NASA Contractor Report 178026

ICASE REPORT NO. 85-57

NASA-CR-178026
19860009521

ICASE

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Contract Nos. NAS1-17070, NAS1-18107

November 1985

INSTITUTE FOR COMPUTER APPLICATIONS IN SCIENCE AND ENGINEERING
NASA Langley Research Center, Hampton, Virginia 23665

Operated by the Universities Space Research Association

National Aeronautics and
Space Administration

Langley Research Center
Hampton, Virginia 23665

DISPLAY 20/6/1
86N18991*# ISSUE 9 PAGE 1478 CATEGORY 59 RPT#: NASA-CR-178026
ICASE-85-57 NAS 1.26:178026 CNT#: NAS1-17070 NAS1-18107 AF-AFOSR-84-0070
85/11/00 37 PAGES UNCLASSIFIED DOCUMENT
UTTL: Multigrid method for nearly singular and slightly indefinite problems
TLSP: Final Report
AUTH: A/BRANDT, A.; B/TAASAN, S. PAA: A/(Weizmann Inst. of Science, Rehovot, Israel)
CORP: National Aeronautics and Space Administration. Langley Research Center, Hampton, Va. AVAIL.NTIS
SAP: HC A03/MF A01
COI: UNITED STATES Submitted for publication
MAJS: /*COMPUTATION/*COMPUTATIONAL GRIDS/*DIFFERENTIAL EQUATIONS/*EIGENVECTORS/*NUMERICAL ANALYSIS/*RELAXATION METHOD (MATHEMATICS)
MINS: / ALGORITHMS/ APPROXIMATION/ CONVERGENCE/ EIGENVALUES/ LINEAR EQUATIONS
ABA: Author

MULTIGRID METHOD FOR NEARLY SINGULAR AND SLIGHTLY INDEFINITE PROBLEMS

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ABSTRACT

This paper deals with nearly singular, possibly indefinite problems for which the usual multigrid solvers converge very slowly or even diverge. The main difficulty is related to some badly approximated smooth functions which correspond to eigenfunctions with nearly zero eigenvalues. A modification to the usual coarse-grid equations is derived, both in Correction Scheme and in Full Approximation Scheme. With this modification, the algorithm exhibits the usual multigrid efficiency.

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*Sponsored by the Air Force Wright Aeronautical Laboratories, Air Force Systems Command, Unites State Air Force under Grant AFOSR 84-0070.

**Research was supported by the National Aeronautics and Space Administration under NASA Contract Nos. NAS1-17070 and NAS1-18107 while the author was in residence at ICASE, NASA Langley Research Center, Hampton, VA 23665-5225.

CONTENTS

INTRODUCTION

Usual multigrid for indefinite problems is sometimes found to be very inefficient. A strong limitation exists on the coarsest grid to be used in the process. This limitation is not so much a result of the indefiniteness (existence of eigenvalues with different signs) itself, but of the nearness to singularity, that is, the existence of nearly zero eigenvalues. These eigenvalues are badly approximated (e.g., they may even have a different sign) on coarse grids, hence the corresponding eigenfunctions, which are usually smooth ones, cannot efficiently converge. As a remedy, one could avoid using grids which are too coarse, but in many cases this would degrade efficiency.

This trouble of the coarse-grid approximation has been resolved by introducing a modification to the usual coarse-grid equations, based on the observation that there are just few smooth eigenfunctions which are not well represented on the coarse-grid, and these can be controlled by specially added relations. This modifiction removes the restriction on the coarseness of the grids that can be used.

Another issue when dealing with indefinite problems is the choice of relaxation. Mode analysis shows that the Gauss-Seidel relaxation is suitable for such problems if fine enough grids are considered. Indeed, even though some smooth components diverge with this relaxation, on fine enough grids this divergence is slow and can, therefore, easily be corrected by the coarse-grid corrections. On coarser grids, however, the divergence of smooth components in Gauss-Seidel relaxation is faster, hence, another relaxation scheme is needed. We have used for that purpose the Kaczmarz relaxation, which always converges.

The multigrid algorithm obtained here has good asymptotic convergence rates for problems in which the indefiniteness is not too high, i.e., the number of eigenvalues with the "wrong" sign (positive in our text) is small. For higher indefiniteness another method has been developed and will be reported elsewhere.

2. RELAXATION

Generally, in order to achieve good multigrid performances, the relaxation involved need to have good smoothing properties on one hand, and at most slow divergence on the other hand. We discuss below Gauss-Seidel and Kaczmarz relaxations and their proper use in our context.

2.1. Gauss-Seidel

Fourier analysis of Gauss-Seidel relaxation even for slightly indefinite problems shows that on fine grids high frequencies converge very fast. The reason for this is that the principal part for indefinite problems is the same as that of definite ones. Smooth components may diverge on such grids, but slowly enough to be handled by the coarse-grid correction. For example, in case of the operator $\Delta + k^2$ in two dimensions the worst divergence factor per sweep of smooth components is $1/(1 - \frac{1}{2} k^2 h^2)$, h being the mesh size. On coarse grids, typically when this factor becomes larger than 1.2 or so, Gauss-Seidel relaxation can no longer be used.

2.2. Kaczmarz Relaxation

Given an equation

$$Ax = b \tag{2.1}$$

where A is an $n \times n$ nonsingular matrix, define a new unknown y such that

$$A^* y = x \tag{2.2}$$

where A^* is the adjoint of A. The equation obtained for y is

$$AA^* y = b. \tag{2.3}$$

The matrix AA^* is symmetric positive definite for any A which is nonsingular. Hence, Gauss-Seidel relaxation for equation (2.3) will converge. It induces a relaxation on equation (2.1) via the relation (2.2). This relaxation of (2.1) is called Kaczmarz relaxation. Its i-th step is

$$x_j \leftarrow x_j + \bar{a}_{ij}\, \delta_i \qquad (j = 1,\cdots,n)$$

$$\delta_i = (b_i - \textstyle\sum_j a_{ij}\, x_j)/\sum_j |a_{ij}|^2$$

where $\bar{a}_{ij}$ is the complex conjugate of a_{ij}. For general smoothing properties of this relaxation, see [1] Section 1.1 and [2].

Kaczmarz relaxation converges whenever solution exists, and can therefore be used on coarse grids. Moreover, when more than one solution exists the convergence is to the one closest to the initial approximation (Tanabe [3]).

Hence, this relaxation would not allow the growth of error eigenfunctions corresponding to $\lambda = 0$, and would similarly allow only very slow change in eigenfunctions corresponding to λ close to 0.

