

## GMRES AND INTEGRAL OPERATORS\*

C. T. KELLEY<sup>†</sup> AND Z. Q. XUE<sup>†</sup>

**Abstract.** In this paper we show how the properties of integral operators and their approximations are reflected in the performance of the GMRES iteration and how these properties can be used to smooth the GMRES iterates by an implicit application of Nyström interpolation, thereby strengthening the norm in which convergence takes place. The smoothed iteration has very similar properties to Broyden's method. We present an example to illustrate the ideas.

**Key words.** integral equations, GMRES iteration, Broyden's method

**AMS subject classifications.** 65F10, 65J10, 65R20

**1. Introduction.** In this paper we consider the performance of the GMRES [27] iteration for linear equations of the form

$$(1.1) \quad Au = u - Ku = f$$

with  $K$  a compact operator on a separable Hilbert space  $H$ . An example of such an operator is an integral operator on  $H = L^2[0, 1]$  of the form

$$(1.2) \quad Ku(x) = \int_0^1 k(x, y)u(y) dy$$

where  $k$  is continuous.

Our setting is that of [15] where issues similar to those raised in this paper were considered in the context of Broyden's method [4] for linear and nonlinear equations. Broyden's method has also been considered as a linear equation solver in [5], [12], [13], [25], and [20]. Let  $H$  be a separable real Hilbert space and let  $X \subset H$  be a Banach space such that the inner product  $(\cdot, \cdot)$  in  $H$  is continuous from  $X \times X \rightarrow \mathbb{R}$ . This implies that there is  $C_X$  such that

$$(1.3) \quad \|u\|_H \leq C_X \|u\|_X$$

for all  $u \in X$ . Let  $K \in \mathcal{COM}(H, X)$ , which is the space of compact operators from  $H$  to  $X$ . Of course, we may also regard  $K$  as an element of  $\mathcal{COM}(H)$ , which is the space of compact operators on  $H$ . In the context of the integral operator (1.2) with continuous  $k$ ,  $H = L^2[0, 1]$ ,  $X = C[0, 1]$ , and  $C_X = 1$ .

Algorithms such as GMRES and Broyden's method, which depend on notions of orthogonality, could use the Hilbert space inner product of  $H$  to solve equations in which the right-hand side  $f \in X$ . However, a convergence theory based entirely on a Hilbert space formulation would show that the resulting sequence is convergent in the topology of  $H$  but not necessarily in that of the Banach space  $X$  in which the problem may have been originally posed. Hence, we face an apparent conflict between the topology in which the problem was posed and the inner product (and hence Hilbert space) nature of the algorithm. This issue was resolved in [15] in the context of Broyden's method. For the linear equations context of this paper the result of [15] is that the Broyden iterations converge  $q$ -superlinearly in the topology of  $X$  provided  $K \in \mathcal{COM}(H, X)$  and  $f \in X$ .

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Nyström interpolation [24], i.e., replacing an approximate solution  $u$  by  $\bar{u} = f + Ku$ , can be used to create approximations accurate in stronger norms than the original [17] to improve the overall accuracy of a discrete approximation [28] and as a method for smoothing an intergrid transfer in multilevel schemes [1], [3], [14]. We have the first purpose in mind here. Following GMRES with a Nyström interpolation would, as we shall see, result in accuracy in the  $X$ -norm. The cost, however, would be an additional application of  $K$ .

The purpose of this paper is to show how GMRES can be modified to incorporate Nyström interpolation at a very small cost in both computational effort and algorithmic complexity. The result is an algorithm that has the simultaneous  $X$  and  $H$  convergence property of Broyden's method. The example we give in §4 compares GMRES, both with and without Nyström interpolation, and Broyden's method as primary solvers and not in the context of a multilevel method, where they could be either used as coarse mesh solvers or as the primary solver in a nested iteration approach. The reasons for this are that the independence of our results to mesh size can best be illustrated if the solvers perform the same task for each mesh. The merits of our implicit Nyström interpolation carry over to the multilevel situation, enabling coarse mesh solvers to be accurate in the appropriate discrete  $X$ -norm, which is important for the convergence theory.

