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Finite Element Methods for Spherically Symmetric Elliptic Equations

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1. Introduction

In this paper we consider the numerical solution of elliptic partial differential equations in spherical domains. There are numerous applications in engineering and the physical sciences in which the solution of a spherical elliptic equation is desired; see the references in [12]. When all the functions involved are spherically symmetric (that is, they depend only on distance from the center of the domain), the problem can be replaced by an equivalent two-point boundary value problem. The resulting problem is singular, but nevertheless has a smooth solution. It should therefore be possible to approximate the solution accurately using the Rayleigh-Ritz Galerkin method with a piecewise polynomial subspace on a quasiuniform mesh. We will obtain optimal-order error bounds, showing that this procedure is theoretically well-founded. Instead of the usual Sobolev norms, we use norms which are appropriate to the original n-dimensional setting of the problem.

The problem has been considered, in 2 and 3 dimensions, by Russell and Shampine [12]. They obtain error bounds for approximation procedures specially designed to deal with the apparent singularity at the origin. In particular, they treat collocation in which the basis is augmented by singular basis functions, singular patch bases (L-splines), and a finite difference scheme of Jamet [8] designed to handle the singularity. Crouzeix and Thomas [1] and Reddien [11] consider this problem as part of a wider class and obtain similar results.

Dupont and Wahlbin [4] and Jesperson [9] have analyzed an approximation procedure similar to ours, and have obtained error bounds of optimal order in the usual Sobolev norms. The import of their results, together with those of this paper, is that no special measures are required for this problem: the Rayleigh-Ritz Galerkin method using high-order piecewise polynomial spaces on a uniform mesh is a highly effective numerical method.

2. Spherically Symmetric Elliptic Problems

Let B(a) be the open sphere of radius a in R^n, i.e.,

$$B(a) \equiv \{\underline{x} \in R^n \mid r(\underline{x}) < a\},$$

where $r(\underline{x}) \equiv \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2}$, and $B \equiv B(1)$ be the open unit sphere.

Consider the partial differential equation

$$- \Delta U + QU = F \quad \text{in } B, \tag{1}$$

$$U = 0 \quad \text{on } \partial B, \tag{2}$$

where F and Q are given functions defined on B. We say that a function defined on B is <u>spherically symmetric</u> if it depends only on distance r from the origin. If F and Q are spherically symmetric then an obvious symmetry argument shows that U is, too (a change in coordinate systems by rotation around any axis passing through the origin leaves the problem, and hence its solution, unchanged).

Let u(r), f(r), and q(r) be functions such that

$$F(\underline{x}) = f(r(\underline{x})),$$

$$Q(\underline{x}) = q(r(\underline{x})),$$

$$U(\underline{x}) = u(r(\underline{x})).$$

Then u(r) can be obtained as the solution of the singular two-point boundary value problem

$$- D(r^{n-1}Du) + r^{n-1}q(r)u = r^{n-1}f(r), \qquad 0 < r < 1, \tag{3}$$

$$Du(0) = u(1) = 0, \tag{4}$$

where $D \equiv \frac{d}{dr}$.

We note that in case n = 3, the well-known change of variables v = ru results in the nonsingular problem

$$- D^2v + qv = rf, \qquad 0 < r < 1,$$

$$v(0) = v(1) = 0.$$

However, we know of no such trick in two dimensions!

For real-valued functions f,g defined on (0,a) we let

$$(f,g)_{B(a)} \equiv \int_0^a r^{n-1} f(r)g(r)\, dr,$$

and

$$\| f \|_{B(a)} \equiv (f,f)_{B(a)}^{1/2}.$$

Furthermore, we define $J^m(a)$ (respectively $J_0^m(a)$) to be the closure of the C^∞ functions (respectively the C^∞ functions which vanish in a neighborhood of a) with respect to the norm

$$\| f \|_{m,B(a)} \equiv \left(\sum_{j=0}^{m} \| D^j f \|_{B(a)}^2 \right)^{1/2}.$$

We assume that the coefficient $q \in C(I)$ is such that there exist positive constants λ and Λ such that

$$\lambda^2 \| Du \|^2_{B(a)} \leq [u,u]_{B(a)} \leq \Lambda^2 \| Du \|^2_{B(a)} \tag{5}$$

for all $u \in J^1(a)$, where

$$[u,v]_{B(a)} \equiv \int_0^a r^{n-1} [DuDv + quv] \, dr.$$

Our approximation-theoretic results in the spaces J^m will rely on the following basic fact, proved in Courant and Hilbert [2].