3. TROUBLES WITH THE COARSE-GRID APPROXIMATION

Having settled the question of relaxation, another difficulty is encountered: some coarse grids do not well approximate some smooth components. To understand this situation, suppose the error on the fine-grid (grid h) contains a smooth eigenfunction ϕ^h, so that the corresponding residual is $L^h \phi^h = \lambda^h \phi^h$. The corresponding equations on the coarse-grid (grid H) are

$$L^H V^H = \lambda^h I_h^H \phi^h$$

where I_h^H is the fine-to-coarse transfer, i.e., some local averaging. Since ϕ^h is a smooth eigenfunction of L^h, $I_h^H \phi^h$ is approximately an eigenfunction of L^H, but with slightly different eigenvalue λ^H. The solution of the coarse-grid equations is approximately

$$\tilde{V}^H = \frac{\lambda^h}{\lambda^H} I_h^H \phi^h.$$

After interpolating the $\tilde{V}^H$ as a correction to the fine-grid solution, the new error is approximately

$$\phi^h - I_H^h \tilde{V}^H \approx \left(1 - \frac{\lambda^h}{\lambda^H}\right)\phi^h$$

where I_H^h is the interpolation operator and since ϕ^h is a smooth function, we assume that $I_H^h I_h^H \phi^h \approx \phi^h$. Thus, due to the coarse-grid correction the error is reduced by the factor $|1 - \lambda^h/\lambda^H|$; hence a condition for good convergence is

$$|1 - \frac{\lambda^h}{\lambda^H}| \ll 1 \tag{3.1}$$

for any eigenfunction ϕ^h which has poor convergence by relaxation.

When λ^h, λ^H are close to zero, relation (3.1), even if it holds on fine enough grids, it may strongly be violated on coarse grids. Such coarse grids cannot then be used in the multigrid process. Without them, however, efficiency may very much degenerate. We will therefore present a new method in which restriction (3.1) is removed.

4. MODIFIED COARSE-GRID EQUATIONS: Two-Grid Case

The modification described here is based on the assumption that there are only few smooth eigenfunctions for which relation (3.1) is violated. Denote by H_0 the subspace spanned by these badly approximated eigenfunctions. We assume for the description below that H_0 is known. In Section 6 we present a method for approximating H_0.

4.1. Correction Scheme (CS) Version

Assume first that H_0 is spanned by one function ϕ^h, and let u^h be the exact solution of the fine-grid (grid h) equation

$$L^h u^h = F^h. \tag{4.1}$$

Suppose the current approximation $\tilde{u}^h$ to u^h satisfies

$$\langle u^h, \phi^h \rangle = \langle \tilde{u}^h + \eta\phi^h, \phi^h \rangle. \tag{4.2}$$

If η were known we would have the approximation $\tilde{u}^h + \eta\phi^h$ on the fine-grid instead of $\tilde{u}^h$. This would yield the coarse-grid (grid H) equation

$$L^H v^H = I_h^H [F^h - L^h \tilde{u}^h - \eta L^h \phi^h] \tag{4.3}$$

where v^H approximates the error $v^h = u^h - \tilde{u}^h - \eta\phi^h$. Since by (4.2) the latter does not have components in H_0, equation (4.3) could be used to accelerate fine-grid convergence. However, since η is not known, we need to add another equation on the coarse grid which will enable us to solve also for η. A reasonable choice for such an equation is an approximation of equation (4.2), namely

$$\langle v^H, \bar{I}_h^H \phi^h \rangle = 0 \tag{4.4}$$

where $\bar{I}_h^H$ is some fine-to-coarse transfer, not necessarily identical with I_h^H. Equations (4.3), (4.4) form the <u>modified CS equations</u>.

Suppose now that H_0 is spanned by $\{\phi_1^h, \cdots, \phi_N^h\}$ and $\langle \phi_j^h, \phi_k^h \rangle = \delta_{jk}$. Because of linearity, the corrected CS equations for this case will be

$$L^H v^H = I_h^H R^h - \sum_{j=1}^{N} \eta_j I_h^H L^h \phi_j^h \tag{4.5a}$$

$$\langle v^H, \phi_j^H \rangle = 0 \qquad j = 1, \cdots, N \tag{4.5b}$$

where $R^h = F^h - L^h \tilde{u}^h$, $\tilde{u}^h$ being the current fine-grid approximation, and $\phi_j^H = \bar{I}_h^H \phi_j^h$. The coarse-grid correction will finally be done either by

$$\tilde{u}^h \leftarrow \tilde{u}^h + I_H^h \left[\tilde{v}^H + \sum_{j=1}^{N} \tilde{\eta}_j \phi_j^H \right] \tag{4.6a}$$

or by

$$\tilde{u}^h \leftarrow \tilde{u}^h + I_H^h \tilde{v}^H + \sum_{j=1}^{N} \tilde{\eta}_j \phi_j^h \tag{4.6b}$$

depending on whether or not ϕ_j^h are stored on the fine grid, $\tilde{u}$ and $\tilde{\eta}_j$ being the computed (approximate) solutions to equations (4.5). The difference between (4.6a) and (4.6b) is usually unimportant, so ϕ_j^h need not be stored. The only case where (4.6b) must be used is when the fine-grid problem is much closer to singularity than the coarse-grid one. In that case $\tilde{\eta}_j$ may be large; therefore, $I_H^h \tilde{\eta}_j \phi_j^H$ may have large high frequency components, which will magnify the residuals on the fine grid. By doing (4.6b) one avoids introducing high frequency components that arise from interpolating $\tilde{\eta}_j \phi_j^H$, and therefore the mentioned difficulty is removed. See Section 7, Tables 5 and 6.

4.2. Full Approximation Scheme (FAS) Version

The Full Approximation Scheme is essential for nonlinear problems or when local refinement is used. It is important, therefore, to derive the modified equations in that formulation too. This derivation can be done directly from (4.5), but to gain an additional insight we do it independently. The usual FAS equation on the coarse grid is

$$L^H u^H = F^H + \tau_h^H(\tilde{u}^h) \tag{4.7}$$

where $\tau_h^H(\tilde{u}^h) = L^H \bar{I}_h^H \tilde{u}^h - I_h^H L^h \tilde{u}^h$ is the "fine-to-coarse (defect) correction," $F^H = I_h^H F^h$, $\tilde{u}^h$ is the current approximation on the fine grid, and $\bar{I}_h^H$ is the fine-to-coarse solution transfer (see [1, Sections 8.1-8.2]).

