m|\\ n+m \text{ even}}}^{\infty} b_n^m Q_n^m(r). \tag{38}$$

Here for later convenience we assume that $a_n^m \equiv 0$ for $n > \hat{M}$, where \hat{M} is defined in the same way as in Eq. (22).

Consider L = r(d/dr). Substituting (37) into (38) and using (15) recursively, we obtain

$$b_n^m = na_n^m + (2n + \gamma - 1) \sum_{\substack{p=n+2\\p+n \text{ even}}}^{\infty} a_p^m.$$
 (39)

Shifting the index n in (39) to obtain b_{n+2}^m and eliminating the summation term, we obtain the recurrence formula for L = r(d/dr),

$$b_n^m = \frac{2n + \gamma - 1}{2n + \gamma + 3}b_{n+2}^m + \frac{(2n + \gamma - 1)(n + \gamma + 1)}{2n + \gamma + 3}a_{n+2}^m + na_n^m.$$
(40)

The b_n^m can be solved backwards numerically and stably with the starting value $b_{M+2}^m \equiv 0$. A backwards recurrence relation for the inverse of r(d/dr) can be obtained by solving (40) for

 a_n^m . This recurrence relation is also numerically stable with the starting value $a_{M+2}^m \equiv 0$, except for the indeterminate coefficient a_0^0 . This term serves as the integration constant implicit in $(r(d/dr))^{-1}$.

If $L = r^2$, using (17) and (37) with (38) we obtain for $n \ge |m|$,

$$b_{n}^{m} = \frac{(n - |m|)(n + |m| + \beta - 1)}{(2n + \gamma - 5)(2n + \gamma - 3)} a_{n-2}^{m}$$

$$+ \frac{2n(n + \gamma - 1) + 2|m|(|m| + \beta - 1) + (\gamma - 3)(\beta + 1)}{(2n + \gamma - 3)(2n + \gamma + 1)} a_{n}^{m}$$

$$+ \frac{(n - |m| + \gamma - \beta)(n + |m| + \gamma - 1)}{(2n + \gamma + 3)(2n + \gamma + 1)} a_{n+2}^{m},$$
 (41)

where $a_{|m|-2}^m \equiv 0$. If $\gamma = 3$ and n = m = 0, the second term on the right-hand side is taken as $(\beta + 1)/(\gamma + 1)a_n^m$. With Eq. (41) we can compute b_n^m for $|m| \le n \le \hat{M} + 2$. A backwards recurrence relation for the $1/r^2$ operator can be obtained by solving (41) for a_{n-2}^m . Starting values are $a_{M+2}^m \equiv 0$ and $a_{M+4}^m \equiv 0$. However, this recurrence is numerically unstable. The a_n^m can be computed stably and inexpensively by solving (41) with a tri-diagonal LU decomposition without pivoting. Here it is important that the function represented by b_n^m behave as $O(r^{|m|+2|p|+2})$ as $r \to 0$, where p is integer; otherwise, the resulting $g_m(r)$ can behave poorly near the coordinate singularity.

We now consider $L = r^2H$, where H is the Helmholtz operator

$$H = \frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{m^2}{r^2} - \kappa,$$
 (42)

where κ is some constant. Note that L can be written as $L = (r(d/dr))^2 - m^2 - \kappa r^2$ so that the operators constructed above can be exploited. Substituting (37), (39), and (41) into (38), we obtain for $n \ge |m|$,

$$b_{n}^{m} = (n^{2} - m^{2})a_{n}^{m} + (2n + \gamma - 1)$$

$$\times \left\{ \sum_{\substack{p=n+2\\p+n \text{ even}}}^{\infty} (n+p)a_{p}^{m} + \sum_{\substack{p=n+2\\p+n \text{ even}}}^{\infty} (2p+\gamma-1) \sum_{\substack{q=p+2\\q+p \text{ even}}}^{\infty} a_{q}^{m} \right\}$$