Throughout this paper we assume that  $A$  is a nonsingular linear operator on  $H$  and  $X$ . We consider convergence rate estimates of the form

$$(1.4) \quad \|r_k\|_H \leq \tau_k \|r_0\|_H,$$

where  $r_k = f - Au_k$ , and the sequence of real numbers  $\{\tau_k\}$  converges to zero and is independent of the right-hand side  $f$  of (1.1).

Rates of convergence of the form (1.4) can be derived from resolvent integration [21], [22] for any  $K$  such that  $I - K$  has bounded inverse and 1 is in the unbounded component of the resolvent set of  $K$ . If  $K$  is compact, more precise information can be obtained. In fact the GMRES iterates converge  $r$ -superlinearly to the solution in a way that is independent of the right-hand side. This means that the sequence  $\{\tau_k\}$  converges  $q$ -superlinearly to zero; i.e.,

$$\lim_{k \rightarrow \infty} \frac{\tau_{k+1}}{\tau_k} = 0.$$

In the case of normal or diagonalizable (similar to normal) compact operators a  $q$ -superlinearly convergent sequence  $\{\tau_k\}$  can be directly related to spectral properties of  $K$  in a very simple way. In [18] assumptions on the rate of decay of the spectrum were used for this. In order to illustrate how the smoothing properties of  $K$  might influence the convergence rate, below we present a slight extension of the result in [18]. While this result follows from the general theory in [22], we believe that its direct and brief proof is worth inclusion. We denote by  $\kappa_H(A)$  the  $H$ -norm condition number of  $A$ ;

$$\kappa_H(A) = \|A\|_H \|A^{-1}\|_H.$$

**THEOREM 1.1.** *Let  $H$  be a separable Hilbert space,  $K \in \mathcal{COM}(H)$ , let  $A = I - K$  be nonsingular, and let  $S$  be a nonsingular bounded operator on  $H$  such that*

$$L = SKS^{-1}$$

*is normal. Let  $\{\lambda_i\}$  be the eigenvalues of  $A$  ordered so that*

$$(1.5) \quad |\lambda_i - 1| \geq |\lambda_{i+1} - 1| \quad \text{for } i \geq 1;$$

then for all  $k \geq 1$  the GMRES residuals  $r_k$  satisfy

$$(1.6) \quad \|r_k\| \leq \kappa_H(S) \|r_0\| 2^k \prod_{i=1}^k |1 - \lambda_i^{-1}|.$$

*Proof.* For  $k = 1, \dots$  define

$$(1.7) \quad p_k(z) = \prod_{i=1}^k (1 - \lambda_i^{-1} z).$$

Since  $p_k(0) = 1$  for all  $k$  we have [27]

$$(1.8) \quad \|r_k\|_H \leq \kappa_H(S) \|r_0\|_H \sup_m |p_k(\lambda_m)|.$$

For  $k$  fixed,  $p_k(\lambda_m) = 0$  for  $1 \leq m \leq k$ . For  $m > k$ ,

$$\begin{aligned} |p_k(\lambda_m)| &\leq \prod_{i=1}^k |1 - \lambda_i^{-1} \lambda_m| = \prod_{i=1}^k |\lambda_i^{-1}| |\lambda_i - \lambda_m| \\ &\leq \prod_{i=1}^k |\lambda_i^{-1}| (|\lambda_i - 1| + |1 - \lambda_m|) \leq \prod_{i=1}^k |\lambda_i^{-1}| 2|\lambda_i - 1| \\ &= 2^k \prod_{i=1}^k |1 - \lambda_i^{-1}|. \end{aligned}$$

This completes the proof.  $\square$

Since  $\lambda_i \rightarrow 1$ , the sequence

$$\tau_k = 2^k \prod_{i=1}^k |1 - \lambda_i^{-1}|$$

is  $q$ -superlinearly convergent. If, say,  $K$  is normal (so  $S = I$ ) and the eigenfunctions of  $K$  are smooth, then the rate of convergence of  $\lambda_i$  to one reflects both the smoothness of the kernel  $k$  and the convergence rate of the sequence  $\{\tau_k\}$ .