In the present case, however, we wish to approximate on the coarse-grid only the part of the error which is free of H_0 components; hence, the H_0 components of the correction, $\sum \eta_j \phi_j^h$, should be considered part of the fine grid approximation, replacing (4.7) by

$$L^H u^H = F^H + \tau_h^H\left(\tilde{u}^h + \sum_{j=1}^{N} \eta_j \phi_j^h\right). \tag{4.8}$$

The additional conditions, ensuring that the coarse-grid correction is indeed approximtely free of H_0 components, can be written as

$$\langle u^H, \phi_j^H\rangle = \langle \bar{I}_h^H \tilde{u}^h, \phi_j^H\rangle + \eta_j \langle \phi_j^H, \phi_j^H\rangle, \quad (j = 1,\cdots,N). \tag{4.9}$$

Equations (4.8) and (4.9) together should determine u^H and $\eta_1,\cdots,\eta_N$. Once an approximate solution $(\tilde{u}^H, \tilde{\eta}_1,\cdots,\tilde{\eta}_N)$ has been calculated, the correction to the fine grid solution can be done analogously to either (4.6a) or (4.6b), but the former option yields here a particularly simple formula, namely

$$\tilde{u}^h \leftarrow \tilde{u}^h + I_H^h(\tilde{u}^H - \bar{I}_h^H \tilde{u}^h) \tag{4.10a}$$

which is just the usual FAS correction formula. The latter option, which must be used in some extreme cases, reads

$$\tilde{u}^h \leftarrow \tilde{u}^h + I_H^h \left(\tilde{u}^H - I_h^H \tilde{u}^h - \sum_{j=1}^{N} \eta_j \phi_j^H\right) + \sum_{j=1}^{N} \eta_j \phi_j^h \,. \tag{4.10b}$$

Equation (4.8) is not in a form convenient for calculations on grid H. In case the problem is linear, a more convenient form is

$$L^H u^H = \bar{F}^H + \sum_{j=1}^{N} \eta_j \psi_j^H \tag{4.11}$$

where

$$\begin{aligned} \bar{F}^H &= F^H + \tau_h^H(\tilde{u}^h) \\ &= I_h^H R^h + L^H(I_h^H \tilde{u}^h) \end{aligned} \tag{4.12}$$

and $\psi_j^H = \tau_h^H(\phi_j^h)$. The solution of (4.9) and (4.11) thus involves the $2N+1$ input functions $\bar{F}^H$, $\psi_1^H,\cdots,\psi_N^H$, $\phi_1^H,\cdots,\phi_N^H$, of which $\bar{F}^H$ should be calculated and stored whenever the algorithm switches from level h to level H, while the other $2N$ functions can be calculated and stored once for all. The same equations can be used also for nonlinear problems, but with ψ_j^H generally calculated by

$$\psi_j^H = \varepsilon^{-1}\{\tau_h^H(\tilde{u}^h + \varepsilon\phi_j^h) - \tau_h^H(\tilde{u}^h)\}, \tag{4.13}$$

with sufficiently small positive ε. The dependence of ψ_j^H on $\tilde{u}^h$ is very crude (e.g., no dependence at all when L^h is linear); hence it will usually be unnecessary to update them on a new switch to level H.

5. GENERAL MULTIPLE GRID EQUATIONS

Suppose a sequence of discretization with mesh sizes $h_1 > h_2 > \cdots > h_M$ is given, where $h_j = 2h_{j+1}$. Let the h_k-grid equations be

$$L^k u^k = F^k$$

where L^k approximates L^{k+1} for $k < M$, and L^M approximate some differential operator L.

Usually, if level M well approximates the differential equation (even in terms of H_0 components) then level $M - 1$ will approximate level M well enough for acceleration purposes. Hence, modified coarse-grid equations may not be needed on level $M - 1$. Denote by ℓ the finest level on which modified equations are needed. We describe now the modified equations on levels $k \leq \ell$, assuming the subspace of bad components, H_0, is spanned on level ℓ by the orthogonal set $\{\phi_1^\ell, \cdots, \phi_N^\ell\}$.

5.1. CS Version

For $k \leq \ell$ the equations to be solved for v^k, η_j^k on level k are

$$L^k v^k = f^k - \sum_{j=1}^{N} \eta_j^k I_{\ell+1}^k L^{\ell+1} \phi_j^{\ell+1} \qquad (5.1a)$$

$$\langle v^k, \phi_j^k \rangle = \rho_j^k \qquad (j = 1, \cdots, N) \qquad (5.1b)$$

where

$$f^k = I_{k+1}^k (\tilde{f}^{k+1} - L^{k+1} \tilde{v}^{k+1}) \qquad (k < \ell) \qquad (5.2a)$$

$$\tilde{f}^k = f^k - \sum_{j=1}^{N} \tilde{\eta}_j^k \, I_{\ell+1}^k \, L^{\ell+1} \, \phi_j^{\ell+1} \qquad (k \leq \ell) \tag{5.2b}$$

$$\tilde{f}^{\ell+1} = f^{\ell+1} \tag{5.2c}$$

$$\rho_j^k = \rho_j^{k+1} - \langle \tilde{v}^{k+1}, \phi_j^{k+1} \rangle \qquad (k < \ell, \; j = 1,\cdots,N) \tag{5.2d}$$

$$\rho_j^{\ell} = 0 \qquad (j = 1,\cdots,N) \tag{5.2e}$$

$$\phi_j^k = \bar{I}_{k+1}^k \, \phi_j^{k+1} \qquad (k < \ell; \; j = 1,\cdots,N) \tag{5.2f}$$

$$\bar{I}_{\ell+1}^k = \bar{I}_{k+1}^k \, \bar{I}_{\ell+1}^{k+1}, \qquad I_{\ell+1}^k = I_{k+1}^k \, I_{\ell+1}^{k+1} \tag{5.2g}$$

$\bar{I}_{k+1}^k$, I_{k+1}^k are fine-to-coarse grid transfers, not necessarily the same. $\tilde{v}^k$, $\tilde{\eta}_j^k$ are the current approximation to v^k, η_j^k respectively. Initial approximations are $\tilde{v}^k = 0$, $\tilde{\eta}_j^k = 0$. The input functions for level k are thus f^k, ϕ_j^k and $I_{\ell+1}^k \, L^{\ell+1} \, \phi_j^{\ell+1}$, $(j = 1,\cdots,N)$, of which only f^k should be updated on every new switch from level $k + 1$.

For efficient relaxation, instead of storing f^k one should store $\tilde{f}^k$ and update it whenever the $\tilde{\eta}_j^k$ are changed.