Lemma 1: If $f \in J_0^1(a)$, then

$$\| f \|_{B(a)} \leq a \, \| Df \|_{B(a)}. \tag{6}$$

Inequalities (5) and (6) show that the bilinear form $[\ ,\ ]_B$ is positive definite over the space J_0^1. Thus, for each $f \in J^0$ there exists a unique $u \in J_0^1$, called the generalized solution of (3) - (4), such that

$$[u,v]_B = (f,v)_B, \quad \text{for all } v \in J_0^1.$$

This differential equation is exceedingly well-behaved. In fact, we know that the size of the solution is bounded in terms of the size of the data.

Lemma 2: There exists a constant Γ such that, for all $f \in J^0$, the generalized solution u of (3) - (4) satisfies

$$\| D^2 u \|_B \leq \Gamma \| f \|_B.$$

Proof: See [13].

We now state a variant of the Sobolev lemma. Let $\lfloor x \rfloor$ denote the greatest integer not exceeding x.

Lemma 3: Let $u \in J^m(a)$. There exists a positive constant C_n such that, for all $r \in [0,a]$,

$$(u(r))^2 \leq C_n \sum_{j=0}^{m} a^{2j-n} \| D^j u \|^2_{B(a)}, \tag{7}$$

where $m = \lfloor \frac{n}{2} \rfloor + 1$.

Proof: See Friedman [7].

In the cases n = 2 or 3, (7) applies with m = 2.

Let S_n be a finite-dimensional subspace of J_0^1. The function $\tilde{u} \in S_n$ is the Rayleigh-Ritz Galerkin (RRG) approximation to u if

$$[\tilde{u},v_n]_B = (f,v_n)_B, \qquad \text{for all } v_n \in S_n.$$

Since the RRG approximation is the projection of u on S_n with respect to the inner product $[\cdot,\cdot]_B$, we have the error bounds

$$[u - \tilde{u},u - \tilde{u}]_B = \inf_{v_n \in S_n} [u - v_n,u - v_n]_B,$$

and by (5),

$$\| D(u - \tilde{u}) \|_B \leq \lambda^{-1}\Lambda \inf_{v_n \in S_n} \| D(u - v_n) \|_B. \tag{8}$$

Let Δ be a partition of [0,1]:

$$\Delta\colon 0 = x_0 < x_1 < x_2 < \dots < x_N = 1,$$

and $h \equiv \max\limits_{1 \leq i \leq N} (x_i - x_{i-1})$. We assume that the partition is quasiuniform, meaning that the global mesh ratio,

$$M_\Delta \equiv \max_{1 \leq i,j \leq N} \frac{x_i - x_{i-1}}{x_j - x_{j-1}}$$

is bounded independent of N.

As approximating subspaces we will use spaces of piecewise polynomials with respect to the partition Δ:

$$S_0^k(\Delta,\nu) \equiv \{s \in C^\nu[0,1]) \mid s(1) = 0, \text{ and } s \text{ is a polynomial of degree} < k \text{ on each of the intervals } (x_{i-1}, x_i),\ 1 \leq i \leq N \}.$$

3. Spherical Spline Approximation

We first consider approximation by polynomials in a neighborhood of the origin.

Lemma 4: Let $v \in J^m(a)$, $m \geq 1$. There exists a polynomial $T_a v$ of order m satisfying

$$\| D^j(v - T_a v) \|_{B(a)} \leq a^{m-j} \| D^m v \|_{B(a)} \tag{9}$$

for all $0 \leq j \leq m$.

