JOURNAL OF COMPUTATIONAL PHYSICS 96, 241–257 (1991)

Spectral Collocation Methods and Polar Coordinate Singularities

HENNER EISEN,* WILHELM HEINRICHS, AND KRISTIAN WITSCH

Heinrich-Heine-Universität Düsseldorf,
Lehrstuhl für Angewandte Mathematik,
Universitätsstraße 1, D-4000 Düsseldorf 1, Germany

Received July 19, 1989; revised February 8, 1990

This paper considers the numerical solution of elliptic differential equations on the unit disk. Using polar coordinates, the disk is mapped onto a rectangle. The resulting transformed problem is solved by a method related to collocation. Since the origin is a coordinate singularity, some natural trial functions are singular there and a special technique is applied to use zero as a collocation point. For Poisson and Helmholtz equations, a fast algorithm with an operation count of $\mathcal{O}(N^2 \log N)$ is presented. Numerical results show the different stability and convergence properties of the algorithms.

1. INTRODUCTION

Consider an elliptic differential operator A of second order defined on the unit disk

$$B := \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 \leqslant 1\}. \tag{1}$$

B is the image of the set

$$B^\circ := [0, 1] \times \mathbb{R}_{2\pi} \tag{2}$$

under the polar coordinate mapping

$$P : \mathbb{R}_0^+ \times \mathbb{R}_{2\pi} \to \mathbb{R}^2 \tag{3}$$

$$(r, \varphi) \mapsto (r \cos \varphi, r \sin \varphi). \tag{4}$$

Here $\mathbb{R}_{2\pi}$ denotes the set of equivalence classes of real numbers where two real numbers ϕ and ψ are equivalent if there exists an integer k such that $\phi - \psi = 2\pi k$. Thus, each function defined on $\mathbb{R}_{2\pi}$ is equivalent to a 2π-periodic function defined on $\mathbb{R}$. $\mathbb{R}_0^+$ denotes the set of non-negative real numbers.

* Work based on [3].

0021-9991/91 $3.00

For an arbitrary function f° on B° we define the corresponding function f on B by

$$f(x, y) := f^\circ \circ P^{-1}(x, y) \qquad \text{if} \quad (x, y) \neq 0 \tag{5}$$

$$f(0, 0) := \frac{1}{2\pi} \int_{\mathbb{R}_{2\pi}} f^\circ(0, \varphi)\, d\varphi \qquad \text{if} \quad (x, y) = 0. \tag{6}$$

Thus, f is continuous if $\lim_{x \to 0} f$ exists on $B \backslash \{0\}$.

Let U be the interior of B and S its boundary. The natural way of applying spectral methods to the problem

$$Au = f \qquad \text{on } U \tag{7}$$

$$u = g \qquad \text{on } S \tag{8}$$

is to compute the transformed differential operator A° and to solve the transformed differential equation

$$A^\circ u^\circ = f^\circ \qquad \text{on } U^\circ \tag{9}$$

$$u^\circ = g^\circ \qquad \text{on } S^\circ, \tag{10}$$

where $U^\circ := [0, 1) \times \mathbb{R}_{2\pi}$ and $S^\circ := \{1\} \times \mathbb{R}_{2\pi}$. Its numerical solution u_N° is expanded using trial functions

$$\Psi_{nk}^\circ(r, \varphi) := r^n e^{ik\varphi}, \tag{11}$$

as

$$u_N^\circ = \sum_{n=0}^{N} \sum_{k=-N+1}^{N} a_{nk} \Psi_{nk}^\circ. \tag{12}$$

For the case of collocation, we choose $N+1$ points $r_m \in [0, 1]$ (where $r_0 = 1$ and $r_i < r_j$ for $i > j > 0$ is assumed) and $2N$ points $\varphi_j \in \mathbb{R}_{2\pi}$. We then determine the coefficients a_{nk} from the system of equations

$$A^\circ u_N^\circ(r_m, \varphi_j) = f^\circ(r_m, \varphi_j), \qquad m = 1, ..., N; \qquad j = 0, ..., 2N-1 \tag{13}$$

$$u_N^\circ(r_0, \varphi_j) = g^\circ(r_0, \varphi_j), \qquad j = 0, ..., 2N-1. \tag{14}$$

This is straightforward if all r_m are different from zero. But a special problem arises in the case of $r_N = 0$. Since the polar coordinate mapping is not invertible at $r = 0$, it is not possible to evaluate $A^\circ u_N^\circ(0, \varphi_j)$ for arbitrary u_N°.

In order to obtain optimal convergence, the r_m are normally chosen as Gauss–Legendre or Gauss–Lobatto points. In particular, the Chebychev extremals are preferred since they allow the application of FFT. Unfortunately, $r = 0$ occurs as a collocation point just when FFT is most efficiently applicable (N a power of 2).

2. Regularity of Trial Functions

We consider trial functions of type (11). To obtain well-conditioned matrices, it is more convenient to use orthogonal polynomials than monomials with respect to the radial coordinate. But monomials allow a simpler investigation of regularity. The following results can be applied to orthogonal polynomials by expanding them in monomials.

Due to the coordinate singularity, the functions Ψ_{nk} are not necessarily as regular on B as the functions Ψ°_{nk} are on B°. For instance, Ψ_{10} is the euclidian norm which is not differentiable at 0 while Ψ_{0k} is discontinuous there for every $k \neq 0$. Similar problems arise in all singular coordinate systems. We refer to Orszag [11], Boyd [1], and Canuto, Hussaini, Quarteroni, and Zang [2]. To classify the regular and irregular functions Ψ_{nk}, there are a few important theorems. Although not very complicated, we do not know any reference where a clear mathematical formulation and proofs of them are published. So we will do this here.