$$- \kappa \left\{ \frac{(n-|m|)(n+|m|+\beta-1)}{(2n+\gamma-5)(2n+\gamma-3)} a_{n-2}^{m} + \frac{2n(n+\gamma-1)+2|m|(|m|+\beta-1)+(\gamma-3)(\beta+1)}{(2n+\gamma-3)(2n+\gamma+1)} a_{n-2}^{m} + \frac{(n-|m|+\gamma-\beta)(n+|m|+\gamma-1)}{(2n+\gamma+3)(2n+\gamma+1)} a_{n+2}^{m} \right\}, \tag{43}$$

where $a_{|m|-2}^m \equiv 0$. After some shifting of indices, we can eliminate the summation terms to obtain

$$b_{n}^{m} = \frac{1}{(2n+\gamma+5)(2n+\gamma+7)}$$

$$\times \left\{ 2(2n+\gamma-1)(2n+\gamma+7)b_{n+2}^{m} - (2n+\gamma-1)(2n+\gamma+1)b_{n+4}^{m} - \kappa \frac{(n-|m|)(n+|m|+\beta-1)(2n+\gamma+5)(2n+\gamma+7)}{(2n+\gamma-5)(2n+\gamma-3)} a_{n-2}^{m} + \left[(n-|m|)(n+|m|)(2n+\gamma+5)(2n+\gamma+7) - \kappa \frac{2n+\gamma+7}{(2n+\gamma-3)} (2(\gamma-\beta)n+4|m|(|m|+\beta-1)+(\gamma-3)(\beta+1)) \right] a_{n}^{m} + \left[2(2n+\gamma-1)(2n+\gamma+7)(n^{2}+(\gamma+3)n+m^{2}+\gamma+1) + \kappa(2n^{2}+2(\gamma+3)n+6|m|(|m|+\beta-1)+(\gamma-1)(3\beta-\gamma+2)) \right] a_{n+2}^{m} + \left[(n-|m|+\gamma+3)(n+|m|+\gamma+3)(2n+\gamma-1)(2n+\gamma+1) + \kappa \frac{2n+\gamma-1}{2n+\gamma+9} (2(\gamma-\beta)n-4|m|(|m|+\beta-1)+(\gamma+1)(2\gamma-3\beta+3)) \right] a_{n+4}^{m} - \kappa \frac{(n-|m|+\gamma-\beta+4)(n+|m|+\gamma+3)(2n+\gamma-1)(2n+\gamma+1)}{(2n+\gamma+9)(2n+\gamma+11)} a_{n+6}^{m} \right\},$$

where $a_{|m|-2}^m \equiv 0$. If $\gamma = 3$ and n = m = 0, the factor that multiplies to a_n^m is taken as $-\kappa(\gamma + 7)(\beta + 1)$. Solving for b_n^m backwards with starting values $b_{M+4}^m \equiv 0$ and $b_{M+6}^m \equiv 0$, we can compute $r^2Hg_m(r)$ stably. Coefficients for $Hg_m(r)$ can be found by using the $1/r^2$ operator.

A backwards recurrence relation for the inverse of r^2H can be obtained by solving (44) for a_{n-2}^m . If $\kappa = 0$, we solve for a_n^m to obtain the recurrence relation. However, the former is unstable for all m and the later becomes unstable as |m| increases. We now present a numerically stable procedure to solve

$$Hg_m(r) = h_m(r) (45)$$

for $g_m(r)$, where $h_m(r)$ is a polynomial of degree at most \hat{M} . Here we seek $N = (\hat{M} - |m|)/2 + 1$ nonzero coefficients for $g_m(r)$ by the tau method. For clarity, we consider the case N = 6. Without boundary conditions the equation $r^2Hg_m(r) = r^2h_m(r)$ in matrix form in accordance with (41) and (44) is