Proof: Let $T_a v$ be the first m terms of the Taylor series for v at a, i.e.,

$$T_a v(x) = v(a) + Dv(a)(x-a) + \ldots + \frac{D^{m-1} v(a)}{m-1!} (x - a)^{m-1}.$$

Since $D^{m-1}(v - T_a v) \in J_0^1(a)$, we may apply inequality (6), obtaining

$$\| D^{m-1}(v - T_a v) \|_{B(a)} \leq a \| D^m(v - T_a v) \|_{B(a)}$$
$$= a \| D^m v \|_{B(a)}.$$

To prove (9), we note that $D^j(v - T_a v)(a) = 0$ for all $0 \leq j < m-1$. We may therefore apply (6) to each of the remaining derivatives, and use the result for D^{j+1} to obtain the result for D^j.

Q.E.D.

Theorem 1: For each integer $2 \leq m \leq k$, there exists a positive constant $K = K(k,m,n)$, depending on the global mesh ratio, such that for each $f \in J^m \cap J_0^1$ there exists an approximation $\hat{f} \in S_0^k(\Delta,\nu)$ to f satisfying

$$\| D^j(f - \hat{f}) \|_B \leq K h^{m-j} \| D^m f \|_B. \tag{10}$$

Proof: The details of the proof may be found in [13]. We will sketch the main ideas here.

The approximation whose existence is asserted can be explicitly constructed. Let $\{B_i\}_{i=1}^d$ be the B-spline basis functions for the space $S_0^k(\Delta,\nu)$. In [3], de Boor and Fix construct a set of linear functionals $\{\lambda_i\}$ dual to the B-spline basis, i.e.,

$$\lambda_i(B_j) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}.$$

The approximation

$$F_\Delta f \equiv \sum_{i=1}^{d} \lambda_i(f) B_i$$

is called the quasiinterpolant of f.

The functional λ_i is a linear combination of derivatives, evaluated at some point $\tau_i \varepsilon$ support(B_i). Moreover, difference approximations may be used instead of derivatives.

We assume that $\tau_i = x_1$ for all i such that x_1 is in the support of B_i, and that the points used in the corresponding difference approximations are all contained in the interval $(0,x_1)$. It can be shown that there exists a constant C such that, for all such i,

$$|\lambda_i(f)| \leq C \, \| f \|_{L^\infty(0,x_1)} . \tag{11}$$

To obtain error bounds for the quasiinterpolant in the weighted norm $\| \; \|_B$, we use the fact that the quasiinterpolant of any polynomial of degree < k is that polynomial [3]. Considering first the interval $(0, x_1)$,

$$\| D^j(f - F_\Delta f) \|_{B(x_1)} \leq \| D^j(f - T_{x_1} f) \|_{B(x_1)} + \| D^j F_\Delta(T_{x_1} f - f) \|_{B(x_1)} .$$

Let $R = f - T_{x_1} f$. By (11),

$$\| D^j F_\Delta(T_{x_1} f - f) \|_{B(x_1)} \leq \sum_{i=1}^{d} |\lambda_i(R)| \; \| D^j \, B_i \|_{B(x_1)}$$

$$\leq C \, \| R \|_{L^\infty(0,x_1)} \sum_{i=1}^{d} \| D^j \, B_i \|_{B(x_1)} .$$

All but k of the basis functions vanish in $(0,x_1)$. For those that don't, it is readily shown that

$$\| D^j B_i \|_{B(x_1)} \leq K \, x_1^{(n/2)-j} .$$

Together with the Sobolev lemma and the bounds for R given in Lemma 4, this yields

$$\| D^j F_\Delta(T_a f - f) \|_{B(x_1)} \leq K x_1^{m-j} \| D^m f \|_{B(x_1)}. \tag{12}$$

A similar argument gives the same result for the intervals (x_i, x_{i+1}), $2 \leq i \leq k$. In the remaining intervals, the support of any basis function which is nonzero in the interval is bounded away from zero. Using this fact, an approximation result analogous to (12) is easily obtained. Combining these results yields (10).

Q.E.D.