Theorem 1. *Ψ_{nk} is n-times continuously differentiable if and only if it is a polynomial.*

Proof. The functions Ψ_{nk} are homogeneous of degree n, i.e., $\Psi_{nk}(tz) = t^n \Psi_{nk}(z)$ for all $z = (x, y) \in \mathbb{R}^2$ and all $t > 0$. Derivatives of functions which are homogeneous of degree j are homogeneous of degree $j-1$. Thus, the nth derivative of Ψ_{nk} is homogeneous of degree 0; i.e.,

$$\Psi^{(n)}_{nk}(tz) = \Psi^{(n)}_{nk}(z) \qquad \text{for all} \quad z \neq 0, \qquad t > 0. \tag{15}$$

Since $\Psi^{(n)}_{nk}$ is continuous, it follows $\lim_{t \to 0} \Psi^{(n)}_{nk}(tz) = \Psi^{(n)}_{nk}(0)$ and

$$\Psi^{(n)}_{nk}(z) = \Psi^{(n)}_{nk}(0) = \text{const} \tag{16}$$

for all $z \in B$. Since a derivative of Ψ_{nk} is constant Ψ_{nk} is a polynomial. ∎

To investigate whether Ψ_{nk} is n-times continuously differentiable, there is

Theorem 2. *Ψ_{nk} is a polynomial if and only if*

$$n - k \in 2\mathbb{Z} \tag{17}$$

(parity condition) and

$$n \geqslant |k|. \tag{18}$$

Proof. On $B \backslash \{0\}$ there is an explicit formula for the $\Psi_{nk} = \Psi^\circ_{nk} \circ P^{-1}$. We use the equalities $x = r\cos\varphi$, $y = r\sin\varphi$, $r = \sqrt{x^2+y^2}$, and $e^{i\varphi} = \cos\varphi + i\sin\varphi$. Therefore,

$$e^{ik\varphi} = (e^{i\varphi})^k \overset{r \neq 0}{=} \left(\frac{x+iy}{\sqrt{x^2+y^2}}\right)^k. \tag{19}$$

Thus,

$$r^n e^{ik\varphi} = (\sqrt{x^2+y^2})^n \frac{1}{(\sqrt{x^2+y^2})^k} (x+iy)^k \tag{20}$$

$$= (x^2+y^2)^{(n-k)/2} (x+iy)^k = \Psi_{nk}(x, y). \tag{21}$$

If $(n-k)$ is odd, Ψ_{nk} is never a polynomial because

$$\frac{\partial^n}{\partial x^n}\bigg|_{y=0} (\sqrt{x^2+y^2})^{n-k} (x+iy)^k = \begin{cases} n! & \text{for} \quad x>0 \\ -n! & \text{for} \quad x<0. \end{cases} \tag{22}$$

Thus, Ψ_{nk} has a partial derivative which cannot be continuously extended to B and is therefore not a polynomial on B.

To complete the proof, we have to consider only the case where $n-k$ is even. Factorizing

$$(x^2+y^2) = (x+iy)(x-iy), \tag{23}$$

we obtain

$$\Psi_{nk}(x, y) = (x+iy)^{(n+k)/2} (x-iy)^{(n-k)/2}. \tag{24}$$

If $|k| > n$, either the exponent of $(x+iy)$ or of $(x-iy)$ is negative in (24). Since the factors $(x+iy)$ and $(x-iy)$ are relatively prime, Ψ_{nk} cannot be a polynomial in this case.

If $|k| \leqslant n$, both exponents in (24) are non-negative. Thus, Ψ_{nk} is a polynomial on $B\backslash\{0\}$ which can be extended continuously to B (as done in (6)). ∎

Although not every function Ψ_{nk} is n-times differentiable, there is

THEOREM 3. *If $n \geqslant 2$ then Ψ_{nk} is at least $(n-1)$-times differentiable.*

Proof. Since Ψ_{nk} is homogeneous of degree n it follows that

$$\frac{\|\Psi_{nk}(z) - 0\|}{\|z-0\|^{n-1}} \leqslant \left(\sup_{\zeta \in B} \Psi_{nk}(\zeta)\right) \|z\| \to 0 \tag{25}$$

as $z \to 0$. Thus the $(n-1)$th derivative of Ψ_{nk} exists at $z=0$ and is zero. ∎

3. Collocation Equations at the Origin

If $r=0$ is a collocation point, we have to replace the $2N$ formal collocation equations

$$A^\circ u_N^\circ(0, \varphi_j) = f^\circ(0, \varphi_j), \qquad j = 0, ..., 2N-1 \tag{26}$$

which are contained in (13) by $2N$ well-defined equations. The problem is that u_N could consist of trial functions which are not twice differentiable. Thus, it is not possible to evaluate the differential operator in (26). On the other hand, we know that the solution u of $Au=f$ is at least twice Hölder-continuously differentiable if f is Hölder-continuous (see, for example, Gilbarg and Trudinger [4]). In version 1 of our method, we obtain the first equation by the modified collocation condition

$$A \sum_{(n,k)\in P} a_{nk}\Psi_{nk}(0,0)=f(0,0). \tag{27}$$

Here P denotes the set of index pairs belonging to twice differentiable trial functions, i.e. (by Theorems 2 and 3),

$$P := \{(n,k)\in \mathbb{Z}: (n\geqslant |k| \text{ and } n-k\in 2\mathbb{Z}) \text{ or } n>2\}. \tag{28}$$

Equation (27) implies that the twice differentiable part of u_N satisfies the collocation condition at the origin.