where **x** denotes a nonzero element and $\hat{\mathbf{A}}$ and \mathbf{B} are column vectors whose elements are $\hat{a}_{[m]}^{m}$, $\hat{a}_{[m]+2}^{m}$, ..., \hat{a}_{M}^{m} and $b_{[m]}^{m}$, $b_{[m]+2}^{m}$, ..., b_{M}^{m} from top to bottom, respectively. The \hat{a}_{n}^{m} and b_{n}^{m} represent the coefficients of the functions $g_{m}(r)$ and $h_{m}(r)$. The hat $\hat{}$ is to account for the fact that we have not imposed the boundary condition. The second matrix on the right-hand side (T) represents the operator r^{2} given in (41). The matrix on the left-hand side (L) and the first matrix on the right-hand side (S) represents the operator $r^{2}H$ given in (44). By writing $\mathbf{R} \equiv \mathbf{ST}$, we can write Eq. (46) as $\mathbf{L}\hat{\mathbf{A}} = \mathbf{RB}$.

Let **A** be the column vector of coefficients $a_{|m|}^m$, $a_{|m|+2}^m$, ..., $a_{|m|}^m$ of $g_m(r)$ that satisfy (46) or (45) subject to the constraint of a boundary condition of the form

$$\mathbf{c} \cdot \mathbf{A} = s. \tag{47}$$

For example, the Dirichlet boundary condition at r=1 is represented by $c_i = Q_{|m|+2(i-1)}^m(r=1)$ for $1 \le i \le N$ and $s = g_m(r=1)$. Using a tau method to impose (47) requires A to satisfy

$$(\mathbf{R}^{-1}\mathbf{L})\mathbf{A} = \mathbf{B} + \tau_1 \mathbf{z},\tag{48}$$

where \mathbf{z} is the column vector $z_i \equiv \delta_{iN}$ and τ_1 is determined from (47). We note that a modified tau method of the form

$$\mathbf{L}\mathbf{A} = \mathbf{R}\mathbf{B} + \tau_1 \mathbf{z} \tag{49}$$

is not equivalent to (48); the solution to (49) leads to large errors near the boundary and should not be used.

To solve (47) and (48) efficiently and stably, we define the auxiliary matrix L' to be equal to L with the exception that a new row [1, 0, ..., 0] is added to the top of the matrix and the bottom row is cast off; i.e., for $1 \le j \le N$,

$$L'_{ij} = L_{i-1,j}, \quad 2 \le i \le N,$$

$$L'_{1i} = \delta_{1i}.$$
(50)

The matrix L' is penta-diagonal. It can be stably inverted with an LU decomposition without pivoting. We also define the column vector Y equal to RB with the modification that the bottom element is moved to the top; i.e.,

$$Y_{i} \equiv \sum_{j=1}^{N} R_{i-1,j} B_{j}, \quad 2 \le i \le N,$$

$$Y_{1} \equiv \sum_{j=1}^{N} R_{N,j} B_{j}.$$
(51)

Then

$$\mathbf{A} = \overline{\mathbf{A}} + \tau_1 \mathbf{G}_1 + \tau_2 \mathbf{G}_2, \tag{52}$$

where $\widetilde{\mathbf{A}}$ is the column vector $(\mathbf{L}')^{-1}\mathbf{Y}$, \mathbf{G}_2 is the column vector $(\mathbf{G}_2)_i \equiv (\mathbf{L}')_{i,1}^{-1}$, $\mathbf{G}_1 \equiv (\mathbf{L}')^{-1}\mathbf{G}_3$, and \mathbf{G}_3 is the column vector $(\mathbf{G}_3)_i \equiv R_{i-1,N}$ for $2 \le i \le N$ with $(\mathbf{G}_3)_1 \equiv R_{NN}$. The τ_1 and τ_2 are

$$\tau_1 = [(Y_1 - \mathbf{F} \cdot \overline{\mathbf{A}})(\mathbf{c} \cdot \mathbf{G}_2) - (\mathbf{F} \cdot \mathbf{G}_2)(s - \mathbf{c} \cdot \overline{\mathbf{A}})]/\xi$$
 (53)