Note that η_j^{k-1} is designed to be a correction to η_j^k. Thus, the coarse-grid corrections for $2 \leq k \leq \ell$ will be done by the replacements

$$\tilde{\eta}_j^k \leftarrow \tilde{\eta}_j^k + \tilde{\eta}_j^{k-1} \qquad (j = 1,\cdots,N) \tag{5.3a}$$

$$\tilde{f}^k = \tilde{f}^k - \sum_{j=1}^{N} \tilde{\eta}_j^{k-1} \, I_{\ell+1}^k \, L^{\ell+1} \, \phi_j^{\ell+1} \tag{5.3b}$$

$$\tilde{v}^k \leftarrow \tilde{v}^k + I_{k-1}^k \tilde{v}^{k-1} \tag{5.3c}$$

while for $k = \ell + 1$ use

$$\tilde{v}^{\ell+1} \leftarrow \tilde{v}^{\ell+1} + I_\ell^{\ell+1}\left(\tilde{v}^\ell + \sum_{j=1}^N \tilde{\eta}_j^\ell \phi_j^\ell\right) \tag{5.3d}$$

or

$$\tilde{v}^{\ell+1} \leftarrow \tilde{v}^{\ell+1} + I_\ell^{\ell+1} \tilde{v}^\ell + \sum_{j=1}^N \tilde{\eta}_j^\ell \phi_j^{\ell+1}, \tag{5.3e}$$

(see discussion in Section 4.1 for the use of (5.3d) versus (5.3c)).

5.2. FAS Version

For $k \leq \ell$ the equations to be solved for u^k, η_j^k on level k are given by

$$L^k u^k = \bar{F}^k + \sum_{j=1}^N \eta_j^k \psi_j^k \tag{5.4a}$$

$$\langle u^k, \phi_j^k \rangle = \sigma_j^k + \eta_j^k \alpha_j^k \qquad (j = 1,\cdots,N) \tag{5.4b}$$

where

$$\psi_j^k = \varepsilon^{-1}\left\{\tau_{k+1}^k(\tilde{u}^{k+1} + \varepsilon\phi_j^{k+1}) - \tau_{k+1}^k(\tilde{u}^{k+1})\right\} + I_{k+1}^k \psi_j^{k+1} \qquad (k \leq \ell) \tag{5.5a}$$

(hence $\psi_j^k = \tau_{k+1}^k(\phi_j^{k+1}) + I_{k+1}^k \psi_j^{k+1}$ in the linear case)

$$\psi_j^{\ell+1} = 0 \qquad (j = 1,\cdots,N) \tag{5.5b}$$

$$\tau_{k+1}^k(\tilde{u}^{k+1}) = L^k \bar{I}_{k+1}^k \tilde{u}^{k+1} - I_{k+1}^k L^{k+1} \tilde{u}^{k+1} \tag{5.5c}$$

$$\phi_j^k = \bar{I}_{k+1}^k \phi_j^{k+1} \qquad (j = 1,\cdots,N) \tag{5.5d}$$

$$\bar{F}^k = L^k \bar{I}_{k+1}^k \tilde{u}^{k+1} + I_{k+1}^k (\tilde{F}^{k+1} - L^{k+1} \tilde{u}^{k+1}) \tag{5.5e}$$

$$\tilde{F}^k = \bar{F}^k + \sum_{j=1}^{N} \tilde{\eta}_j^k \psi_j^k \qquad (k \leq \ell) \tag{5.5f}$$

$$\tilde{F}^{\ell+1} = \bar{F}^{\ell+1} \tag{5.5g}$$

$$\sigma_j^k = \langle \bar{I}_{k+1}^k \tilde{u}^{k+1}, \phi_j^k \rangle + \begin{cases} 0 & (k = \ell) \\ \tilde{\sigma}_j^{k+1} - \langle \tilde{u}^{k+1}, \phi_j^{k+1} \rangle & (k < \ell) \end{cases} \tag{5.5h}$$

$$\tilde{\sigma}_j^k = \sigma_j^k + \tilde{\eta}_j^k \alpha_j^k \qquad (j = 1,\cdots,N) \tag{5.5i}$$

$$\alpha_j^k = \langle \phi_j^k, \phi_j^k \rangle \qquad (j = 1,\cdots,N) \tag{5.5j}$$

and $\tilde{\eta}_j^k$, $\tilde{u}^k$ are the current approximations to η_j^k, u^k respectively. Intital approximations are $\tilde{\eta}_j^k = 0$, $\tilde{u}^k = \bar{I}_{k+1}^k \tilde{u}^{k+1}$. The input functions are $\bar{F}^k$, $\phi_1^k,\cdots,\phi_N^k$, $\psi_1^k,\cdots,\psi_N^k$, of which only $\bar{F}^k$ must be recalculated each time the level k problem is formulated.

For efficient relaxation, instead of storing $\bar{F}^k$ and σ_j^k $(j = 1,\cdots,N)$ one should store $\tilde{F}^k$ and $\tilde{\sigma}_j^k$ and update them whenever $\tilde{\eta}_j^k$ is updated. Initially (when the level k problem is set up) $\tilde{F}^k = \bar{F}^k$ and $\tilde{\sigma}_j^k = \sigma_j^k$.

The coarse-grid corrections will be done by the replacements

$$\tilde{\eta}_j^k \leftarrow \tilde{\eta}_j^k + \tilde{\eta}_j^{k-1} \qquad (2 \leq k \leq \ell;\ j = 1,\cdots,N) \tag{5.6a}$$

$$\tilde{F}^k \leftarrow \tilde{F}^k + \sum \tilde{\eta}_j^{k-1}\ \psi_j^k \qquad (2 \le k \le \ell) \tag{5.6b}$$

$$\tilde{\sigma}_j^k \leftarrow \tilde{\sigma}_j^k + \tilde{\eta}_j^{k-1}\ \alpha_j^{k-1} \qquad (2 \le k \le \ell;\ j = 1,\cdots,N) \tag{5.6c}$$

$$\tilde{u}^k \leftarrow \tilde{u}^k + I_{k-1}^k\left(\tilde{u}^{k-1} - \bar{I}_k^{k-1}\ \tilde{u}^k\right) \qquad (2 \le k \le M). \tag{5.6d}$$

In case, for some $2 \le k \le \ell+1$, the grid k problem is much closer to singularity than grid $k+1$ problem, (5.6d) should be replaced by

$$\tilde{u}^k \leftarrow \tilde{u}^k + I_{k-1}^k\left(\tilde{u}^{k-1} - \bar{I}_k^{k-1}\ \tilde{u}^k - \sum_{j=1}^{N} \tilde{\eta}_j^{k-1}\ \phi_j^{k-1}\right) + \sum_{j=1}^{N} \tilde{\eta}_j^{k-1}\ \phi_j^k \tag{5.6e}$$

which is the analogue of both (5.3c) and (5.3e). Of course, (5.6e) can always be used, but (5.6d) is somewhat simpler (cf. end of Section 4.1).