All partial derivatives up to order 2 of Ψ_{nk} are zero at the origin if $n>2$. Thus, the set P in (27) may be restricted to the set

$$P' := \{(0,0), (0, \pm 2), (1, \pm 1), (2,0), (2, \pm 2)\}. \tag{29}$$

We still need $2N-1$ further equations. The trial functions Ψ_{0k} are discontinuous if $k\neq 0$. In order to obtain a continuous numerical solution u_N we require the $2N-1$ conditions

$$a_{0k}=0 \qquad \text{for} \quad k=-N+1,\dots,N; \qquad k\neq 0. \tag{30}$$

Thus, with (27) and (30) we have obtained $2N$ linearly independent equations to replace (26).

Instead of (27), it is also possible to require that the derivative of the zeroth Fourier mode vanishes at the origin (version 2). This more familiar condition is motivated by the continuity of u' and equivalent to

$$a_{10}=0. \tag{31}$$

4. Numerical Results for Poisson's Problem

In this section we give a few numerical results where the ideas presented above have been applied to Poisson's problem

$$-\Delta u=f \qquad \text{on } U, \qquad u=g \qquad \text{on } S \tag{32}$$

with the exact solution $u(x,y)=e^{x+y}$. The transformed differential operator of Δ is

$$\Delta^\circ=\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}. \tag{33}$$

We compose u_N using only real-valued trial functions

$$u_N^\circ(r, \varphi) = \sum_{n=0}^{N} r^n \left(\sum_{k=0}^{N-1} a_{nk} \cos k\varphi + \sum_{k=1}^{N} b_{nk} \sin k\varphi \right). \tag{34}$$

The collocation points used are

$$\{(r_m, \varphi_j) : r_m = \cos m\pi/(2N),\ \varphi_j = (j + 1/2)\,\pi/N,\ m = 0, ..., N,\ j = 0, ..., 2N-1\}. \tag{35}$$

Tables I and II contain the discrete error

$$E_\infty := \max_{(r,\varphi) \in M} |u^\circ(r, \varphi) - u_N^\circ(r, \varphi)|, \tag{36}$$

where

$$M := \{(r_m, \varphi_j) : r_m = \cos(m\pi/(2N)),\ \varphi_j = j\pi/(2N),\\ m \in \{0, ..., N\},\ j \in \{0, ..., 4N-1\}\}. \tag{37}$$

The numerical solution contains trial functions that are not infinitely differentiable because their indices violate (17) or (18). This part of u_N is measured by the quantities

$$\Sigma_{k>n} := \sum_{|k|>n} (|a_{nk}| + |b_{nk}|) \tag{38}$$

$$\Sigma_{k+n \bmod 2} := \sum_{k+n \in 2\mathbb{Z}+1} (|a_{nk}| + |b_{nk}|) \tag{39}$$

$$\Sigma := \sum_{|k|>n \text{ or } k+n \in 2\mathbb{Z}+1} (|a_{nk}| + |b_{nk}|). \tag{40}$$

TABLE I

Collocation for Poisson's Problem on the Unit Disk (Version 1)

N	E_∞	$\Sigma_{n+k \bmod 2}$	$\Sigma_{k>n}$	Σ
2	2.949×10^{-1}	1.620×10^{0}	1.280×10^{-1}	1.620×10^{0}
3	9.935×10^{-2}	8.675×10^{-1}	1.249×10^{-1}	8.819×10^{-1}
4	2.198×10^{-2}	4.751×10^{-1}	6.029×10^{-2}	4.834×10^{-1}
5	2.380×10^{-3}	1.783×10^{-1}	3.130×10^{-2}	1.859×10^{-1}
6	7.623×10^{-5}	7.132×10^{-2}	1.194×10^{-2}	7.476×10^{-2}
7	2.771×10^{-5}	1.883×10^{-2}	2.595×10^{-3}	1.960×10^{-2}
8	3.273×10^{-6}	5.458×10^{-3}	5.795×10^{-4}	5.632×10^{-3}
9	1.900×10^{-7}	1.164×10^{-3}	1.141×10^{-4}	1.200×10^{-3}
10	2.231×10^{-9}	2.697×10^{-4}	2.184×10^{-5}	2.769×10^{-4}
11	8.548×10^{-10}	4.765×10^{-5}	3.191×10^{-6}	4.870×10^{-5}
12	6.816×10^{-11}	9.185×10^{-6}	4.639×10^{-7}	9.337×10^{-6}
13	2.728×10^{-12}	5.481×10^{-6}	3.048×10^{-6}	6.815×10^{-6}
14	3.306×10^{-12}	5.589×10^{-5}	3.435×10^{-5}	7.113×10^{-5}
15	9.555×10^{-12}	4.056×10^{-4}	1.848×10^{-4}	4.843×10^{-4}
16	8.612×10^{-12}	2.733×10^{-3}	1.111×10^{-3}	3.213×10^{-3}

TABLE II

Collocation for Poisson's Problem on the Unit Disk (Version 2)

N	E_∞	$\Sigma_{n+k \bmod 2}$	$\Sigma_{k>n}$	Σ
2	9.589×10^{-2}	1.236×10^{0}	1.280×10^{-1}	1.236×10^{0}
3	9.310×10^{-2}	7.463×10^{-1}	1.250×10^{-1}	7.607×10^{-1}
4	2.185×10^{-2}	4.737×10^{-1}	6.030×10^{-2}	4.820×10^{-1}
5	2.365×10^{-3}	1.823×10^{-1}	3.131×10^{-2}	1.900×10^{-1}
6	6.037×10^{-5}	7.223×10^{-2}	1.194×10^{-2}	7.567×10^{-2}
7	2.777×10^{-5}	1.920×10^{-2}	2.596×10^{-3}	1.997×10^{-2}
8	3.272×10^{-6}	5.508×10^{-3}	5.796×10^{-4}	5.681×10^{-3}
9	1.902×10^{-7}	1.178×10^{-3}	1.141×10^{-4}	1.215×10^{-3}
10	2.040×10^{-9}	2.713×10^{-4}	2.184×10^{-5}	2.785×10^{-4}
11	8.545×10^{-10}	4.802×10^{-5}	3.225×10^{-6}	4.909×10^{-5}
12	6.817×10^{-11}	9.303×10^{-6}	4.835×10^{-7}	9.463×10^{-6}
13	2.747×10^{-12}	4.335×10^{-6}	1.952×10^{-6}	5.169×10^{-6}
14	7.810×10^{-13}	2.486×10^{-5}	5.691×10^{-6}	2.711×10^{-5}
15	3.073×10^{-12}	2.687×10^{-4}	1.268×10^{-4}	3.232×10^{-4}
16	4.767×10^{-12}	2.358×10^{-3}	8.626×10^{-4}	2.736×10^{-3}