$$\tau_2 = [(s - \mathbf{c} \cdot \overline{\mathbf{A}})(\mathbf{F} \cdot \mathbf{G}_1 - R_{NN}) - (\mathbf{c} \cdot \mathbf{G}_1)(Y_1 - \mathbf{F} \cdot \overline{\mathbf{A}})]/\xi \quad (54)$$

with

$$\xi \equiv (\mathbf{F} \cdot \mathbf{G}_1 - R_{NN})(\mathbf{c} \cdot \mathbf{G}_2) - (\mathbf{F} \cdot \mathbf{G}_2)(\mathbf{c} \cdot \mathbf{G}_1)$$
 (55)

and **F** is equal to the last row of **L**. Note that if **A** is to be found repeatedly for different values of **B**, then in a preprocessing step **L**' is decomposed into its LU factors. The factors are stored along with the values of G_1 , G_2 , F, $(F \cdot G_1)$, $(F \cdot G_2)$, $(c \cdot G_1)$, $(c \cdot G_2)$, and ξ . Each evaluation of \overline{A} requires O(5N) operations to find Y, O(5N) operations to find \overline{A} from Y, O(2N) operations to find τ_1 and τ_2 , and O(N) to compute \overline{A} from (52). Thus we can solve the Helmholtz equation $Hg_m(r) = h_m(r)$ for $g_m(r)$ in O(13N) operations.

5. EXAMPLES

5.1. Bessel Function Eigenproblem

In this section we discuss the problem of choosing appropriate α and β . We consider the Bessel function eigenproblem

$$\frac{1}{r}\frac{d}{dr}r\frac{dy}{dr} - \frac{m^2}{r^2}y = -\lambda y \tag{56}$$

and the spherical Bessel function eigenproblem

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{dy}{dr} - \frac{m(m+1)}{r^2}y = -\lambda y$$
 (57)

on [0, 1], where we assume that $m \ge 0$. Although our main interest lies in polar coordinates, the spherical Bessel function eigenproblem is considered in order to show the importance of choosing a correct weight function. In (56) and (57) our boundary conditions are the boundedness at the origin and y(1) = 0. The solution to (56) is the mth-order Bessel function $J_m(r_{mn}r)$, where r_{mn} is the nth zero of $J_m(r)$ and the eigenvalue is $\lambda_{mn} = r_{mn}^2$. They are orthogonal with respect to the weight function $w_b(r) = r$. The solution to (57) is the spherical Bessel function $j_m(r'_{mn}r) \equiv \sqrt{\pi/(2r'_{mn}r)}J_{m+1/2}(r'_{mn}r)$, where r'_{mn} is the nth zero of $j_m(r)$ and the eigenvalue is $\lambda_{mn} = r'_{mn}^2$. They are orthogonal with respect to the weight function $w_s(r) = r^2$. Because both $J_m(r)$ and $j_m(r)$ behave as $O(r^m)$ as $r \to 0$, it is appropriate to expand y(r) as

$$y_{M}(r) = \sum_{\substack{p=|m|\\p+m \text{ even}}}^{|m|+M} a_{p} Q_{p}^{m}(\alpha, \beta; r).$$
 (58)

The matrix representing (56) follows directly from (43) with $\kappa = 0$ and the matrix for (57) can be constructed similarly. For expansion (58), only $y_M(1) = 0$ is imposed explicitly by the tau method. Expansions by $Q_n^m(1, 1; r)$, $Q_n^m(\frac{1}{2}, 1; r)$, $Q_n^m(1, 2; r)$, and $Q_n^m(\frac{1}{2}, 2; r)$ are considered to investigate the effects of the values of α and β .

As a counterexample, we also solve (56) and (57) following the procedure of Gottlieb and Orszag [11, pp. 152–153] by representing y(r) as

$$y_M(r) = \sum_{\substack{p=0\\p \text{ even}}}^M b_p T_p(r), \quad m \text{ even},$$
 (59)

$$y_M(r) = \sum_{\substack{p=1 \ p \text{ odd}}}^{M+1} b_p T_p(r), \quad m \text{ odd},$$
 (60)

where $T_p(r)$ is the Chebyshev polynomial of degree p. The boundary condition $y_M(1) = 0$ is imposed for all m. In addition, a "pole condition" is applied for $m \ge 2$ at the origin: $(dy_M/dr)|_{r=0} = 0$ if m is odd and $y_M(0) = 0$ if m is even. The tau method is used to impose these conditions. The number of coefficients is the same for (58), (59), and (60) and is equal to M/2 + 1.

