

# Towards Robust Two-Level Methods For Indefinite Systems

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We present a black-box two-level solver for indefinite algebraic linear system of equations arising from the finite element discretization. Numerical experiments show the applicability of the method to 3D Helmholtz equations and shear banding problems with strain softening.

## 1.0 Introduction

Despite the fact that iterative solution techniques are recently gaining recognition among practitioners and finding their way into commercial software arena, the current state of the art in iterative methods remains unsatisfactory in many respects. Users of large production codes such as ANSYS, NASTRAN, ALGOR, SDRC, EMRC and ANSYS often observe many “bad” cases resulting from poorly conditioned or indefinite systems for which their iterative solvers converge prohibitively slow or systematically break. Consequently and perhaps rightfully so, a number of commercial software houses, including ABAQUS, refrain from utilizing iterative solver technology primarily because of its lack of robustness.

For positive definite systems iterative solvers developed into mature technology, and in many cases, far more effective than the direct methods. For such systems the multilevel solution techniques possess an optimal rate of convergence by which computational work required to obtain a fixed accuracy is linearly proportional to the number of unknowns, whereas for indefinite systems not even convergence is guaranteed. Numerical analysis of multilevel methods for indefinite systems shows that convergence is only guaranteed provided that the coarse model is sufficiently fine [1]. For some “bad” cases coarsening factor required might be close to one effectively turning the multilevel solver into a direct method.

Indefinite problems arise in many areas of scientific computing. Examples falling into this category are: Helmholtz equations, Galerkin or least squares methods with constraints, and problems with indefinite constitutive tensor arising as a result of damage/localization in solids or shocks in fluids.

The manuscript is organized as follows. After briefly describing the principles of multilevel methods in Section 2, we present a numerical example which demonstrates the critical role of the prolongation operator and serves as a motivation for developing a family of two-level methods for indefinite systems. Attention is restricted to symmetric systems.

Complex symmetric algebraic systems are transformed into real symmetric systems prior to the solution (Section 6.1). In Section 4 we conduct a convergence analysis on a model problem and identify key factors affecting the convergence of two-level schemes. Section 5 details various approaches for constructing efficient prolongators. In Section 6 we test various two-level schemes on a sequence of examples involving Helmholtz equation on bounded domains and shear banding problems with strain softening. A brief discussion of future research directions conclude the manuscript.

## 2.0 Principles of multilevel methods

Consider a linear or linearized system of equations within a Newton-Raphson or related scheme

$$Ku = f \quad u \in R^n \quad f \in R^n \quad (1)$$

where  $K$  is an  $n \times n$  symmetric sparse matrix.

The following notation is adopted in this section. Auxiliary model functions are denoted with subscript 0. For example,  $u_0 \in R^m$ ,  $m < n$  denotes the discrete values of the solution in the auxiliary model. We also denote the prolongation operator from the coarse to the fine model by  $\tilde{Q}$ :

$$\tilde{Q}: R^m \rightarrow R^n \quad (2)$$

The restriction operator  $\tilde{Q}^T$  from the fine-to-coarse model is conjugated with the prolongation operator, i.e.,

$$\tilde{Q}^T: R^n \rightarrow R^m \quad (3)$$

In this section superscripts are reserved to indicate the iteration count. Let  $r^i$  be the residual vector in the  $i$ -th iteration defined as

$$r^i = f - Ku^i \quad (4)$$

where  $u^i$  is the current approximation of the solution in the  $i$ -th iteration.