4. Error Bounds for the RRG Approximation

We now consider the error in the RRG approximation to the generalized solution u of (3) - (4), and show that the RRG approximation $\tilde{u} \in S_0^k(\Delta, \nu)$ approximates u to optimal order.

Theorem 2: Let u be the generalized solution of (3) - (4). Let $\tilde{u} \in S_0^k(\Delta, \nu)$ be the RRG approximation to u. If $u \in J^m \cap J_0^1$, $2 \leq m \leq k$, then

$$\| D(u - \tilde{u}) \|_B \leq \lambda^{-1} \Lambda K h^{m-1} \| D^m u \|_B \tag{13}$$

$$\| u - \tilde{u} \|_B \leq (\Lambda K)^2 \Gamma h^m \| D^m u \|_B. \tag{14}$$

Proof: The error bound (13) follows immediately from (8) and the result of Theorem 1. Inequality (14) also follows, via Nitsche's trick, from Theorem 1 [10].

5. Computational Aspects of the Method

We have shown that the Rayleigh-Ritz approximation $\tilde{u}$ to the solution u of (3) - (4) is optimally accurate in the natural norms for this problem. We would like to think of this approximation as inducing a smooth, accurate approximation of the solution U of the original problem (1) - (2). For this to happen, the odd derivatives of $\tilde{u}$ must vanish at 0. Unless we impose this requirement on the subspace, it will not be fulfilled.

There are two ways this can be done. We can simply force the elements of the space $S_0^k(\Delta, \nu)$ to have odd derivatives which vanish at 0.

Alternatively we consider, rather than (3) - (4), the two-point boundary value problem

$$- D(|x|^{n-1}Du) + |x|^{n-1}q(x)u = |x|^{n-1}f(x),$$
$$-1 < x < 1, \quad u(-1) = u(1) = 0,$$

also derived from (1) - (2). We then define $SS_0^k(\Delta,\nu)$ to be the space of C^ν piecewise polynomials of degree $< k$ (vanishing at -1 and 1) with respect to a partition which is symmetric about 0:

$$\Delta: -1 = x_{-N} < x_{-N+1} < \ldots < x_0 = 0 < x_1 < \ldots < x_N = 1,$$

where $x_{-i} = x_i$, $1 \leq i \leq N$.

It can be shown that the results of Theorems 1 and 2 hold for the space $SS_0^k(\Delta,\nu)$ [13].

The B-spline basis functions then have a symmetry property, derived from the symmetry of the mesh: if $B_0, \ldots, B_d$ are the basis functions $(d+1 = \dim(SS_0^k(\Delta,\nu)))$ numbered in the natural left-to-right order, then

$$B_i(-x) = B_{d-i}(x), \quad -1 < x < 1, \quad 0 \leq i \leq d.$$

Clearly, $\tilde{u} = \sum_{i=0}^{d} \alpha_i B_i$ is even if the vector $\underline{\alpha}$ is symmetric about its middle:

$$\alpha_i = \alpha_{d-i}, \qquad 0 \leq i \leq d. \tag{15}$$

The symmetry property (15) will hold for the RRG approximation's coefficients, even though we do not impose it. The coefficients are obtained as the solution of the linear system

$$A\underline{\alpha} = \underline{f}, \tag{16}$$

where $A = [a_{ij}]$, $\underline{f} = [f_i]$, and

$$a_{ij} \equiv \int_{-1}^{1} |x|^{n-1}(DB_iDB_j + qB_iB_j)\, dx,$$

$$f_i \equiv \int_{-1}^{1} |x|^{n-1} f\, B_i\, dx.$$

Clearly, because of the symmetry of the data and the basis functions, the matrix A will be symmetric about the alternate diagonal and the vector $\underline{f}$ will be symmetric about its middle. This shows that the coefficients of $\tilde{u}$ will satisfy (15). Thus $\tilde{u}$ is even, and all its odd derivatives of order $\leq \nu$ vanish at 0.