The smallest eigenvalue of the Bessel eigenproblem (56) was found numerically for m = 0, m = 7, and m = 49 for several values of M and the fractional errors in the computed eigenvalues are shown in Fig. 1. We note that a similar result is obtained if we examine larger eigenvalues instead of the smallest one. The figures show that the eigenvalues for expansion with $\alpha = 1$ and $\beta = 1$ converges faster than those with other values of α and β . This behavior becomes less obvious for m = 49, but the convergence for $Q_n^m(1, 1; r)$ becomes no worse than other expansions. On the other hand, another choice of α and β gives the fastest convergence for the spherical Bessel eigenproblem. In Fig. 2 we plot the fractional errors in the computed eigenvalues to the smallest exact eigenvalues of the spherical Bessel eigenproblem (57) for m = 0, m = 7, and m = 49 for several values of M. The behavior is similar to that of Bessel eigenproblem, however in this case $Q_n^m(1, 2; r)$ expansion gives the fastest convergence. These results show that it is desirable to choose β according to the natural dimension of the problem to obtain the best result. The figures also suggest that the choice $\alpha = 1$ always gives a faster convergence than $\alpha = \frac{1}{2}$

Figures 1 and 2 also show that the Chebyshev expansion works as well as other expansions for m = 0. However, the convergence deteriorates significantly as m becomes large. This can be understood by the fact that the oscillatory part of the Bessel function moves towards the outer boundary as m increases and the function becomes tougher to resolve accurately for the Chebyshev expansion. On the other hand, the oscillatory part of $Q_n^m(r)$ behaves similarly with the Bessel function as m increases and the exponential convergence is maintained even

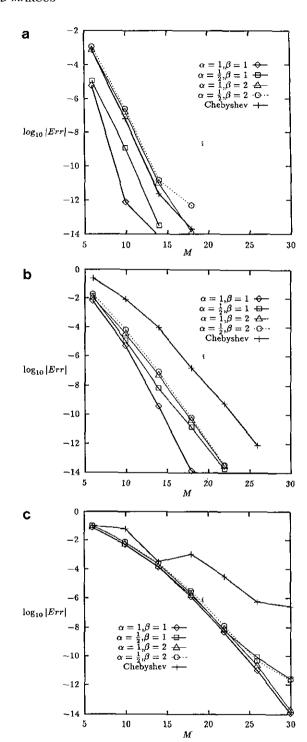


FIG. 1. Fractional error *Err* in computed eigenvalue to the smallest exact eigenvalue $\lambda = 5.78318596295$ of Bessel eigenproblem with m = 0 (a), $\lambda = 122.907600204$ of Bessel eigenproblem with m = 7 (b), and $\lambda = 3144.17045658$ of Bessel eigenproblem with m = 49 (c).

for m = 49 with a relatively small number of coefficients. The behavior of the Bessel function is common to many problems for which the physics at the coordinate singularity is no different from other parts of the domain. In such cases the solution will

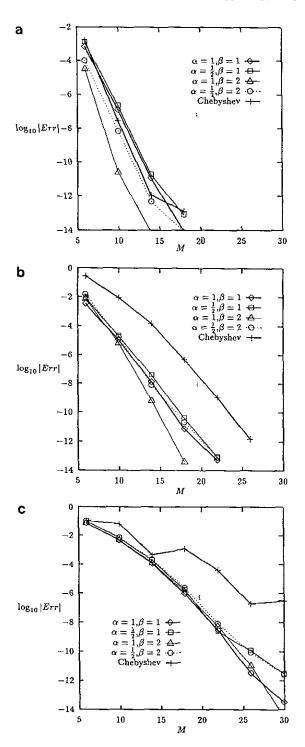


FIG. 2. Fraction error Err in computed eigenvalue to the smallest exact eigenvalue $\lambda = 9.86960440109$ of spherical Bessel eigenproblem with m = 0 (a), $\lambda = 135.886399537$ of spherical Bessel eigenproblem with m = 7 (b), and $\lambda = 3202.99085698$ of spherical Bessel eigenproblem with m = 49 (c).