**2. Convergence in a stronger norm.** In this section we show how, given a rate estimate like (1.4) for the sequence of residuals, the GMRES iteration can be modified to produce a sequence that converges with the same rate in the norm of  $X$ . This will lead to a modified form of GMRES that uses information at hand to perform Nyström interpolation implicitly without the need for an additional application of the operator  $K$ . Proposition 2.1 is a coupling of the convergence rate derived above with the standard smoothing result for Nyström interpolation [2]. We provide the simple proof to help clarify the ideas.

**PROPOSITION 2.1.** *Let  $\{u_k\}$  be the sequence of GMRES iterates. Assume that (1.4) holds for some sequence  $\{\tau_k\}$ . Let  $\tilde{u}_k = u_k + r_k$ . Then*

$$(2.1) \quad \|\tilde{u}_k - u^*\|_X \leq \|K\|_{\mathcal{L}(H, X)} \kappa_H(A) \tau_k \|u_0 - u^*\|_X.$$

*Proof.* First note that (1.4) implies that

$$(2.2) \quad \|u_k - u^*\|_H \leq \tau_k \kappa_H(A) \|u_0 - u^*\|_H.$$

Since

$$\bar{u}_k = u_k + r_k = f + Ku_k,$$

continuity of  $K$  as a map from  $H$  to  $X$  implies that

$$\|\bar{u}_k - u^*\|_X = \|K(u_k - u^*)\|_X \leq \|K\|_{\mathcal{L}(H,X)} \|u_k - u^*\|_H.$$

This completes the proof.  $\square$

The interpolant  $\bar{u}_k$  is as easy to compute as  $u_k$  upon exit from the main loop in GMRES. An algorithmic description of GMRES follows.

ALGORITHM 2.1. *Algorithm gmres*( $u, f, A, \epsilon$ )

1.  $r = f - Au$ ,  $v_1 = r/\|r\|_H$ ,  $\rho = \|r\|_H$ ,  $\beta = \rho$ ,  $k = 1$
2. While  $\rho > \epsilon\|b\|_H$  do
  - (a)  $v_{k+1} = Av_k$   
for  $j = 1, \dots, k$ 
    - i.  $h_{jk} = (v_{k+1}, v_j)$
    - ii.  $v_{k+1} = v_{k+1} - h_{jk}v_j$
  - (b)  $h_{k+1,k} = \|v_{k+1}\|_H$
  - (c)  $v_{k+1} = v_{k+1}/\|v_{k+1}\|_H$
  - (d)  $e_1 = (1, 0, \dots, 0)^T \in R^{k+1}$   
Minimize  $\|\beta e_1 - H_k y\|_{R^{k+1}}$  to obtain  $y \in R^k$
  - (e)  $\rho = \|\beta e_1 - H_k y\|_{R^{k+1}}$
  - (f)  $k = k + 1$
3.  $u_k = u_0 + V_k y$

In step 3  $V_k : R^k \rightarrow H$  is defined by

$$V_k y = \sum_{j=1}^k y_j v_j.$$

We can use the fact that

$$r_k = f - Au_k = V_{k+1}(\beta e_1 + H_k y) = r_0 + V_{k+1} H_k y$$

to recover  $\bar{u}_k$  with no additional operator–vector products involving  $A$ . In fact if  $z = H_k y$  and we define a vector

$$w = (w_1, w_2, \dots, w_{k+1})^T \in R^{k+1}$$

by  $w_i = z_i + y_i$  for  $1 \leq i \leq k$  and  $w_{k+1} = z_{k+1}$ , we have

$$(2.3) \quad \bar{u}_k = \bar{u}_0 + V_{k+1} w,$$

which can simply replace the computation of  $u_k$  in step 3 of gmres. We will refer to the resulting algorithm as *smoothed GMRES*. Note that smoothed GMRES differs from GMRES only in the final output, where (2.3) is used to compute the final result.