It does not cost any more, in work and storage, to use the (-1,1) problem than the (0,1) problem. Because of the symmetries of A, only 1/4 of its elements need to be computed. Moreover, using an algorithm of Evans and Hatzopoulos [5] which takes advantage of symmetry about the alternate diagonal, the equations (16) can be solved in half the time required by the usual band Cholesky algorithm.

The effect of numerical quadrature (used to compute the matrix A and the right-hand side vector $\underline{f}$) on the accuracy of the RRG approximation has been analysed by Fix for nonsingular problems [6]. He showed that if the integrals are computed using composite Gaussian quadrature with k-1 points in each interval, then the error due to the quadrature is asymptotically as small as the discretization error. We have been able to show that k points is sufficient for this type of singular problem [13], but conjecture that this result can be improved, and that k-1 points also suffice here. The numerical results of the next section strongly support this viewpoint.

6. Numerical Results

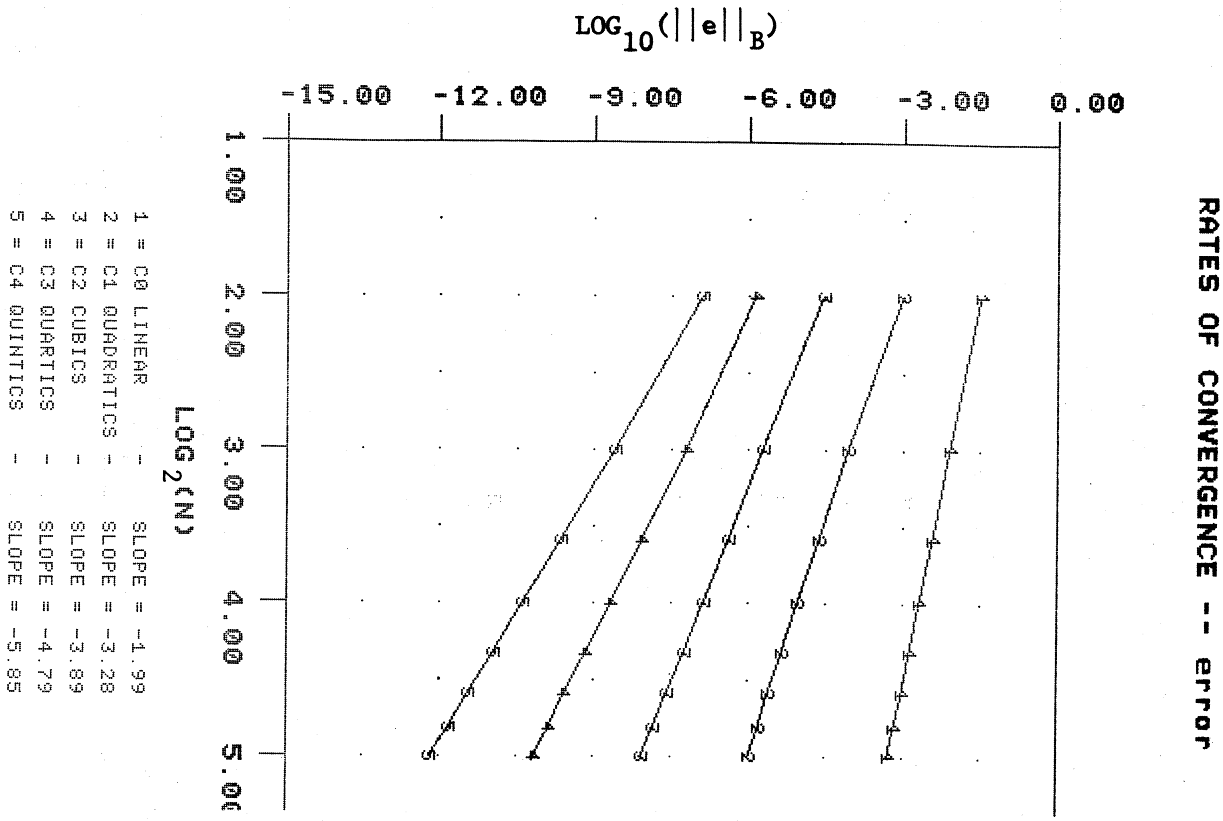
In this section we present the results of a numerical experiment, which illustrates the utility of the computational procedure analyzed in the previous sections. Following Russell and Shampine [12], we consider the problem