The problem of the coarse model correction consists of finding the stationary values of the following functional on the subspace  $R^m$ :

$$(1/2)K(u^i + \tilde{Q}u_0^i), u^i + \tilde{Q}u_0^i) - (f, u^i + \tilde{Q}u_0^i) \Rightarrow \text{stationary } u_0^i \in R^m \quad (5)$$

where  $(\cdot, \cdot)$  denotes the bilinear form defined by

$$(u, v) = \sum_{j=1}^n u_j v_j \quad u, v \in R^n \quad (6)$$

A direct solution of (5) yields a classical two-level procedure. Alternatively, one may introduce an additional auxiliary model for  $u_0$  and so forth, leading to a natural multilevel sequence. In the present manuscript we will consider a two-level process resulting from (5) which yields

$$K_0 u_0^i = \tilde{Q}^T (f - Ku^i) \quad (7)$$

where  $K_0 = \tilde{Q}^T K \tilde{Q}$  is the restriction of the matrix  $K$ . The resulting classical two-level algorithm can be viewed as a two-step procedure:

a) *Coarse model correction*

$$\begin{aligned} r^i &= f - Ku^i \\ u_0^i &= K_0^{-1} \tilde{Q}^T r^i \\ \tilde{u}^i &= u^i + \tilde{Q}u_0^i \end{aligned} \quad (8)$$

where  $\tilde{u}^i$  is a partial solution obtained after the coarse model correction.

b) *Smoothing*

$$u^{i+1} = \tilde{u}^i + D(f - K\tilde{u}^i) \quad (9)$$

where  $D$  is an inverse of smoothing preconditioner.

Let  $u$  be the exact solution of the source problem, then the error resulting from the coarse model correction (8) can be cast into the following form

$$\tilde{e}^i = u - \tilde{u}^i = (I_n - CK)e^i \quad (10)$$

where  $I_s \in \mathcal{R}^{s \times s}$  is an identity matrix and  $C = \tilde{Q}K_0^{-1}\tilde{Q}^T$  is an inverse of the coarse model preconditioner. Likewise the influence of smoothing on error reduction is given by:

$$e^{i+1} = u - u^{i+1} = (I_n - DK)\tilde{e}^i \quad (11)$$

Furthermore if we denote

$$\begin{aligned} M &= I_n - DK \\ T &= I_n - CK \end{aligned} \quad (12)$$

then the error in the two-level process with  $\nu$  pre- and post-smoothing iterations is given as:

$$e^{i+1} = M^\nu T M^\nu e^i \quad (13)$$

In practice, however, the solution increment  $u^{k+1} - u^k$  obtained from a single two-level cycle is used in the determination of the search direction within the framework of the Conjugate Gradient (CG) method for positive definite systems and QMR [2] or GMRES [3] for indefinite systems.

### 3.0 Motivation and goals

Consider a spectral decomposition of the prolongation operator  $\tilde{Q}$

$$\tilde{Q} = \Phi^0 \alpha^0 + \tilde{\Phi}^1 \tilde{\alpha}^1 = \Phi \alpha \quad (14)$$

where  $\Phi^0 \in \mathcal{R}^{n \times m}$ ;  $K\Phi^0 = \Phi^0 \lambda^0$ ;  $\tilde{\Phi}^1 \in \mathcal{R}^{n \times (n-m)}$ ;  $K\tilde{\Phi}^1 = \tilde{\Phi}^1 \tilde{\lambda}^1$ ;  $\alpha^0 \in \mathcal{R}^{m \times m}$ ;

$$\tilde{\alpha}^1 \in \mathbb{R}^{(n-m) \times m}; \lambda^0 = \text{diag}(\lambda_1^0, \lambda_2^0, \dots, \lambda_m^0); \lambda^1 = \text{diag}(\lambda_1^1, \lambda_2^1, \dots, \lambda_{n-m}^1) \text{ and} \\ |\lambda_i^0| < |\tilde{\lambda}_j^1| \forall 1 \leq i \leq m, 1 \leq j \leq n-m.$$

Note that if  $\tilde{\alpha}^1$  vanishes, the prolongation operator is optimal for a given  $m$  and as such the term  $\tilde{\Phi}^1 \tilde{\alpha}^1$  can be viewed as an error in the optimal prolongation. Without loss of generality we will consider the normalized form of the prolongation operator  $\tilde{Q}$ , such that  $\|\tilde{Q}\|_2 = 1$ . Let  $\varepsilon = \|\tilde{\alpha}^1\|_2 / \|\alpha^0\|_2$  denote a measure of quality of the prolongation operator, i.e., if  $\varepsilon = 0$  the prolongation operator is optimal for a given  $m$ .