Observe, indeed, that in the linear case

$$\psi_j^k = \tau_{k+1}^k\left(\phi_j^{k+1}\right) + I_{k+1}^k\ \psi_j^{k+1} = L^k\ \phi_j^k - I_{\ell+1}^k\ L^{\ell+1}\ \phi_j^{\ell+1}$$

and by identifying u^k with $\bar{I}_{k+1}^k\ \tilde{u}^{k+1} + v^k + \sum \eta_j^k\ \phi_j^k$ the equivalence of the FAS and the CS is easily seen.

5.3. Solution Process for Modified Equations

We refer in this section to the FAS version, namely the equation

$$L^k\ u^k = \bar{F}^k + \sum_{j=1}^{N} \eta_j^k\ \psi_j^k \tag{5.7a}$$

$$\langle u^k,\ \phi_j^k \rangle = \sigma_j^k + \eta_j^k\ \alpha_j^k \qquad (j = 1,\cdots,N), \tag{5.7b}$$

where the unknowns are the function u^k and the constants $\eta_1^k,\cdots,\eta_N^k$. The CS version is treated similarly. As before, $\tilde{u}^k$, $\tilde{\eta}_j^k$, $\tilde{F}^k$ and $\tilde{\sigma}_j^k$ will denote the current (stored) approximations to u^k, η_j^k, the right-hand side of (5.7a) and the right-hand side of (5.7b), respectively.

In relaxing equations (5.7) we distinguish between the following:

(i) a local relaxation sweep

Relax $L^k u^k = \tilde{F}^k$ for $\tilde{u}^k$ by either Gauss-Seidel or Kaczmarz, keeping $\tilde{\eta}_j^k$, and therefore also $\tilde{F}^k$, fixed.

(ii) a global step

This will be the step for updating $\eta_1^k,\cdots,\eta_N^k$, and the H_0 components in u^k by using (5.7b) together with (approximatley) the H_0 components of (5.7a). Most generally this is done by solving simultaneously for β_j, $\hat{\eta}_j$ $(j = 1,\cdots,N)$ the system of $2N$ equations:

$$\langle L^k\left(u^k + \sum_{i=1}^{N} \beta_i \phi_i^k\right), \phi_j^k\rangle = \langle \tilde{F}^k + \sum_{i=1}^{N} \hat{\eta}_i \psi_i^k, \phi_j^k\rangle \qquad (j = 1,\cdots,N) \quad (5.8a)$$

$$\langle u^k + \beta_j \phi_j^k, \phi_j^k\rangle = \tilde{\sigma}_j^k + \hat{\eta}_j \alpha_j^k \qquad (j = 1,\cdots,N) \quad (5.8b)$$

and then introducing the following changes

$$\tilde{u}^k \leftarrow \tilde{u}^k + \sum_{j=1}^{N} \beta_j \phi_j^k \qquad (5.9a)$$

$$\tilde{\eta}_j^k \leftarrow \tilde{\eta}_j^k + \hat{\eta}_j \qquad (j = 1,\cdots,N) \quad (5.9b)$$

$$\tilde{F}^k \leftarrow \tilde{F}^k + \sum_{j=1}^{N} \hat{\eta}_j \psi_j^k \qquad (5.9c)$$

$$\tilde{\sigma}_j^k = \tilde{\sigma}_j^k + \hat{\eta}_j \alpha_j^k \qquad (j = 1,\cdots,N). \tag{5.9d}$$

The local relaxation is used to smooth the error in u^k and therefore should be done at all levels. On the other hand, it may be enough to do step (ii) on the coarsest grids only, since it deals with global variables (η_j^k) and with global changes to u^k. Thus, step (ii) will be done on grids $k \leq m$, where usually $m < \ell$. This will usually reduce the storage requirement of the algorithm, since there is no need to store ϕ_j^k on levels $m < k \leq \ell$. In fact, it is often unnecessary to store even ψ_j^k for $m < k \leq \ell$. Indeed for $m < k \leq \ell$ these functions are only used in the interpolation step (5.6b), which can be skipped in case of a V cycle, because as a smooth change to $\tilde{F}^k$, its effect on the subsequent relaxation on level k is negligible. On the other hand, step (5.6b) cannot be skipped in case it is followed by a switch back to the coarser $(k-1)$ grid, since in this case the smooth update to $\tilde{F}^k$ is essential. Thus, in case of W cycles, ψ_j^k must be stored for all levels $k \leq \ell$. Generally, $m < \ell$ can be used only if no intermediate level k $(m < k \leq \ell)$ is much closer to singularity than level $k+1$.

5.4. Summary. Work and Storage

A cycle for improving $\tilde{u}^k$ and $\tilde{\eta}^k = (\eta_1^k,\cdots,\eta_N^k)$ $(k \leq \ell)$ is denoted by

$$(\tilde{u}^k, \tilde{\eta}^k) \leftarrow \mathrm{CMG}(\tilde{u}^k, \tilde{\eta}^k, L^k, \tilde{F}^k, \tilde{\sigma}^k)$$

and is defined recursively by the following steps (A) through (D).

(A) Make the following $\nu_1(k)$ times

(a) a local step for $L^k u^k = \tilde{F}^k$

(b) for $k \leq m$ make a global step defined in (5.8), (5.9). For $k = 1$, choose $\nu_1(k)$ to guarantee convergence to small residuals, or solve the equations directly, and then terminate the cycle. If $k > 1$, continue.

(B) Starting with $\tilde{u}^{k-1} = \bar{I}_k^{k-1} \tilde{u}^k$, $\tilde{\eta}_j^{k-1} = 0$ $(j = 1,\cdots,N)$ make the cycle

$$(\tilde{u}^{k-1}, \tilde{\eta}^{k-1}) \leftarrow CMG(\tilde{u}^{k-1}, \tilde{\eta}^{k-1}, L^{k-1}, \tilde{F}^{k-1}, \tilde{\sigma}^{k-1})$$

$\gamma(k)$ times, where $\tilde{F}^{k-1}$, $\tilde{\sigma}_j^{k-1}$ are defined by (5.5) with k replaced by $k - 1$.