For small N, we observe the well-known exponential convergence. For larger N, this is disturbed by rounding errors because the monomials in the radial part of the trial functions lead to rather ill-conditioned matrices. A somewhat surprising feature is that the Σ's are relatively large compared to the numerical error E_∞.

5. Smooth Least Squares Solutions

Since the non-smooth trial functions are well-known, by Theorems 1 and 2, we might expand u_N using only smooth trial functions. This would require fewer collocation points. The problem is how to choose them, because there is no longer a natural distribution such as the cartesian product of one-dimensional distributions.

Another way is to use only smooth trial functions but the same collocation points as in (35). This results in an overdetermined system of equations $Mx = b$ whose least squares solution can be computed.

We have applied this to the problem of the previous section. Tables III and IV contain the numerical results. The columns marked by "$\Sigma = 0$" contain the errors of the numerical solution which consists only of totally smooth trial functions. In addition, we have computed a solution which only satisfies either the smoothness condition (18) (the corresponding columns are marked by "$\Sigma_{k>n} = 0$") or the condition (17) ("$\Sigma_{n+k \bmod 2} = 0$").

The linear least squares problems have been solved by the QR-algorithm. This can also be done by solving the normal equations $MM^{\mathrm{T}}x = M^{\mathrm{T}}b$ by the Cholesky

TABLE III

Linear Least Squares Solutions of Overdetermined Collocation (Version 1)

	$\Sigma_{k>n}=0$		$\Sigma_{n+k \bmod 2}=0$		$\Sigma=0$
N	E_∞	Σ	E_∞	Σ	E_∞
2	2.949×10^{-1}	1.492×10^{0}	2.242×10^{-1}	6.762×10^{-2}	2.293×10^{-1}
3	9.936×10^{-2}	6.846×10^{-1}	8.968×10^{-2}	3.537×10^{-2}	8.984×10^{-2}
4	2.207×10^{-2}	3.599×10^{-1}	2.138×10^{-2}	7.452×10^{-3}	2.076×10^{-2}
5	2.380×10^{-3}	1.109×10^{-1}	2.331×10^{-3}	3.183×10^{-3}	2.378×10^{-3}
6	7.624×10^{-5}	4.437×10^{-2}	1.377×10^{-4}	6.330×10^{-4}	1.149×10^{-4}
7	2.771×10^{-5}	1.053×10^{-2}	2.756×10^{-5}	1.147×10^{-4}	2.752×10^{-5}
8	3.276×10^{-6}	3.121×10^{-3}	3.322×10^{-6}	1.760×10^{-5}	3.269×10^{-6}
9	1.900×10^{-7}	6.044×10^{-4}	1.900×10^{-7}	2.405×10^{-6}	1.887×10^{-7}
10	2.232×10^{-9}	1.423×10^{-4}	5.133×10^{-9}	3.266×10^{-7}	3.863×10^{-9}
11	8.549×10^{-10}	2.322×10^{-5}	8.547×10^{-10}	3.371×10^{-8}	8.484×10^{-10}
12	6.814×10^{-11}	4.464×10^{-6}	6.834×10^{-11}	3.947×10^{-9}	6.809×10^{-11}
13	2.730×10^{-12}	8.933×10^{-7}	2.723×10^{-12}	3.418×10^{-10}	2.712×10^{-12}
14	4.317×10^{-12}	7.455×10^{-6}	5.373×10^{-14}	3.597×10^{-11}	4.152×10^{-14}
15	9.010×10^{-12}	4.702×10^{-5}	3.619×10^{-14}	2.932×10^{-12}	2.309×10^{-14}
16	2.001×10^{-11}	3.475×10^{-4}	3.619×10^{-14}	1.259×10^{-12}	2.598×10^{-14}

TABLE IV

Linear Least Squares Solutions of Overdetermined Collocation (Version 2)

	$\Sigma_{k>n}=0$		$\Sigma_{n+k \bmod 2}=0$		$\Sigma=0$
N	E_∞	Σ	E_∞	Σ	E_∞
2	9.589×10^{-2}	1.108×10^{0}	2.106×10^{-1}	6.762×10^{-2}	2.158×10^{-1}
3	9.311×10^{-2}	5.634×10^{-1}	9.582×10^{-2}	3.537×10^{-2}	8.951×10^{-2}
4	2.193×10^{-2}	3.585×10^{-1}	2.134×10^{-2}	7.452×10^{-3}	2.072×10^{-2}
5	2.365×10^{-3}	1.149×10^{-1}	2.318×10^{-3}	3.183×10^{-3}	2.365×10^{-3}
6	6.001×10^{-5}	4.527×10^{-2}	1.372×10^{-4}	6.330×10^{-4}	1.154×10^{-4}
7	2.776×10^{-5}	1.090×10^{-2}	2.758×10^{-5}	1.147×10^{-4}	2.750×10^{-5}
8	3.274×10^{-6}	3.170×10^{-3}	3.322×10^{-6}	1.760×10^{-5}	3.269×10^{-6}
9	1.902×10^{-7}	6.184×10^{-4}	1.899×10^{-7}	2.405×10^{-6}	1.888×10^{-7}
10	2.035×10^{-9}	1.438×10^{-4}	5.142×10^{-9}	3.266×10^{-7}	3.873×10^{-9}
11	8.545×10^{-10}	2.359×10^{-5}	8.546×10^{-10}	3.371×10^{-8}	8.484×10^{-10}
12	6.813×10^{-11}	4.514×10^{-6}	6.834×10^{-11}	3.947×10^{-9}	6.809×10^{-11}
13	2.730×10^{-12}	7.809×10^{-7}	2.723×10^{-12}	3.419×10^{-10}	2.712×10^{-12}
14	1.647×10^{-12}	7.744×10^{-6}	5.351×10^{-14}	3.597×10^{-11}	4.174×10^{-14}
15	3.210×10^{-12}	4.566×10^{-5}	3.331×10^{-14}	2.810×10^{-12}	2.420×10^{-14}
16	1.025×10^{-11}	4.586×10^{-4}	3.419×10^{-14}	1.157×10^{-12}	2.509×10^{-14}