As a motivation we consider a linearized shear banding problem, illustrated in Figure 1, where the material in the band is softening, and thus giving rise to an indefinite system of algebraic equations. The specimen has been discretized with  $8 \times 8 \times 8$  hexahedral elements totaling 2187 degrees-of-freedom. We assume that a shear band (or a softening zone) develops on the diagonal plane of two layers of elements [18] as shown in Figure 1. Let  $E_{band}$  and  $E$  be the stiffnesses inside and outside the shear band, respectively. We consider three material models having the ratio  $E_{band}/E$  equal to: (i) 0.1 (positive definite system with oscillatory coefficients), (ii) - 0.1 (weakly indefinite system), and (iii) - 0.5 (strongly indefinite system). The three problems have been analyzed with the two-level method outlined in Section 2 and with prolongators generated by different values of  $\varepsilon$ . For all problems considered the coarse model had 250 degrees-of-freedom, or approximately 11% of the modes in the source mesh. The QMR accelerator [2] and the SSOR smoother have been employed. Note that for  $\varepsilon = 0$  the eigenmodes corresponding to the lowest eigenvalues in the absolute value comprise the prolongation operator.

Figure 1 shows the iteration count versus the prolongation quality parameter  $\varepsilon$ . It can be seen that for positive definite system with oscillatory coefficients and for weakly indefinite system the performance of the two-level method is only mildly sensitive to the quality of prolongation. On the other hand, it is evident that highly indefinite systems are very sensitive to the quality of prolongation operator making it a key factor affecting the performance of two- or multi- level methods for indefinite systems.

Although this approach is impractical due to the large computational effort in approximating  $\Phi^0$  to the desired accuracy, it still shows that it is possible to construct a robust multilevel solver for indefinite problems. Furthermore, it is used in the present work to motivate the efficient construction of local approximations to the eigenvector columns of  $\Phi^0$  as discussed in the sequel. As an alternative, we will examine the feasibility of cost-efficient utilization of normal equations. For highly indefinite systems for which positive and negative eigenvalues are of the same order of magnitude, it might be necessary to apply a two- or multi- level scheme to normal equations. For such 'hard' cases we will transform the indefinite source system into a positive definite one,  $K^2 x = f$ , (provided that  $K$  is not singular), where  $x \in R^n$  is defined as  $u = Kx$ .