As an algorithm for the solution of linear compact fixed point problems, smoothed GMRES shares two properties with Broyden's method. Both converge superlinearly to the solution in the topologies of both  $H$  and  $X$  and both require storage of the iteration history. Older implementations of Broyden's method require storage of two vectors for each iteration, [10], [23], [7]. However recent work for linear [9] and nonlinear [16] problems show how to use only a single vector, making the two algorithms competitive.

**3. Discrete problems.** While we state and prove our results in the infinite-dimensional setting they apply equally well when  $K$  is an approximation of some compact operator and  $X$  and  $H$  are both  $R^N$  for some  $N$  with different norms, say, discrete approximations of  $L^2$  (for  $H$ ) and  $L^\infty$  or  $C^l$  (for  $X$ ) norms.

To illustrate this point, consider the integral operator defined by (1.2). A standard approximation by an  $N$ -point quadrature rule would lead to the discrete problem

$$(3.1) \quad u_i - \sum_{j=1}^N k(x_i, x_j) w_j = f(x_i),$$

where  $\{x_i\}$  and  $\{w_i\}$  are the nodes and weights of the quadrature rule. Assume that  $f$  and  $k$  are  $l$  times continuously differentiable. Define  $H$  to be  $R^N$  with the inner product

$$(u, v)_H = \sum_{j=1}^N u_j v_j w_j$$

and associated norm

$$\|u\|_H = \left( \sum_{j=1}^N u_j^2 w_j \right)^{1/2}.$$

We give  $C^l[0, 1]$  the norm

$$\|u\|_{C^l} = \|u\|_\infty + \|d^l u / dx^l\|_\infty.$$

If we replace  $\|d^l u / dx^l\|_\infty$  with a  $l$ th divided difference we may define an approximate  $C^l$  norm on  $R^N$ . If  $X$  is  $R^N$  with such an approximate  $C^l$  norm, then the matrix

$$K_{ij} = k(x_i, x_j) w_j$$

satisfies, with  $C$  independent of  $N$

$$\|Ku\|_X \leq C\|u\|_H,$$

and the development in the above section may be applied for each level of discretization  $N$  with the constants in the estimates being independent of  $N$ .

For example, if  $l = 1$ , and the nodes of quadrature rule are  $\{ih\}_{i=0}^{N-1}$  with  $h = 1/(N-1)$ , we may define the divided difference  $D_1 u \in R^{N-1}$  by

$$(3.2) \quad (D_1 u)_i = (u_{i+1} - u_i) / h$$

and the  $X$ -norm by

$$\|u\|_X = \|u\|_\infty + \|D_1 u\|_\infty.$$

In §4 we present an example showing how smoothed GMRES can capture the smoothing properties of the Broyden iteration that are missed by GMRES alone.

**4. Example.** As an example we consider the source iteration operator from linear transport theory [19], [26]. We will describe the equation and its discretization only briefly and refer to [19] and [26] for more details. We consider the equation

$$(4.1) \quad \mu \frac{\partial \psi}{\partial x}(x, \mu) + \psi(x, \mu) = \frac{c(x)}{2} \int_{-1}^1 \psi(x, \mu') d\mu'$$

for  $x \in (0, \tau)$  with boundary conditions

$$(4.2) \quad \psi(0, \mu) = F_l(\mu), \quad \mu > 0; \quad \psi(\tau, \mu) = F_r(\mu), \quad \mu < 0.$$

In (4.1) and (4.2) the intensity  $\psi$  is the unknown real valued function of  $x$  and  $\mu$ .  $\tau < \infty$ ,  $c \in C([0, \tau])$ , and  $F_l$  and  $F_r$  are given continuous real valued functions of  $\mu$ . It is known [6] that the boundary value problem (4.1)–(4.2) has a unique solution if  $0 \leq c(x) < 1$ .