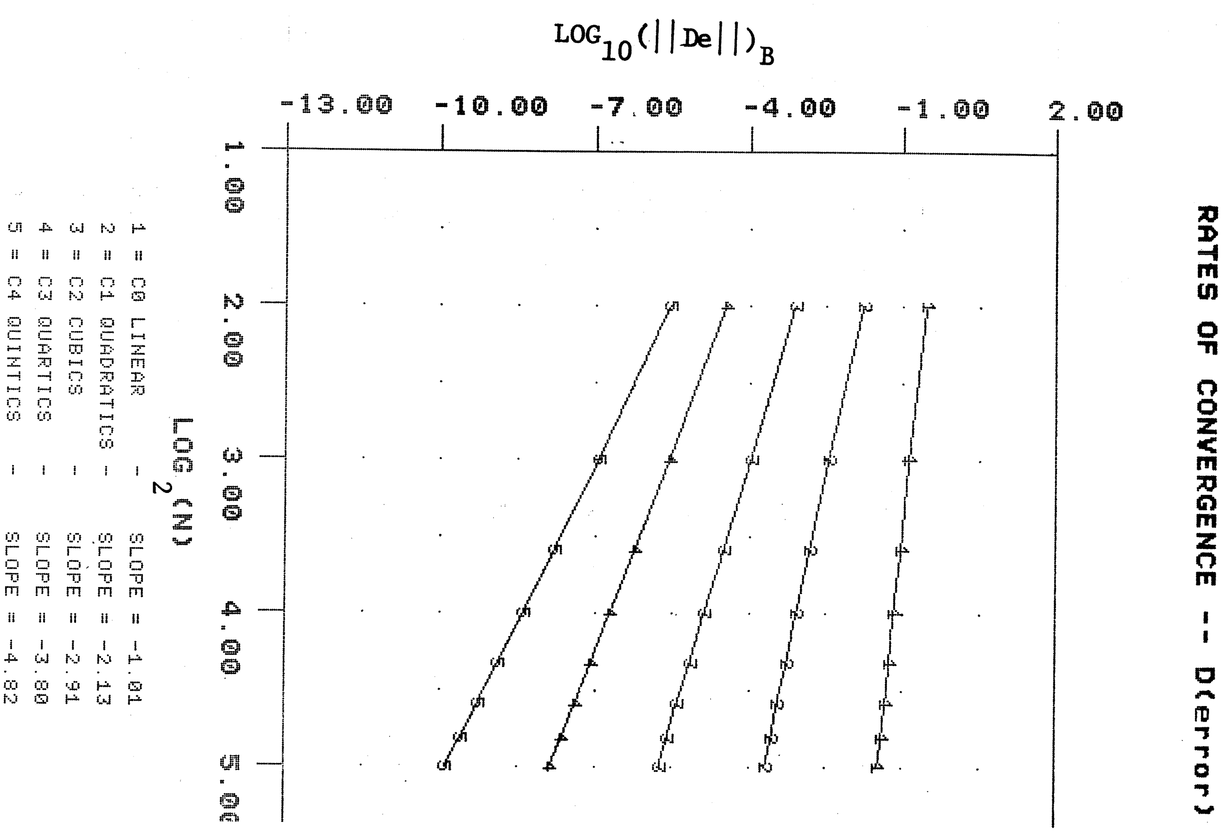
$$- D(x^2 Du) + 4x^2 u = - 20x^2$$

$$Du(0) = u(1) = 0,$$

which has the solution $u(x) = \dfrac{5 \sinh 2x}{x \sinh 2} - 5$.

The RRG approximations to u from several of the $S_0^k(\Delta,\nu)$ subspaces were computed, and the error graphed below. All computations were performed in double precision on a PDP-10 (with 54 binary digits). The integrals required were computed using composite Gaussian quadrature with k-1 nodes in each interval of the mesh. We give the norms $\|e\|_B$ and $\|De\|_B$ of the error and its derivative (computed with composite k+1 node Gaussian quadrature rules.)