algorithm within about half the CPU time. But due to the squared condition number, the rounding errors increase faster if N is increased. For our example, we first observe bigger errors E_∞ if $N \geqslant 10$ ($\Sigma_{k>N}=0$), $N \geqslant 12$ ($\Sigma_{n+k \bmod 2}=0$), or $N \geqslant 13$ ($\Sigma=0$).

The most obvious result is that one obtains better-conditioned problems and a smaller non-smooth part of u_N if its expansion takes (17) into account. The effect of using (18) (only or additionally) is much less significant.

We can take advantage of this behavior if we use orthogonal polynomials Q_n instead of monomials r^n for the radial part of the trail functions. If the weight function is symmetric, the corresponding orthogonal polynomials are either even or odd. Thus, (17) can also be satisfied for functions $Q_n e^{ik\varphi}$. In this case, we do not have to deal with overdetermined systems of equations any longer if we just halve the density of collocation points with respect to the radial coordinate. Applying FFT, it is possible to obtain fast and stable algorithms. This is applied in the next sections.

As regards the two different ways of handling the coordinate origin, version 1 using (27) and version 2 using (31), version 2 is often slightly better if the parity condition $\Sigma_{n+k \bmod 2}=0$ is not enforced. For the other cases, where enforcing $\Sigma_{n+k \bmod 2}=0$ implies (31) automatically, there are no significant differences. The advantage of version 1 is that condition (27) can be used with a non-overdetermined set of collocation points even if $\Sigma_{n+k \bmod 2}=0$ is enforced (as mentioned in the previous paragraph).

6. Separable Equations

If the coefficients of the transformed operator do not depend on φ, we can make a numerical separation approach. We consider for example Poisson's equation (32). We restrict our considerations to homogeneous boundary conditions $u=0$ on S. Solutions to inhomogeneous boundary conditions can be computed by adding an auxiliary function u_g, where $u_g=g$ at all collocation points in S,

$$\{\varphi_j\colon \varphi_j = j\pi/N,\ j=0, ..., 2N-1\}. \tag{41}$$

A good choice for u_g is a linear combination of the (harmonic) functions $r^n e^{\pm in\varphi}$.

To solve the transformed differential equation

$$-\Delta^\circ u^\circ = f^\circ \qquad \text{on } U^\circ, \qquad u^\circ = 0 \qquad \text{on } S^\circ \tag{42}$$

numerically, our procedure starts by evaluating the right-hand side f° at the collocation points (N even)

$$\{(r_m, \varphi_j)\colon r_m = \cos m\pi/N,\ \varphi_j = j\pi/N,\ m=0, ..., N/2,\ j=0, ..., 2N-1\}. \tag{43}$$

These values are partially interpolated with respect to the φ-coordinate. This can be done by $\mathcal{O}(N^2 \log N)$ arithmetic operations since it requires the application of $(N/2+1)$ FFTs. We obtain

$$f^\circ(r_m, \varphi_j) = \sum_{k=-N+1}^{N} \widehat{f_k^\circ}(r_m)\, e^{ik\varphi_j}, \tag{44}$$

where $(\widehat{f_k^\circ}(r))_{k=-N+1,...,N}$ is the discrete partial Fourier transform (interpolant) of f° which we have only evaluated at the points r_m. We, analogously, represent the numerical solution u_N° by its discrete transform

$$u_N^\circ(r_m, \varphi_j) = \sum_{k=-N+1}^{N} \widehat{u_{Nk}^\circ}(r_m)\, e^{ik\varphi_j}. \tag{45}$$

Our goal is to obtain a collocation solution; i.e.,

$$-\Delta^\circ u_N^\circ(r, \varphi) = f^\circ(r, \varphi) \tag{46}$$

should hold if (r, φ) is a collocation point (43). If we insert (45) and (44) into (46) we obtain the $2N$ ordinary differential equations

$$\left(-\frac{1}{r}\frac{d}{dr} r \frac{d}{dr} + \frac{k^2}{r^2}\right) \widehat{u_{Nk}^\circ}(r) = \widehat{f_k^\circ}(r) \tag{47}$$

for $k = -N+1, ..., N$.