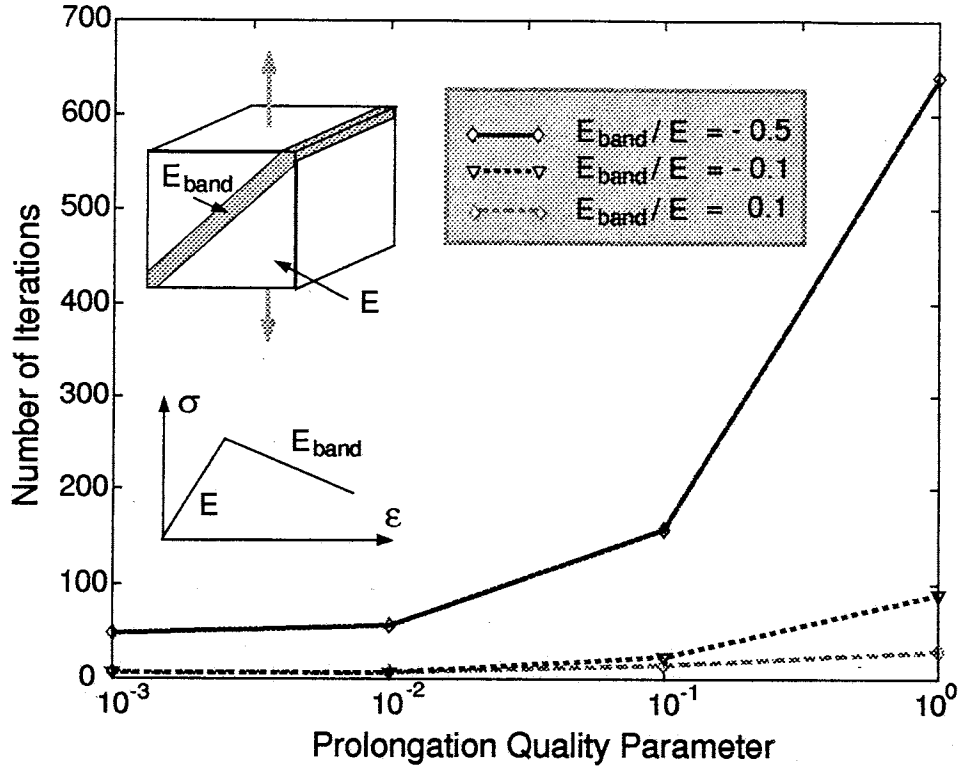


Figure 1: Iteration count versus prolongation quality parameter for various indefinite systems

## 4.0 Convergence studies

In this section we study the rate of convergence of two-level methods applied to a linear system of equations:

$$K^P x = f \quad (15)$$

arising from either the source system,  $\rho = 1$ , or normal equations,  $\rho = 2$ .

### 4.1 The prolongation operator

We will consider the following model problem:  $\alpha^0 \in \mathcal{R}^{m \times m}$ ,  $\tilde{\alpha}^1 = \alpha^1 \in \mathcal{R}^{m \times m}$ , are both diagonal matrices, i.e.,  $\alpha_{km}^i = 0$ ,  $i, j = 0, 1$  for  $k \neq m$ . We assume that  $2m < n$  and define  $\Phi^1 \in \mathcal{R}^{n \times m}$  by choosing arbitrary  $m$  columns from  $\tilde{\Phi}^1$  to express the error in the prolongation operator as  $\Phi^1 \alpha^1$ . Furthermore, let  $\lambda^1 \in \mathcal{R}^{m \times m}$  be the corresponding eigenvalues of  $\Phi^1$ .

We will seek to enhance the quality of the initial or tentative prolongation operator  $\tilde{Q}$  by means of smoothing denoted as

$$Q = S^p \tilde{Q} \quad (16)$$

where  $S \in \mathcal{R}^{n \times n}$  is a prolongation smoother,  $p$  represents the number of times it is applied, and  $Q \in \mathcal{R}^{n \times m}$  is termed as the *enhanced prolongator*.

For positive definite systems the concept of smoothing or weighted interpolation has been utilized in [6] and [7]. Our studies in [11] indicated that for positive definite systems with efficient two- or multi- level preconditioners the computational savings resulting from prolongation smoothing are often very limited due to minor reduction in iteration count but increased cost associated with prolongation enhancement.

The prolongation smoother  $S$  can be defined either with respect to the source or normal equations. It has the following structure:

$$S = I_n - P^{-1} K^\beta \quad (17)$$

where  $P$  is a preconditioner of  $K^\beta$ . The exponent  $\beta$  can be either one or two. Its value might be different from  $p$ . For example, we may select to apply an iterative method to the source system, but to smooth the prolongation with respect to the normal equations. For the purpose of convergence studies, we will consider the simplest form of prolongation smoother based on Richardson preconditioner given as

$$P^{-1} = \frac{1}{\hat{\lambda}^\beta} I_n \quad (18)$$

where  $\hat{\lambda}$  is an upper bound of the maximal eigenvalue of  $K$  in the absolute value.