The intensity can be computed directly once the flux

$$(4.3) \quad f(x) = \frac{1}{2} \int_{-1}^1 \psi(x, \mu') d\mu'$$

is known. By integrating forward ( $\mu > 0$ ) and backward ( $\mu < 0$ ) in  $x$  we derive the integral equation for  $f$ ,

$$(4.4) \quad f(x) - \int_0^\tau k(x, y) f(y) dy = g(x)$$

where

$$k(x, y) = \frac{1}{2} E_1(|x - y|) c(y),$$

$$E_1(|x - y|) = \int_0^1 \exp\left(\frac{-|x - y|}{v}\right) \frac{dv}{v},$$

and

$$g(x) = \frac{1}{2} \int_0^1 \exp\left(\frac{-x}{v}\right) F_l(v) dv \\ + \frac{1}{2} \int_0^1 \exp\left(\frac{-(\tau - x)}{v}\right) F_r(-v) dv.$$

It is known [6], [8] that the integral operator  $K$  in (4.4) has spectral radius  $< 1$  and hence (4.4) has a unique solution. It is also easy to see from the formula for  $k$  that  $K$  maps  $L^2$  into any of the spaces

$$X_\epsilon^l = C[0, 1] \cap C^l[\epsilon, 1].$$

By examining the formula for  $g$  we see that the solution  $f \in C[0, 1]$  is infinitely differentiable in compact subsets of  $(0, 1]$  and hence lies in any of the spaces  $X_\epsilon^l$ .

We discretize (4.4) with the standard *discrete ordinates* approximation to (4.1), which is not a direct approximation of (4.4) by a quadrature rule at all. We approximate the integral in (4.1) by a 20-point double Gaussian quadrature rule (10-point Gaussian quadratures on each of the intervals  $(-1, 0)$  and  $(0, 1)$ ) in line with the analysis in [26] and then integrate forward and backward with the Crank–Nicolson scheme on a spatial mesh with  $N$  points. The convergence theory developed in [19] and [26] implies that the discrete form  $K$  of the integral operator satisfies

$$\|Ku\|_{l, \epsilon} \leq M(l, \epsilon) \|u\|_H$$

for some  $M(k, \epsilon)$ , which is independent of the spatial mesh. Here  $\|\cdot\|_H$  denotes the scaled Euclidean norm

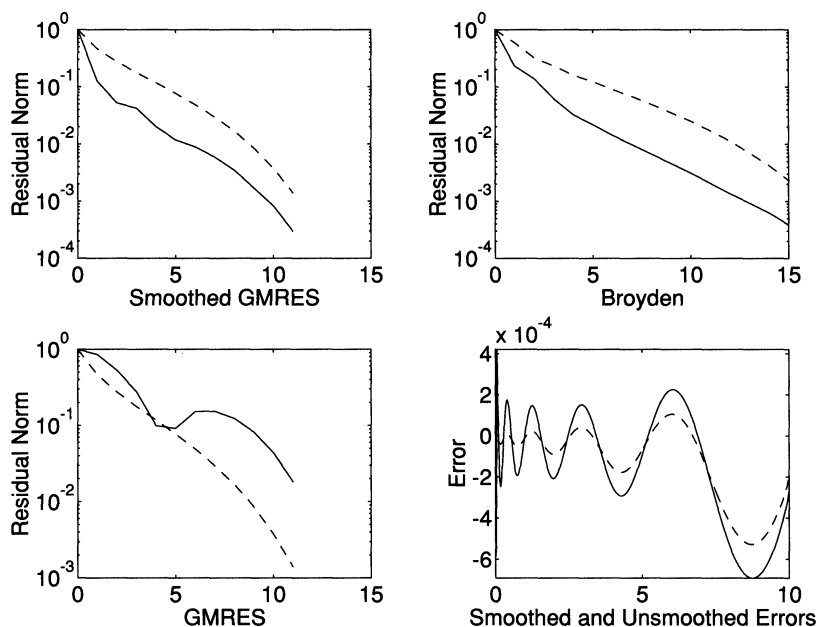


FIG. 4.1.  $N = 401$ .