In order to obtain a numerical solution u_N which satisfies the parity condition (17), we compose $\widehat{u_{Nk}^\circ}(r)$ by using even trial functions if k is even and by odd trial functions if k is odd. This can be described formally by extending the function $\widehat{f_k^\circ}$ to $[-1, 1]$ by

$$\widehat{f_k^\circ}(-r) := \begin{cases} \widehat{f_k^\circ}(r) & k \text{ even} \\ -\widehat{f_k^\circ}(r) & k \text{ odd} \end{cases} \tag{48}$$

and finally restricting the numerical solutions $\widehat{u_{Nk}^\circ}(r)$ to $[0, 1]$. If the equations (47) are solved numerically by collocation at the points

$$r_m = \cos(m\pi/N), \qquad m = 0, ..., N, \tag{49}$$

(46) will hold for all collocation points defined in (43). As already discussed in Section 3, the collocation equations are not well defined at the origin. After the separation approach, the resulting ordinary differential operators are singular for $r=0$. We overcome this problem by multiplying Eq. (47) by r^2 and obtain

$$\left(-r\frac{d}{dr} r \frac{d}{dr} + k^2\right) \widehat{u_{Nk}^\circ}(r) = r^2 \widehat{f_k^\circ}(r). \tag{50}$$

Thus, for the collocation point $r=0$ we obtain the equations

$$k^2\widehat{\mathring{u}_{Nk}}(0)=0. \tag{51}$$

For $k\neq 0$, this would result in $a_0=0$ if we used monomials as trial functions to expand

$$\widehat{\mathring{u}_{Nk}}(r)=\sum_{n=0}^{N} a_n r^n. \tag{52}$$

Thus, the numerical solution u_N to (42) will automatically satisfy (30) and is continuous.

For $k=0$, we consider the limit of the basic equation (47) as $r\to 0$:

$$\lim_{r\to 0}\left(-\frac{d^2}{dr^2}\widehat{\mathring{u}_{N0}}(r)-\frac{1}{r}\frac{d}{dr}\widehat{\mathring{u}_{N0}}(r)\right)=\widehat{\mathring{f}_0}(0). \tag{53}$$

This is possible only if

$$\lim_{r\to 0}\frac{1}{r}\frac{d}{dr}\widehat{\mathring{u}_{N0}}(r) \tag{54}$$

exists. Fortunately, $\widehat{\mathring{u}_{N0}}(r)$ consists of even trial functions only, in order to let u_N satisfy the parity condition (17). If the trial functions are continuously differentiable, $\frac{d}{dr}\big|_{r=0}\widehat{\mathring{u}_{N0}}(0)=0$ and (54) exists. Applying l'Hôpital's theorem, we obtain

$$\lim_{r\to 0}\frac{1}{r}\frac{d}{dr}\widehat{\mathring{u}_{N0}}(r)=\frac{d^2}{dr^2}\bigg|_{r=0}\widehat{\mathring{u}_{N0}}(r). \tag{55}$$

Thus, we can use

$$-2\frac{d^2}{dr^2}\bigg|_{r=0}\widehat{\mathring{u}_{N0}}(r)=\widehat{\mathring{f}_0}(0) \tag{56}$$

as the equation at the collocation point $r=0$.

This separation method is easily extended to Helmholtz' equation

$$-\Delta u+\lambda u=f, \tag{57}$$

where λ denotes a constant. Instead of (47) we have to solve inhomogeneous Bessel's differential equations

$$\left(-\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}+\frac{k^2}{r^2}+\lambda\right)\widehat{\mathring{u}_{Nk}}(r)=\widehat{\mathring{f}_k}(r). \tag{58}$$

Instead of (56) we then have

$$\left(-2\frac{d^2}{dr^2}\bigg|_{r=0}+\lambda\right)\widehat{\mathring{u}_{N0}}(r)=\widehat{\mathring{f}_0}(0). \tag{59}$$

7. Efficient Solution of Bessel's Equation

In this section we deal a lot with subscripted variables. If some of them are used without having defined their values before, these values are assumed to be zero.

If we compute the collocation approximations of (47) in a straightforward manner by solving a full-matrix system for each differential equation, the algorithm would require $\mathcal{O}(N^4)$ operations. This is already an improvement, since a direct approach as described by (13) requires $\mathcal{O}(N^6)$. We will now describe a very efficient algorithm to compute the numerical solution of (47) by $\mathcal{O}(N \log N)$ operations. Thus, the collocation approximation of Poisson's problem is computable by $\mathcal{O}(N^2 \log N)$ operations.

A fast collocation solver for differential equations of the type

$$-r \frac{d}{dr} r \frac{d}{dr} v(r) + k^2 v(r) = r^2 \widehat{f^\circ}, \qquad v(-1) = v(1) = 0, \tag{60}$$

can be derived from the τ-method of C. Lanczos [10]. We compose the numerical solution by the trial functions

$$\Psi_n(r) := (1 - r^2)\, T_n(r), \tag{61}$$

where $T_n(r) = \cos(n \arccos r)$ denotes the Chebychev polynomial of degree n. The advantage of these trial functions is that we do not have to treat the boundary conditions explicitly. Furthermore, they lead to better-conditioned matrices; for further details see Heinrichs [9].

The right-hand side of (60) is interpolated by Chebychev polynomials

$$r_m^2\, g(r_m) = \sum_{l=0}^{N} b_l T_l(r_m), \tag{62}$$

where the r_m are the members of the collocation point set (49). It is possible to compute the coefficients b_l by $\mathcal{O}(N \log N)$ operations applying the fast cosine transform (see, for example, [2]). For further usage we denote by h the function

$$h(r) := \sum_{l=0}^{N} b_l T_l(r). \tag{63}$$

Let A be an arbitrary differential operator such that

$$A \Psi_n(r) = \sum_{p=0}^{N+t} s_{np} T_p(r) \tag{64}$$

holds. Here, t denotes an integer of small absolute value.