(C)
$$\tilde{\eta}_j^k \leftarrow \tilde{\eta}_j^k + \tilde{\eta}_j^{k-1} \qquad (k \leq m;\ j = 1,\cdots,N)$$

$$\tilde{F}^k \leftarrow \tilde{F}^k + \sum_{j=1}^{N} \tilde{\eta}_j^{k-1} \psi_j^k \qquad (k \leq m)$$

$$\tilde{\sigma}_j^k \leftarrow \tilde{\sigma}_j^k + \tilde{\eta}_j^{k-1} \alpha_j^{k-1} \qquad (k \leq m)$$

and interpolation is done either by

$$\tilde{u}^k \leftarrow \tilde{u}^k + I_{k-1}^k (\tilde{u}^{k-1} - \bar{I}_k^{k-1} \tilde{u}^k)$$

or

$$\tilde{u}^k \leftarrow \tilde{u}^k + I_{k-1}^k (\tilde{u}^{k-1} - \bar{I}_k^{k-1} \tilde{u}^k - \sum_{j=1}^{N} \tilde{\eta}_j^{k-1} \phi_j^{k-1}) + \sum_{j=1}^{N} \tilde{\eta}_j^{k-1} \phi_j^k .$$

The second option is necessary in case the grid k problem may be almost singular.

(D) Make steps (a), (b) of (A) $\nu_2(k)$ times.

$\gamma(k) = 2$ corresponds to a W cycle; hence if $\gamma(k) = 2$, the global step has to be done on level k, which implies $m \geq k$. If $\gamma(k) = 1$ we can choose m to be smaller than k. Since equations (5.7) are for $k \leq \ell < M$, this cycle is part of a bigger cycle for $k = M$.

The storage and work required by this algorithm are essentially the same as in the usual multigrid algorithm, since all extra work and storage involved are made on very coarse grids, often only on level 1, sometimes also on level 2. In fact, $\ell = M-1$ should be used only when the finest (grid M) problem is itself a rather poor approximation to the differential problem, so usually $\ell < M-1$, in which case the extra work is negligible compared to the work of relaxing grid M.

6. APPROXIMATION OF SUBSPACE H_0

In the preceding discussion it is assumed that H_0 is accurately known. This section deals with how accurately H_0 needs to be known and how to approximate it.

6.1. Accuracy Needed for H_0

Let ϕ_i^h $(i \geq 1)$ be the smooth eigenfunctions on the finest grid

$$L^h \phi_i^h = \lambda_i^h \phi_i, \qquad \langle \phi_i, \phi_j \rangle = \delta_{ij}, \tag{6.1}$$

and let H_0 be for simplicity spanned by ϕ_1^h alone. Suppose that ϕ_1^h is

not known to the algorithm, and instead ϕ^h is used, where

$$\phi^h = \sum_{i \geq 1} a_i \phi_i^h. \tag{6.2}$$

Suppose an error $v^h = e_1 \phi_1^h$ has emerged on the fine grid so that

$$L^h v^h = e_1 \lambda_1 \phi_1^h, \tag{6.3}$$

and the corresponding modified CS coarse-grid equations are

$$L^H v^H + \eta I_h^H L^h \phi^h = e_1 \lambda_1 \phi_1^H \tag{6.4a}$$

$$\langle v^H, \phi^H \rangle = 0 \tag{6.4b}$$

where $\phi^H = I_h^H \phi^h$, $\phi_i^H = I_h^H \phi_i^H$. For smooth eigenfunctions ϕ_i^h, we can assume that ϕ_i^H are again eigenfunctions

$$L^H \phi_i^H = \lambda_i^H \phi_i^H, \qquad \langle \phi_i^H, \phi_j^H \rangle = \delta_{ij}, \tag{6.5}$$

neglecting changes in eigenfunctions since important to our discussion are only changes in the eigenvalues. If we write the solution to (6.4) as

$$v^H = \sum_{i \geq 1} E_i \phi_i^H \tag{6.6}$$

then (6.4) gives

$$\lambda_i^H E_i + \eta\lambda_i^h a_i = 0 \qquad i \geq 2 \tag{6.7a}$$

$$\lambda_1^H E_1 + \eta\lambda_1^h a_1 = \lambda_1^h e_1 \tag{6.7b}$$

$$\sum_{i\geq 1} a_i E_i = 0. \tag{6.7c}$$

Equations (6.7) imply

$$\eta = \frac{q_1 a_1 e_1}{\beta + q_1 a_1^2} \tag{6.8a}$$

$$E_1 = \eta\beta/a_1, \qquad E_i = -\eta q_i a_i \qquad (i \geq 2). \tag{6.8b}$$

where

$$\beta = \sum_{i\geq 2} q_i a_i^2, \qquad q_i = \frac{\lambda_i^h}{\lambda_i^H}. \tag{6.9}$$

Hence, the coarse-grid correction is

$$\begin{aligned} V^H + \eta\phi^H &= \sum_{i\geq 1} (E_i + \eta a_i)\phi_i^H \\ &= \frac{\beta + a_1^2}{\beta + q_1 a_1^2} q_1 e_1 \phi_1^H + \sum_{i\geq 2} \frac{q_1 a_1 a_i}{\beta + q_1 a_1^2} (1 - q_i) e_1 \phi_i^H. \end{aligned} \tag{6.10}$$

Extra errors have thus been introduced in the directions of $\{\phi_2^H, \phi_3^H, \ldots,\}$; but these should be small (relative to e_1), since q_i should be close to 1 for ϕ_i^H not in H_0 (and also a_i will be small compared to a_1 by the condition below) and, more importantly, these errors can efficiently be reduced by the next coarse-grid correction. Our focus here should thus be the behavior of the ϕ_1^h component. Assuming $I_H^h \phi_1^H \approx \phi_1^h$ by smoothness, the

coarse-grid correction, when interpolated to the fine grid and subtracted from the old fine grid error, gives in this component the new error $\bar{e}_1 \phi_1^h$, where

$$\bar{e}_1 = (1 - q_1)\beta(\beta + q_1 a_1^2)^{-1} e_1. \tag{6.11}$$

The main condition for convergence is therefore

$$\left| \frac{(\lambda_1^h - \lambda_1^H)\beta}{\lambda_1^h a_1^2 + \lambda_1^H \beta} \right| < 1, \tag{6.12}$$

and the convergence factor per cycle is bounded (below) by the left-hand side of (6.12). This bound is indeed small when λ_1^H is a good approximation to λ_1^h, i.e., when $|\lambda_1^h - \lambda_1^H| \ll \lambda_1^h$. But if that is not the situation (which is why one should want to include ϕ_1^h in H_0 in the first place) then the necessary condition for fast convergence is that both $|\lambda_1^h \beta|$ and $|\lambda_1^H \beta|$ are small compared to $\lambda_1^h a_1^2$. Since $q_i \approx 1$ for $i \geq 2$, the condition for fast convergence can be summarized as

$$\sum_{i \geq 2} a_i^2 \ll \min\left(1, \frac{|\lambda_1^h|}{|\lambda_1^H|}\right) a_1^2. \tag{6.13}$$

This condition implies in particular that, if $\lambda_1^h = 0$, that is, if the given problem is singular, then $a_2 = a_3 = \cdots = 0$, i.e., the eigenfunction ϕ_1^h must be known exactly. This seems to be too stringent, but in fact, the increase in accuracy for ϕ_1^h can be obtained as the algorithm proceeds, by doing for each cycle of the original problem, a cycle for improving ϕ_1^h. (See Section 7, Tables 8 and 9.)