satisfy the pole condition naturally and better performance of the $Q_n^m(r)$ expansion is expected. Thus the $Q_n^m(r)$ expansions have some advantages over the Chebyshev expansion for large m even though Orszag [1] and Boyd [14] have suggested that

the exact pole condition is not necessary for eigenvalue problems and boundary value problems.

Based on the results in this section, we will use $\alpha = 1$ and $\beta = 1$ in the next section where we solve the vorticity equation in polar coordinates.

5.2. Vorticity Equation

In this section we apply our method to a simple yet practical problem, the vorticity equation in two dimensions,

$$\frac{\partial \omega}{\partial t} = -\mathbf{u} \cdot \nabla \omega,\tag{61}$$

where the velocity $\mathbf{u} = (u_r, u_\phi)$ satisfies the incompressible continuity equation $\nabla \cdot \mathbf{u} = 0$. The $\omega(t, r, \phi) \equiv (1/r)(\partial/\partial r)$ $(ru_\phi) - (1/r)(\partial u_r/\partial \phi)$ is the vorticity [17]. We introduce the stream function $\psi(t, r, \phi)$ such that $\mathbf{u} = (-(1/r)(\partial\psi/\partial\phi), (\partial\psi/\partial r))$ and write the right-hand side of (61) as

$$J(\psi,\omega) = -\mathbf{u} \cdot \nabla \omega = \frac{1}{r^2} \left(r \frac{\partial \psi}{\partial r} \frac{\partial \omega}{\partial \phi} - r \frac{\partial \omega}{\partial r} \frac{\partial \psi}{\partial \phi} \right). \tag{62}$$

The vorticity is related to ψ by $\omega(t, r, \phi) = \nabla^2 \psi$. Our domain is the unit disk $D = \{(r, \phi) | 0 \le r \le 1, 0 \le \phi < 2\pi\}$ and the boundary condition is $u_r = 0$ at r = 1 or $\psi(t, r = 1, \phi) = 0$. Both ψ and ω are expanded in the form of (22) and (23) and the initial conditions are prepared as the expansion coefficients of $\Phi_n^m(r)$. The $J(\psi, \omega)$ are computed as follows. The $r(\partial/\partial r)$ (see (40)) and $\partial/\partial\phi$ are applied to ψ and ω in function space and the resulting four functions are transformed to the physical space. Then the values of $J(\psi, \omega)$ are computed at each collocation point by simple multiplications. Because neither Gauss-Legendre nor Gauss-Radau quadrature points include the origin, division by r^2 can be carried out straightforwardly. Here, it is important that the multiplication of $1/r^2$ in (62) is carried out in physical space. Otherwise if one transforms $r^2J(\psi,\omega)$ to function space and uses the inverse of the recurrence (41), the result will behave poorly near the coordinate singularity because after the dealiasing the function will no longer be divisible by r^2 exactly. Once $J(\psi, \omega)$ is found, the vorticity at new time step can be found by using a time integration method and the stream function can be found by the procedure to invert the Helmholtz operator in Section 4 with $\kappa = 0$.