A function

$$v_N(r) := \sum_{n=0}^{N} a_n \Psi_n(r) \tag{65}$$

satisfies the differential equation

$$Av_N = h \tag{66}$$

if and only if the coefficients a_n satisfy the system of equations

$$\sum_{n=0}^{N} s_{np} a_n = b_p, \qquad p = 0, ..., N+t. \tag{67}$$

If $t > 0$, the system (67) is overdetermined and generally not solvable. The τ-method for approximately computing v_N consists of simply neglecting the equations of (67) with $p > N$. It is not necessary to neglect such equations if we want only that v_N satisfy (60) at the collocation points (49). Similarily to the s_{np}, we can define coefficients $\tilde{s}_{np}$ which satisfy

$$A\Psi_n(r_m) = \sum_{p=0}^{N} \tilde{s}_{np} T_p(r_m) \tag{68}$$

for all collocation points (49). If the a_n satisfy the system

$$\sum_{n=0}^{N} \tilde{s}_{np} a_n = b_p, \qquad p = 0, ..., N, \tag{69}$$

then v_N satisfies (66) at the collocation points r_m. Since $h(r_m) = r_m^2 \widehat{f^\circ}(r_m)$, v_N is also the collocation solution of (60) where $A = -r(d/dr)\, r(d/dr) + k^2 + r^2\lambda$.

In the special case of the collocation points (43) the $\tilde{s}_{np}$ can be easily computed from the τ-method's s_{np}. At these points the Chebychev polynomials satisfy the equality

$$T_k(r_m) = T_{2N-k}(r_m). \tag{70}$$

Thus, the $\tilde{s}_{np}$ can be computed by

$$\tilde{s}_{np} = s_{np} + s_{n\,2N-p} \tag{71}$$

$$n = 0, ..., N; \qquad p = 0, ..., N-1 \tag{72}$$

$$\tilde{s}_{nN} = s_{nN} \tag{73}$$

$$n = 0, ..., N \tag{74}$$

if $N \geqslant t$.

The s_{np} for simple differential operators are well known. Auxiliary formulas to compute them are presented by Gottlieb and Orszag [5]. If $A = I$ (identity), we have

$$I\Psi_n(r) = \sum_{p=0}^{n+2} s^I_{np} T_p(r), \tag{75}$$

where $s^I_{nn} = \frac{1}{2}$ and $s^I_{nn-2} = s^I_{nn+2} = -\frac{1}{4}$ except that $s^I_{02} = -\frac{1}{2}$ and $s^I_{11} = \frac{1}{4}$.

If $A = r(d/dr)\,r(d/dr)$, we have

$$r\frac{d}{dr}r\frac{d}{dr}\Psi_n(r) = \sum_{p=0}^{n+2} s^D_{np} T_p(r), \tag{76}$$

where $s^D_{nn+2} = (-n^2 - 4n - 4)/4$, $s^D_{nn} = (-2n^2 - 12n - 8)/4$, $s^D_{nn-2} = (-n^2 - 20n - 4)/4$, $s^D_{np} = -6n$ for $p = 1, ..., n-4$ and $n + p \in 2\mathbb{Z}$, $s^D_{n0} = 3n$ for $n \in 2\mathbb{Z}$ and $n \geqslant 4$. Special values for low indices are $s^D_{02} = 2$, $s^D_{11} = -\frac{23}{4}$, $s^D_{20} = -6$, and $s^D_{24} = -4$.

If A is the multiplication by r^2 we have

$$r^2\Psi_n(r) = \sum_{p=0}^{n+4} s^r_{np} T_p(r), \tag{77}$$

where $s^r_{nn} = \frac{1}{8}$, $s^r_{nn-4} = s^r_{nn+4} = s^r_{13} = s^r_{31} = -\frac{1}{16}$, but $s^r_{04} = -\frac{1}{8}$ and $s^r_{22} = \frac{1}{16}$.

Thus, we are able to compute the $\tilde{s}_{np}$ which arise when Bessel's differential operator (multiplied by r^2),

$$-r\frac{d}{dr}r\frac{d}{dr} + k^2 + \lambda r^2, \tag{78}$$

is discretized. The required s_{np} are

$$s_{np} = -s^D_{np} + s^I_{np} + \lambda s^r_{np}, \tag{79}$$

from which the $\tilde{s}_{np}$ can be computed using (71).

Solving (69) results in the matrix formulation

$$\tilde{S}^{\mathrm{T}} a = b, \tag{80}$$

where $a = (a_p)$, $b = (b_p)$, and $\tilde{S}^{\mathrm{T}}$ is the transpose of the matrix $\tilde{S} = (\tilde{s}_{np})$; $n, p = 0, ..., N$; $\tilde{S}^{\mathrm{T}}$ has a special Hessenberg-like structure. By an elimination process, it can be transformed to a band matrix $T\tilde{S}^{\mathrm{T}}$. The matrix T which formally describes this elimination process is

$$T = \begin{pmatrix} 1 & 0 & -1/2 & & & \\ & 1 & 0 & -1 & & \\ & & 1 & 0 & \ddots & \\ & & & 1 & \ddots & -1 \\ & & & & \ddots & 0 \\ & 0 & & & & 1 \end{pmatrix}. \tag{81}$$

Thus, the solution a of (80) can be obtained by solving the equivalent band matrix system

$$T\tilde{S}^{\mathrm{T}}a = Tb. \tag{82}$$

The matrix $T\tilde{S}^{\mathrm{T}}$ and the vector Tb can be computed within $\mathcal{O}(N)$ operations. Thus, the system (80) is also solvable within $\mathcal{O}(N)$ operations.

The total computational work to obtain the collocation solution of (60) is dominated by the interpolation (fast cosine transform) of the right-hand side which requires $\mathcal{O}(N \log N)$ operations.

We still have to show how to handle the case $k^2 = 0$. Computing the $\tilde{s}_{nk}$ and applying the elimination process (82) results in a singular band matrix $T\tilde{S}^{\mathrm{T}}$. We eliminate its subdiagonals. Applying this elimination, the lowest matrix row becomes zero. This zero row is then replaced by the coefficients which arise from Eq. (59). After eliminating this row, an upper triangular band matrix system remains which can be solved easily.