Consequently, the enhanced prolongation is given by:

$$Q = \left( I_n - \frac{1}{\hat{\lambda}^\beta} K^\beta \right)^p (\Phi^0 \alpha^0 + \Phi^1 \alpha^1) = \sum_{i=0}^1 \Phi^i \left[ I_m - \frac{1}{\hat{\lambda}^\beta} (\lambda^i)^\beta \right]^p \alpha^i \quad (19)$$

## 4.2 Auxiliary coarse model stiffness matrix

The auxiliary coarse model stiffness matrix is obtained by restriction:

$$K^0 = Q^T K^p Q = \sum_{i=0}^1 \left[ I_m - \frac{1}{\hat{\lambda}^\beta} (\lambda^i)^\beta \right]^{2p} (\lambda^i)^p (\alpha^i)^2 \quad (20)$$

Before proceeding with the convergence analysis, we investigate the spectral characteristics of  $K^0$ .

$$\|K^0\|_2 = \max_j \{|K_{jj}^0|\} = \max_{j,i} \left\{ \left[ 1 - \left( \frac{\lambda_j^i}{\hat{\lambda}} \right)^{\beta-2p} \right] |\lambda_j^i|^p [C_0(\alpha_i^0)^2 + C_1(\alpha_i^1)^2] \right\} \quad (21)$$

where  $C_i \leq 1$ . From  $\|\tilde{Q}\|_2 = 1$  follows that  $\sum_{i=0}^1 (\alpha_i^j)^2 \leq 1 \forall j$  and we obtain the following estimate:

$$\|K^0\|_2 \leq \max_{j,i} \left\{ \left[ 1 - \left( \frac{\lambda_j^i}{\hat{\lambda}} \right)^{\beta-2p} \right] |\lambda_j^i|^p \right\} \quad (22)$$

Maximizing  $\|K^0\|_2$  with respect to  $\lambda_j^i$  for  $\rho = 1$  yields

$$\|K^0\|_2 \leq \eta \hat{\lambda}^\beta \quad (23)$$

where

$$\eta = \frac{1}{2p\beta} \left( \frac{2p\beta}{2p\beta+1} \right)^{2p+1} \quad (24)$$

We now show that (24) is valid for any tentative prolongation  $\tilde{Q} \in \mathfrak{R}^{n \times m}$  satisfying  $\|\tilde{Q}\|_2 = 1$  or  $\|\alpha\|_2 = 1$ .

$$\|K^0\|_2 = \|(S^p \tilde{Q})^T K^p (S^p \tilde{Q})\|_2 \leq \|\alpha\|_2^2 \|(S^p \Phi)^T K^p (S^p \Phi)\|_2 \quad (25)$$

Since  $K^p \Phi = \Phi \lambda^p$  and  $S^p \Phi = \Phi \left( I_n - \frac{1}{\hat{\lambda}^\beta} \lambda^\beta \right)^p$  we get

$$\|K^0\|_2 \leq \left\| \left( I_n - \frac{1}{\hat{\lambda}^\beta} \lambda^\beta \right)^p \lambda^p \left( I_n - \frac{1}{\hat{\lambda}^\beta} \lambda^\beta \right)^p \right\|_2 = \max_{j,i} \left\{ \left[ 1 - \left( \frac{\lambda_j^i}{\hat{\lambda}} \right)^{\beta-2p} \right] |\lambda_j^i|^p \right\} \quad (26)$$

which is identical to equation (22).

### 4.3 Auxiliary coarse model iteration matrix

The inverse of the coarse model preconditioner (10) is given as:

$$C = Q(K^0)^{-1}Q^T = \sum_{i,j=0}^1 \Phi^i D^{ij} (\Phi^j)^T \quad (27)$$

where

$$D^{ij} = \left[ I_m - \frac{1}{\hat{\lambda}^\beta} (\lambda^i)^\beta \right]^p \alpha^i (K_0)^{-1} \alpha^j \left[ I_m - \frac{1}{\hat{\lambda}^\beta} (\lambda^j)^\beta \right]^p \in \mathfrak{R}^{mxm} \quad (28)$$