To illustrate the absence of the stiffness problem, we consider an initial vorticity distribution configured as a vortex pair

$$\omega_0(x, y) = G(x + 0.25, y) - G(x - 0.05, y),$$
 (63)

where $G(\xi, \eta)$ is a gaussian $G(\xi, \eta) \equiv 100 \exp(-32(\xi^2 + \eta^2))$ and $x = r \cos \phi$ and $y = r \sin \phi$. Vortices are arranged asymmetrically. The solution is such that each vortex circulates in the disk with a half-moon shaped trajectory and the vortex with negative vorticity goes over the coordinate singularity

TABLE I

The CFL Number σ and Fractional Changes in Several Conserved Quantities at t = 10 from the Initial Values

Δt	σ	$\int_D ru_{\phi} r dr d\phi$	$\int_{D} \nabla \psi ^{2} r \ dr \ d\phi$	$\int_{D} \omega^{2} r dr d\phi$
0.001	0.18	-1.1×10^{-7}	-1.0×10^{-3}	-2.9×10^{-2}
0.002	0.36	-3.2×10^{-9}	-1.1×10^{-3}	-2.9×10^{-2}
0.004	0.72	3.1×10^{-7}	-1.5×10^{-3}	-3.0×10^{-2}
0.008	1.44	_	_	_

Note. The third to fifth columns are the fractional changes of angular momentum, energy, and enstrophy.

periodically (the period is approximately two in nondimensional time). We use M=64 to expand ψ and ω in the form of (22) and (23) with $\alpha=1$ and $\beta=1$. The coefficients for n>2M/3 are used for dealiasing. Equation (61) is integrated with a second order leap-frog method up to t=10 with several values of time step Δt and a hyperviscosity type small scale dissipation was used.

Fractional changes in several conserved quantities at t = 10are shown together with the CFL number σ corresponding to Δt in Table I. The CFL number is defined as $\sigma = \Gamma \Delta t / \Delta t$ $2\pi r_c \Delta x$ based on the circulation of vortices $|\Gamma| = 100\pi/32$, the characteristic radius $r_G = 1/\sqrt{32}$ and the characteristic grid size $\Delta x = \pi/M \sim 0.049$. Note that the grid size near the coordinate singularity is $O(\pi r_1/M)$ and if this value is used for Δx , σ will be $O(1/r_1) \sim 27$ times larger. The calculation is stable up to $\Delta t = 0.004$ but unstable for $\Delta t = 0.008$. Although the exact inviscid solution conserves all three quantities in Table I, they are not conserved exactly in our calculation primarily due to the small scale dissipation. However, the fractional errors are small and do not change quadratically as Δt is varied. Thus the time integration error is seen to be small even for $\Delta t =$ 0.004. In terms of the CFL number this upper limit of Δt is reasonable and we observe no significant time step restriction in our method.

In our computation, a large fraction of CPU time is spent for the radial and azimuthal transform to compute $J(\psi, \omega)$. The time to invert Laplacian to find ψ is not significant. The inefficiency of the matrix multiplication compared to the fast Fourier transform is a relatively minor problem for moderate size of M because only $O(M^2/9)$ quadratures are needed for a radial transform if the dealiasing is used. In our computation on CRAY C90, for which the matrix multiplication is particularly fast, the radial transform takes only 1.1 times the azimuthal FFT for M=64, 1.2 times for M=128, and 1.4 times for M=256. However, for larger M, the fast transform [15] becomes more efficient and its application should be considered.

6. CONCLUSION

Our polynomial basis functions coupled with Fourier modes in the azimuthal direction form an orthogonal basis set on the unit disk in polar coordinates. They satisfy the pole conditions exactly, converge spectrally to a & function and satisfy the stable recurrence relations for r^2 , $r(d \neq dr)$, the inverse of r(d/dr)dr) and the Helmholtz operator. The inverses of r^2 and the Helmholtz operator can be computed efficiently and stably by solving these recurrence relations in matrix form. There is some arbitrariness in the parameters α and β and our numerical experiments suggest that β should be chosen according to the physical dimension of the problem. It is also suggested that $\alpha = 1$ gives a better result than $\alpha = \frac{1}{2}$. In time dependent problems our representation is not stiff at the pole and does not suffer from any significant time step restriction. The inefficiency of the matrix transform is a minor problem for moderate size of M. Unlike the representation of Robert and Merilees which becomes ill-conditioned for $M \gtrsim 25$ [3], our representation is well-conditioned for large M.

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