$$\|u\|_H = \left( \frac{1}{N} \sum_{j=1}^N u_j^2 \right)^{1/2},$$

and the discrete  $X_\epsilon^l$  norms are given by

$$(4.5) \quad \|u\|_{l,\epsilon} = \|u\|_\infty + \|D_1^l u_\epsilon\|_\infty.$$

In (4.5) the operator  $D_1$  is defined by (3.2) and  $u_\epsilon$  is the vector defined by

$$(u_\epsilon)_i = \begin{cases} 0, & ih \leq \epsilon, \\ u_i, & ih > \epsilon. \end{cases}$$

We set  $F_l(\mu) = 1$ ,  $F_r(\mu) = 0$  for all  $\mu$ , and  $\tau = 10$ . We set  $c(x) = \exp(-x/100)$ , which is a special case of the class considered in [11]. We performed three sets of computations for  $N = 401$ ,  $N = 801$ , and  $N = 1601$ . We used the initial iterate  $u_0 = 0$  and solved the equation with GMRES, smoothed GMRES, and Broyden's method. We terminated the iteration when the discrete  $H$ -norm residual had been reduced by a factor of  $5/(N-1)^2$ . We used the solution with  $N = 6401$  (terminated when the  $H$ -norm residual had been reduced by a factor of  $10^{-12}$  as a representation of the exact solution). We computed the discrete  $X_\epsilon^l$ -norms with  $\epsilon = .025$ .

For  $N = 401$  (Fig. 4.1),  $N = 801$  (Fig. 4.2), and  $N = 1601$  (Fig. 4.3) we plot relative residual norms as functions of the iteration number in both the discrete  $X_\epsilon^1$ -norm (solid line) and the discrete  $H$ -norm (dashed line). In each figure there are plots of residual histories for both GMRES and smoothed GMRES (SGMRES). In those plots the dashed line is the  $H$ -norm relative residual for both GMRES and SGMRES. The solid line is the relative residual norm in  $X_\epsilon^1$ , which we computed directly in GMRES by explicitly computing the residual and its  $X_\epsilon^1$ -norm or by using (2.3). We also plot the error in the final result as a function of  $x \in [0, \tau]$  for smoothed (dashed line) and unsmoothed (solid line) GMRES. One can clearly see the

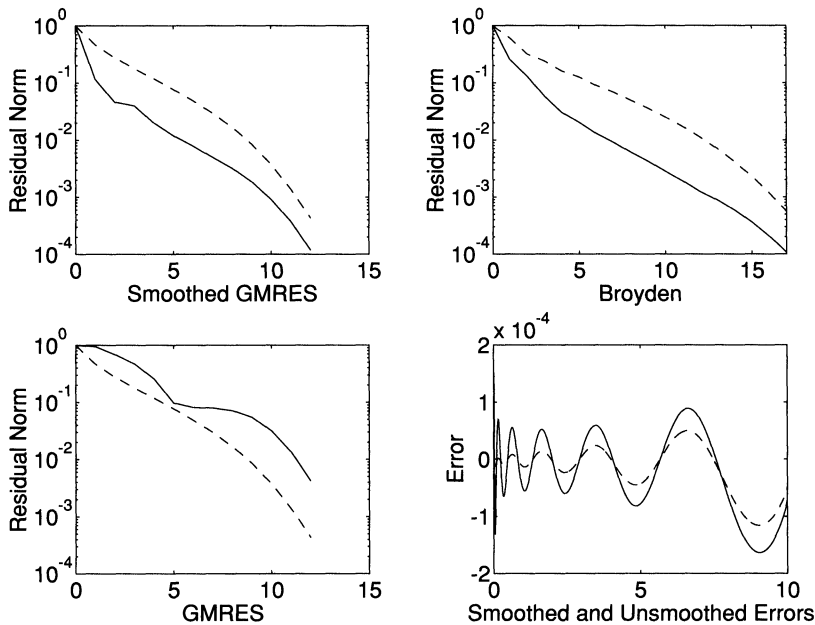


FIG. 4.2.  $N = 801$ .