RATES OF CONVERGENCE -- error
LOG10(||e||B)
0.00
-3.00
-6.00
-9.00
-12.00
-15.00
1.00
2.00
3.00
4.00
5.00
LOG2(N)
1 = C0 LINEAR - SLOPE = -1.99
2 = C1 QUADRATICS - SLOPE = -3.28
3 = C2 CUBICS - SLOPE = -3.89
4 = C3 QUARTICS - SLOPE = -4.79
5 = C4 QUINTICS - SLOPE = -5.85


RATES OF CONVERGENCE -- D(error)
LOG10(||De||)B
2.00
-1.00
-4.00
-7.00
-10.00
-13.00
1.00
2.00
3.00
4.00
5.00
LOG2(N)
1 = C0 LINEAR - SLOPE = -1.01
2 = C1 QUADRATICS - SLOPE = -2.13
3 = C2 CUBICS - SLOPE = -2.91
4 = C3 QUARTICS - SLOPE = -3.80
5 = C4 QUINTICS - SLOPE = -4.82

Jesperson has solved the quasilinear problem

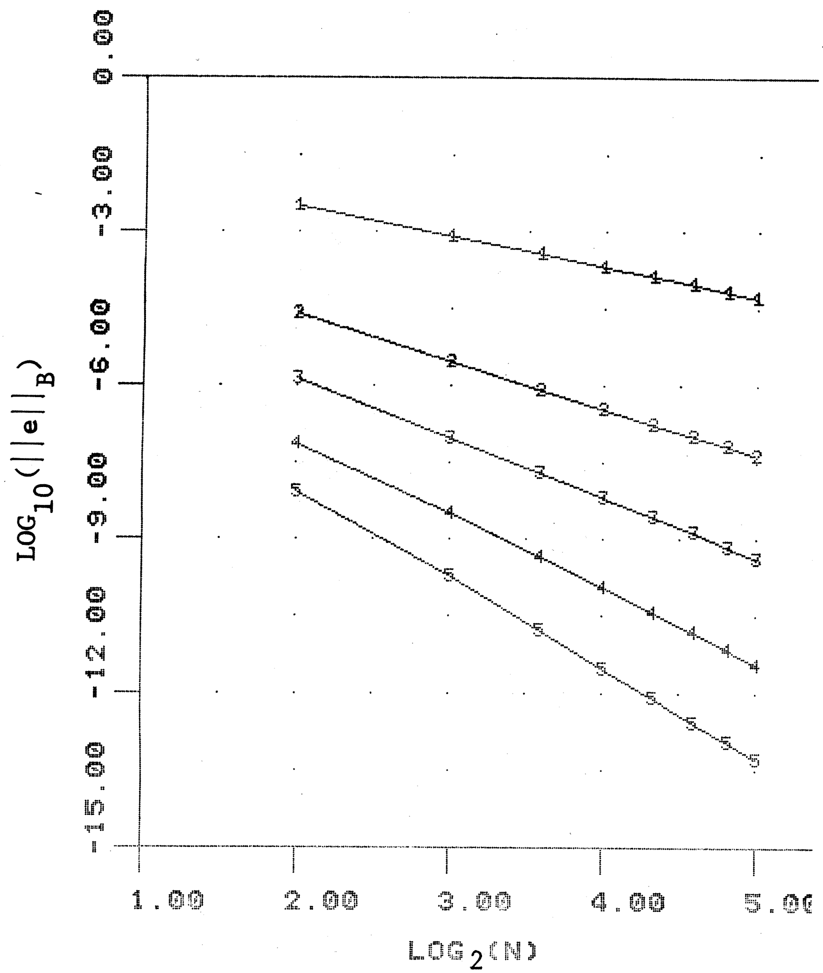
$$- D(x\ Du) = - \frac{64}{49} e^{u}$$

$$Du(0) = u(1) = 0,$$

which has the unique solution $u(x) = 2 \ln(\frac{7}{8 - x^2})$. Our theoretical results can be made to apply to this problem in a routine manner; cf. [14]. The RRG approximations to u were computed using Newton's method with an initial guess of 0; the resulting sequence of linear problems was solved in the manner discussed above. The iteration was stopped when the residual reached $\sim 10^{-15}$. In each case, this required 4 iterations.