On the other hand,(6.13) implies that there is no complication when the coarse-grid problem is singular (see Section 7, Tables 1-4).

Generally, condition (6.13) gives a precise idea as to how closely ϕ_1^h should be approximated.

6.2 Algorithm for Approximating H_0

We motivate the algorithm by considering the case where H_0 is spanned by one function. It is assumed in this discussion that the finest grid problem is well-posed. This implies that errors in components which belong to H_0 show sizeable average residuals on the finest grid.

The method for approximating H_0 is based on the following observation: components which belong to H_0 are spanned by eigenfunctions whose eigenvalues are much closer to zero than others, and exactly such eigenfunctions will converge in Kaczmarz relaxation much slower than other eigenfunctions. Hence, if the coarse-grid equation

$$L^k w^k = 0 \qquad \text{with homogeneous boundary conditions} \tag{6.14}$$

is relaxed, starting with a random approximation, then when convergence has slowed down, the dominant part in the resulting $\tilde{w}^k$ must be a component in H_0; therefore, $\tilde{w}^k$ at this stage can serve as an approximation to a function in H_0 on the coarse grid. H_0 is needed on finer grids. A first candidate will be just an interpolation of $\tilde{w}^k$ to these grids. However, since interpolation introduces high frequency errors which will leave large residuals in equation (6.14) on finer grids, and therefore give the wrong ψ_j^k, one needs to smooth somehow the interpolated $\tilde{w}^k$ from coarser grids. A reasonable way to

do it is to relax (6.14) on fine grids after obtaining a first approximation from coarser grids. This is summarized in the following algorithm.

Algorithm

Repeat the following for $i = 1,\cdots,N$ ($N = \dim H_0$)

(A) Set $k = 1$

(B) $\tilde{W}^k$ = random function if $k = 1$

$\tilde{W}^k = I^k_{k-1}\, \tilde{W}^{k-1}$ if $k > 1$.

(C) Relax (6.14), starting with initial approximation $\tilde{W}^k$, keeping $\tilde{W}^k$ orthogonal to $\{\phi^k_1,\cdots,\phi^k_{i-1}\}$, until convergence becomes slow

(D) $k \leftarrow k + 1$

(E) if $k \leq \ell+1$ go to (A), else $\phi^{\ell+1}_i = \tilde{W}^{\ell+1}$.

(F) Define $\phi^k_i = I^k_{k+1}\, \phi^{k+1}_i$ $(k = \ell,\ell-1,\cdots,1)$.

In case N is not known in advance, stop the above procedure when step (C) no longer reaches slow convergence in just a few sweeps. If, after few cycles of solving the original problem, convergence rate still deteriorates, repeat (A) through (F) once more, replacing the random function in (B) by the residuals left by the original problem on the coarsest grid. If the addition of the new function $\phi^{\ell+1}_i$ to the set $\{\phi^{\ell+1}_1,\cdots,\phi^{\ell+1}_{i-1}\}$ does not improve convergence rate significantly, it means that the accuracy of $\{\phi^{\ell+1}_1,\cdots,\phi^{\ell+1}_i\}$ is not enough and this can be improved by inverse iteration on the grid $k = \ell+1$ (using standard multigrid for doing the inverse iteration). The improvement of the functions $\phi^{\ell+1}_j$ by inverse iteration is done by one multigrid cycle before each multigrid cycle of the original problem. Such an improvement is needed when the original finest grid probelm is much closer to singularity than the next level; see Section 7, Tables 8 and 9.

Finally, if cycles on level $\ell+1$ converge satisfactorily, but not on finer levels, then ℓ should be increased (by 1). The above algorithm can then, of course, be shortened, starting with the known H_0 on level ℓ.

7. NUMERICAL RESULTS

Experiments were performed with the new algorithm using the model problem

$$\begin{cases} (\Delta + k^2)U = F & \text{in } \Omega = (0,1) \times (0,1) \\ U = g & \text{on } \partial\Omega. \end{cases}$$

The tables below show the residual history on the finest level. We denote by M, m, ℓ, h_1 the following:

M -- the finest level,

ℓ -- the finest level on which corrected equations are needed,

m -- the finest level on which the global step is performed,

h_1 -- the mesh size of the coarsest grid (grid 1).

The subspace H_0 was calculated by the algorithm of Section 6.2, where in step (B) 40 relaxations were done on the coarsest grid ($k = 1$) and two on every finer grid ($1 < k \leq \ell$). The algorithm CMG of Section 5.3 was used with

$\nu_1(k) = 2$, $\nu_2(k) = 1$ when Gauss-Seidel relaxation is used,

$\nu_1(k) = \nu_2(k) = 3$ when Kaczmarz relaxation is used,

$\nu_1(k) = 13$ for $k = 1$,

$\gamma(k) = 1$ for $k > 2$, $\gamma(k) = 2$ for $k = 2$.

We give below the discrete first two eigenvalues of the Laplacian for the grids used in the examples of this section. This will enable us to see how far from singularity is each of the different levels used in the process.

h	λ_1^h	λ_2^h
.25	-18.74516600406	-41.37258300203
.125	-19.48683967711	-47.23375184668
.0625	-19.67587286709	-48.81161578777
.03125	-19.72335955067	-49.21342550952

In Tables 1-4 interpolation of corrections was made according to (5.6b); in other tabels the interpolation is specified. Residuals were transferred by 9-point full weighting and the local relaxation was Gauss-Seidel for $kh \leq .5$ and Kaczmarz for $kh > .5$. In all examples $M = 4$, $h_1 = .25$, $\ell = 3$, $m = 2$.

Tables 3, 4 show a case in which the second eigenvalue is very close to zero, and its corresponding eigenspace is two-dimensional. Therefore, only two functions were used in spanning H_0. The algorithm for finding functions in H_0 finds first these eigenfunctions whose eigenvalues are closest to zero. Therefore, the eigenfunction belonging to the first eigenvalue was not used in these computations, and it was not needed as can be seen from the fast convergence shown by these tables. This clearly shows that H_0 is related to almost-singularity, not to indefiniteness.

In Tables 5, 6 we show that in case the finest grid problem is too close to a singularity one must use interpolation of correction according to (5.6e)

(or (5.3e) in the CS version) and not the usual FAS interpolation. In these two tables the exact H_0 was used.