Since all the matrices in (28) are diagonal,  $D^{ij}$  is also diagonal with diagonal components given as

$$\begin{aligned} D_{kk}^{ij} &= \frac{\left[ 1 - \left( \frac{\lambda_k^i}{\hat{\lambda}} \right)^\beta \right]^p \left[ 1 - \left( \frac{\lambda_k^j}{\hat{\lambda}} \right)^\beta \right]^p \alpha_k^i \alpha_k^j}{\sum_{q=0}^1 (\alpha_k^q)^2 \left[ 1 - \left( \frac{\lambda_k^q}{\hat{\lambda}} \right)^\beta \right]^{2p} (\lambda_k^q)^\beta} \\ &= \left\{ \sum_{q=0}^1 \frac{(\alpha_k^q)^2}{\alpha_k^i \alpha_k^j} (\lambda_k^q)^\beta \left[ \frac{[\hat{\lambda}^\beta - (\lambda_k^q)^\beta]^2}{[\hat{\lambda}^\beta - (\lambda_k^i)^\beta][\hat{\lambda}^\beta - (\lambda_k^j)^\beta]} \right]^p \right\}^{-1} \end{aligned} \quad (29)$$

The coarse model iteration matrix (12) is given by

$$T = I_n - Q(K^0)^{-1}Q^T K^p = \Phi \hat{T} \Phi^T \quad (30)$$

where  $\hat{T} \in \mathfrak{R}^{n \times n}$  has the following block structure

$$\hat{T} = \begin{bmatrix} \hat{T}^{11} & \hat{T}^{12} & 0 \\ \hat{T}^{21} & \hat{T}^{22} & 0 \\ 0^T & 0^T & I_{n-2m} \end{bmatrix} \quad \hat{T}^{ij} \in \mathfrak{R}^{mxm} \quad (31)$$

and  $\hat{T}^{ij} \in \mathfrak{R}^{mxm}$  is a diagonal matrix given by

$$\hat{T}_{kk}^{ij} = \delta_{kk}^{ij} - \left\{ \sum_{q=0}^1 \frac{(\alpha_k^q)^2}{\alpha_k^i \alpha_k^j} \left( \frac{\lambda_k^q}{\lambda_k^j} \right)^\beta \left[ \frac{[\hat{\lambda}^\beta - (\lambda_k^q)^\beta]^2}{[\hat{\lambda}^\beta - (\lambda_k^i)^\beta][\hat{\lambda}^\beta - (\lambda_k^j)^\beta]} \right]^p \right\}^{-1} \quad (32)$$

$\delta_{kk}^{ij} \in \mathfrak{R}$  is a Kronecker delta with respect to the superscripts.



#### 4.4 Two-level iteration matrix

For the purpose of convergence studies we consider a relaxation scheme based on the Richardson preconditioner. The corresponding relaxation iteration matrix  $M$  is given as

$$M = I_n - \frac{1}{\hat{\lambda}^\beta} K^\beta \quad (33)$$

Relaxation sweeps can be carried out either with respect to the source system  $\beta = 1$  or normal equations  $\beta = 2$ . The number pre- and post- relaxation sweeps is denoted by  $p$ . The resulting two-level iteration matrix is given by

$$L = M^p T M^p = \Phi \mathcal{P} \begin{bmatrix} F^1 & 0 & \dots & 0 & 0 \\ 0 & F^2 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & F^m & 0 \\ 0 & 0 & \dots & 0 & G \end{bmatrix} \mathcal{P}^T \Phi^T \quad (34)$$

where  $\mathcal{P} \in \mathfrak{R}^{n \times n}$  is a permutation matrix satisfying  $\|\mathcal{P}\|_2 = 1$ ; The block diagonal blocks,  $F^i \in \mathfrak{R}^{2 \times 2}$ , are denoted as