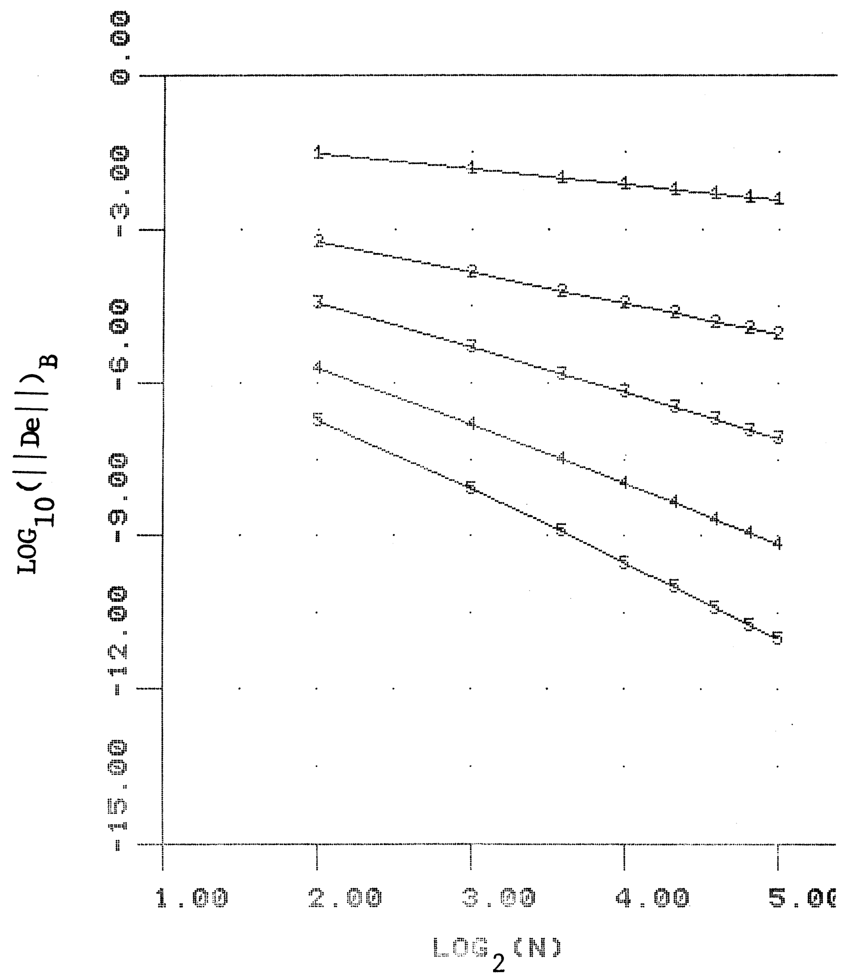
As predicted by the theory, the rate of convergence appears to be h^k (for the error) and h^{k-1} (for the derivative). Apparently, k-1 quadrature nodes per interval are sufficient to obtain the predicted convergence rates.

RATES OF CONVERGENCE -- error



1 = C0 LINEAR - SLOPE = -2.00
2 = C1 QUADRATICS - SLOPE = -3.07
3 = C2 CUBICS - SLOPE = -3.88
4 = C3 QUARTICS - SLOPE = -4.80
5 = C4 QUINTICS - SLOPE = -5.81

RATES OF CONVERGENCE -- D(error)



1 = C0 LINEAR - SLOPE = -1.01
2 = C1 QUADRATICS - SLOPE = -2.01
3 = C2 CUBICS - SLOPE = -2.92
4 = C3 QUARTICS - SLOPE = -3.80
5 = C4 QUINTICS - SLOPE = -4.77

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