Table 7 shows that if ϕ is not known accurately enough, poor results are obtained. ϕ in this example is found by the same procedure described in the beginning of this section.

In Table 8 inverse iteration (done by usual multigrid) was used to improve the accuracy of ϕ. Starting with ϕ obtained as in Table 7, one multigrid cycle of inverse iteration was done to improve ϕ before each multigrid cycle for the original problem. Results are identical to the ones obtained with the exact ϕ (Table 5).

Table 9 shows a case in which the distance of the closest eigenvalue to zero is about 1.10^{-8}. As seen from this table, improving ϕ by only one cycle of inverse iteration per cycle of the original problem is not quite enough to maintain the full speed of the algorithm. Once in few cycles the residuals are magnified, and this happens whenever the L_2-norm of the error in the approximation is reduced significantly. This reduction of the error is due to a correction of the approximate solution by $\eta\phi$. If ϕ is not accurate enough, components other than the desired ones enter to u^h and since their residuals are much higher than those of $\eta\phi$, a magnification of the residuals occurs. (A similar phenomenon can be seen also in Table 7, where the distance from singularity is larger, but ϕ is not improved at all by inverse iterations.) This would not have happened if we allowed the speed of convergence of the inverse-iteration cycles to be slightly faster than that of the main cycles, e.g., by adding an extra inverse-iteration cycle once per several cycles. But this is not really needed, because all that may happen is a minor slowdown at high-accuracy solutions (much below truncation errors) for cases of extreme closeness to singularity.

In fact, we believe that, to obtain solutions with errors smaller than trunction error, all one has generally to do is a one-cycle FMG algorithm for calculating H_0 (meaning one inverse-iteration cycle for level k after step (C) in the algorithm of Section 6.2), followed by a one-cycle FMG algorithm for solving the original problem.

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Table 1: $k^2 = 18.745166$, dim $H_0 = 1$

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.172(+2)
3	.114(+1)
4	.891(-1)
5	.762(-2)
6	.685(-3)
7	.652(-4)
8	.658(-5)
9	.684(-6)
10	.744(-7)

Table 2: $k^2 = 19.486839$, dim $H_0 = 1$

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.174(+2)
3	.114(+1)
4	.892(-1)
5	.763(-2)
6	.687(-3)
7	.654(-4)
8	.661(-5)
9	.688(-6)
10	.749(-7)

Table 3: $k^2 = 41.372583$, dim $H_0 = 2$

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.172(+2)
3	.112(+1)
4	.938(-1)
5	.864(-2)
6	.832(-3)
7	.820(-4)
8	.815(-5)
9	.796(-6)
10	.811(-7)

Table 4: $k^2 = 47.233752$, dim $H_0 = 2$

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.171(+2)
3	.110(+1)
4	.910(-1)
5	.824(-2)
6	.778(-3)
7	.755(-4)
8	.740(-5)
9	.682(-6)
10	.673(-7)

Table 5: $k^2 = 19.723368$, dim $H_0 = 1$, interpolation according to (5.6e).

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.172(+2)
3	.114(+1)
4	.893(-1)
5	.765(-2)
6	.687(-3)
7	.691(-4)
8	.685(-5)
9	.759(-6)
10	.768(-7)

Table 6: $k^2 = 19.723368$, dim $H_0 = 1$, interpolation according to (5.6d).

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.172(+2)
3	.114(+1)
4	.893(-1)
5	.125
6	.102(-1)
7	.162(-1)
8	.132(-2)
9	.909(-3)
10	.742(-4)

Table 7: $k^2 = 19.72336843$, dim $H_0 = 1$, interpolation according to (5.6e), ϕ_1 crudely computed.

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.174(+2)
3	.114(+1)
4	.879(-1)
5	.116
6	.550(-2)
7	.134
8	.427(-1)
9	.465(-2)
10	.534(-3)

Table 8: $k^2 = 19.72336843$, dim $H_0 = 1$, interpolation according to (5.6e). ϕ_1 successively improved.

cycle #	$\|\text{residuals}\|_2$
1	.363(+3)
2	.174(+2)
3	.114(+1)
4	.893(-1)
5	.765(-2)
6	.687(-3)
7	.691(-4)
8	.683(-5)
9	.759(-6)
10	.768(-7)

Table 9: $k^2 = 19.72335955955$, dim $H_0 = 1$, interpolation according to (5.6e).

cycle #	$\|\text{Residuals}\|_2$	$\|\tilde{u}^h - u^h\|_2$
1	.363(+3)	.555
2	.174(+2)	.392
3	.114(+1)	.392
4	.893(-1)	.392
5	.764(-2)	.392
6	.687(-3)	.392
7	.655(-4)	.392
8	.359(-3)	.268(-1)
9	.284(-4)	.268(-1)
10	.219(-5)	.268(-1)

1. Report No. NASA CR-178026 ICASE Report No. 85-57	2. Government Accession No.	3. Recipient's Catalog No.

4. Title and Subtitle	5. Report Date
MULTIGRID METHOD FOR NEARLY SINGULAR AND SLIGHTLY INDEFINITE PROBLEMS	November 1985
	6. Performing Organization Code
7. Author(s)	8. Performing Organization Report No.
Achi Brandt and Shlomo Ta'asan	85-57
	10. Work Unit No.
9. Performing Organization Name and Address	
Institute for Computer Applications in Science and Engineering Mail Stop 132C, NASA Langley Research Center Hampton, VA 23665-5225	11. Contract or Grant No. NAS1-17070; NAS1-18107
12. Sponsoring Agency Name and Address	13. Type of Report and Period Covered
National Aeronautics and Space Administration Washington, D.C. 20546	Contractor Report
	14. Sponsoring Agency Code 505-31-83-01

15. Supplementary Notes

Langley Technical Monitor:
J. C. South Jr.
Final Report

Lecture Notes in Mathematics,
(W. Hackbusch and U. Trottenberg, eds.), Springer-Verlag

16. Abstract

This paper deals with nearly singular, possibly indefinite problems for which the usual multigrid solvers converge very slowly or even diverge. The main difficulty is related to some badly approximated smooth functions which correspond to eigenfunctions with nearly zero eigenvalues. A correction to the usual coarse-grid equations is derived, both in Correction Scheme and in Full Approximation Scheme. The performance of the new algorithm using this correction is essentially as that of usual multigrid for definite problems.

17. Key Words (Suggested by Author(s))	18. Distribution Statement
multigrid indefinite problems	59 - Mathematics and Computer Science 64 - Numerical Analysis Unclassified - Unlimited

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price
Unclassified	Unclassified	37	A03

For sale by the National Technical Information Service, Springfield, Virginia 22161