8. Numerical Results

Tables V and VI contain the numerical errors

$$\max_{(r_m, \varphi_j) \in M} |u(r_m, \varphi_j) - u_N(r_m, \varphi_j)|, \tag{83}$$

where M denotes the set of collocation points (43). The u_N have been computed by the numerical separation approach. Table V contains solutions to Helmholtz equations with various λ. For $\lambda = 5$, we have solved, in addition, the ordinary differential equations by the τ-method. As a test for critical λ, we have chosen $-\lambda = (2.4048)^2$ which is close to the first eigenvalue of $-\Delta$. Table VI contains the errors to Poisson problems with various exact solutions u. The functions $u = r^a$ are not infinitely

TABLE V

Numerical Errors of Even-Parity Collocation Solutions to $-\Delta u + \lambda u = f$, where $u = \cos(3x + 4y + 0.7)$

N	$\lambda = 0$	$\lambda = 1$	$\lambda = 5$	$\lambda = 5$, τ-meth.
8	2.457×10^{-3}	2.143×10^{-3}	4.497×10^{-3}	7.554×10^{-2}
16	1.232×10^{-9}	5.310×10^{-9}	2.103×10^{-8}	1.911×10^{-7}
32	2.012×10^{-15}	1.901×10^{-15}	2.304×10^{-15}	2.359×10^{-15}
	$\lambda = 10$	$\lambda = 30$	$\lambda = 100$	$\lambda = -(2.4048)^2$
8	8.368×10^{-3}	2.139×10^{-2}	5.294×10^{-2}	2.551×10^{2}
16	3.940×10^{-8}	1.024×10^{-7}	2.522×10^{-7}	3.496×10^{-5}
32	1.915×10^{-15}	2.678×10^{-15}	2.984×10^{-15}	2.752×10^{-11}

TABLE VI

Numerical Errors of Even-Parity Collocation Solutions to Various Poisson Problems

N	$u=e^{x+y}$	$u=\cos(7x+8y+0.7)$	
8	2.856×10^{-8}	1.474×10^{0}	
16	2.665×10^{-15}	4.873×10^{-4}	
32	2.665×10^{-15}	7.994×10^{-15}	
	$u=r^{2.5}$	$u=r^{3}$	$u=r^{5}$
8	7.677×10^{-2}	2.922×10^{-2}	1.225×10^{-3}
16	1.647×10^{-2}	4.223×10^{-3}	2.498×10^{-5}
32	3.438×10^{-3}	6.045×10^{-4}	8.505×10^{-7}

differentiable (Theorems 1, 2, and 3). e^{x+y} is included for comparisons with the straightforward program. For $\cos(7x+8y+0.7)$, the magnitude of the rounding error is equal to the truncation error if $N=32$.

All numerical results presented in this paper have been computed on a SIEMENS 7.580-S computer using double precision arithmetic (14 hexadecimal digits mantissa).

9. Conclusions

We have shown how to extend the spectral collocation method to problems on domains which are parametrized by singular coordinate systems. This is possible even if the coordinate singularity is a collocation point. The space spanned by the trial functions is a direct sum of two subspaces which contain either smooth or non-smooth functions. The smooth functions are those functions which are in the differential operator's domain of definition. The collocation equations at the origin are then replaced by a collocation equation to be satisfied by the smooth part of the numerical solution and a continuity condition.

Our numerical results show that it is possible to find a set of collocation points on a disk such that exponential convergence is achieved. For some (separable) differential equations, the numerical solution can be computed within $\mathcal{O}(N^2 \log N)$ operations.

For the case of non-separable equations with a separable principle part, the fast algorithm provides us with an efficient preconditioner for iterative solvers. It should also be possible to use it within a spectral multi-grid algorithm (Zang, Wong, Hussaini [12, 13], Heinrichs [6, 7, 8]).

REFERENCES

1. J. P. BOYD, *Mon. Weather Rev.* **106**, 1184 (1978).
2. C. CANUTO, M. Y. HUSSAINI, A. QUARTERONI, AND T. A. ZANG, *Spectral Methods in Fluid Dynamics* (Springer-Verlag, New York, 1988).
3. H. EISEN, *Spektrale Verfahren für die Poissongleichung auf dem Einheitskreis*, Diploma thesis, Mathematischen Institut der Universität Düsseldorf, 1988 (unpublished).
4. D. GILBARG AND N. S. TRUDINGER, *Elliptic Partial Differential Equations of Second Order*, 2nd ed. (Springer-Verlag, Berlin, 1983).
5. D. GOTTLIEB AND S. A. ORSZAG, *Numerical Analysis of Spectral Methods: Theorie and Applications*, CBMS-NSF Regional Conference Series in Applied Mathematics, No. 104 (SIAM, Philadelphia, 1977).
6. W. HEINRICHS, *Kollokationsverfahren und Mehrgittermethoden bei elliptischen Randwertaufgaben*, GMD-Bericht 168 (Oldenbourg-Verlag, Munich/Vienna, 1987).
7. W. HEINRICHS, *J. Comput. Phys.* **77**, 166 (1988).
8. W. HEINRICHS, *J. Comput. Phys.* **78**, 424 (1988).
9. W. HEINRICHS, *Math. Comput.* **53**, 103 (1989).
10. C. LANCZOS, *Applied Analysis* (Prentice–Hall, Engelwood Cliffs, NJ, 1956).
11. S. A. ORSZAG, *Mon. Weather Rev.* **102**, 56 (1974).
12. T. A. ZANG, Y. S. WONG, AND M. Y. HUSSAINI, *J. Comput. Phys.* **48**, 485 (1982).
13. T. A. ZANG, Y. S. WONG, AND M. Y. HUSSAINI, *J. Comput. Phys.* **54**, 489 (1984).