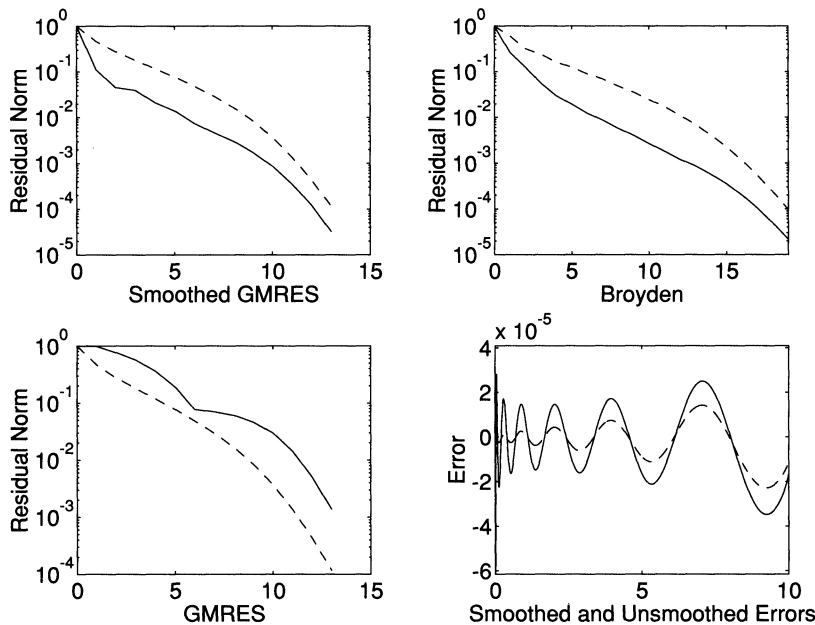


FIG. 4.3.  $N = 1601$ .

effects of the smoothing especially near  $x = 0$  where the errors of the unsmoothed solution oscillate much more strongly.

To show how the smoothing affects the results in other norms, we present in Table 4.1 the norms of the errors in the discrete  $L^\infty$ ,  $X_\epsilon^1$ ,  $X_\epsilon^2$ , and  $X_\epsilon^3$  norms for GMRES and SGMRES. One can see from these tables that the effect of the Nyström interpolation becomes more dramatic as the differentiability in the norms increases.



TABLE 4.1  
Errors in various norms.

Norm	$N = 401$		$N = 801$		$N = 1601$	
	GMRES	SGMRES	GMRES	SGMRES	GMRES	SGMRES
$H$	3.1865e-4	2.3279e-4	7.6028e-5	4.8816e-5	1.7326e-5	9.8239e-6
$L^\infty$	6.9223e-4	5.2749e-4	1.6349e-4	1.1584e-4	6.1573e-5	2.2828e-5
$X_\epsilon^1$	4.0814e-2	8.0632e-3	7.0348e-3	1.2897e-3	3.1247e-3	3.9660e-4
$X_\epsilon^2$	1.9878e+0	2.4950e-1	5.3146e-1	3.0577e-2	2.2838e-1	1.1983e-2
$X_\epsilon^3$	8.3956e+1	7.5656e+0	2.5227e+1	1.6119e+0	9.2401e+0	8.5306e-1

The computations illustrate how the smoothed GMRES iteration gives better performance in the  $X_\epsilon^1$ -norm. The curves for the various values of  $m$  are quite similar, indicating that the infinite-dimensional analysis can be observed numerically. Note also that the  $X_\epsilon^1$  and  $H$  relative residuals for the Broyden iteration, which requires more work than GMRES, are very close, in line with the theory in [15].

The tables and figures were created with MATLAB version 4.0a on a Sun SPARC 20 model 61 workstation running SUN OS 4.1.3.

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