$$F^i = \begin{bmatrix} F_{11}^i & F_{12}^i \\ F_{21}^i & F_{22}^i \end{bmatrix} \quad (35)$$

where

$$F_{kl}^i = (-1)^{k+l} \left( \frac{\lambda_i^0}{\lambda_i^1} \right)^{p(k-1)} \left( \frac{\alpha_i^0}{\alpha_i^1} \right)^{k+l-2} \left\{ \left( \frac{\hat{\lambda}^\beta}{\hat{\lambda}^\beta - (\lambda_i^0)^\beta} \right)^{2p} + \left( \frac{\lambda_i^0}{\lambda_i^1} \right)^p \left( \frac{\alpha_i^0}{\alpha_i^1} \right)^2 \left( \frac{\hat{\lambda}^\beta}{\hat{\lambda}^\beta - (\lambda_i^1)^\beta} \right)^{2p} \right\}^{-1} \quad (36)$$

and  $G$  is a diagonal matrix with diagonal terms given as

$$G_k^1 = \left( 1 - \left( \frac{\lambda_k^1}{\hat{\lambda}} \right)^\beta \right)^{2p} \quad (37)$$

The spectral radius of the iteration matrix denoted as  $\rho(L)$  is given as:

$$\rho(L) = \max_{i,k} \{\rho(F^i), |G_k^1|\} \quad (38)$$

The eigenvalues of  $F^i$  can be computed from

$$\det \begin{bmatrix} F_{11}^i - \lambda & F_{12}^i \\ F_{21}^i & F_{22}^i - \lambda \end{bmatrix} = \lambda^2 - (F_{11}^i + F_{22}^i)\lambda - F_{21}^i F_{21}^i + F_{11}^i F_{22}^i = 0 \quad (39)$$

which yields

$$\lambda^i = \frac{F_{11}^i + F_{22}^i}{2} \pm \sqrt{\left(\frac{F_{11}^i - F_{22}^i}{2}\right)^2 + F_{21}^i F_{21}^i} \leq |F_{11}^i| + |F_{22}^i| + \sqrt{|F_{12}^i F_{21}^i|} \quad (40)$$

Substituting (36) into (40) gives:

$$\rho(F^i) \leq \frac{\varepsilon_i^2 + \varepsilon_i \sqrt{|\Lambda_i|} + |\Lambda_i|}{|\varepsilon_i^2/G_i^0 + \Lambda_i/G_i^1|} \quad \forall i \quad (41)$$

where

$$\Lambda_i = \begin{pmatrix} \lambda_i^0 \\ \frac{1}{\lambda_i} \end{pmatrix}^p \quad \varepsilon_i = \begin{vmatrix} \alpha_i^1 \\ \alpha_i^0 \end{vmatrix} \quad G_i^0 = \left(1 - \frac{(\lambda_i^0)^\beta}{\hat{\lambda}^\beta}\right)^{2p} \quad (42)$$

and  $G_i^1$  as defined in (37). Since  $|\lambda_i^0| \ll |\hat{\lambda}^\beta|$  we approximate  $G_i^0 = 1$ .

To study the convergence characteristics of the two-level method we consider three cases: (i)  $\Lambda_i \geq 0$ , (ii)  $-G_i^1 \varepsilon_i^2 < \Lambda_i < 0$ , and (iii)  $\Lambda_i \leq -G_i^1 \varepsilon_i^2$ . Only cases (i) and (iii) satisfy the convergence criteria,  $\rho(L) < 1$ , provided that:

$$(G_i^1)^{-1} \geq 1 + \frac{\varepsilon_i}{\sqrt{\Lambda_i}} \quad \Lambda_i \geq 0 \quad \forall i \quad (43)$$

$$(G_i^1)^{-1} \geq 1 + \frac{\varepsilon_i}{\sqrt{-\Lambda_i}} + \frac{2\varepsilon_i^2}{(-\Lambda_i)} \quad \Lambda_i \leq -G_i^1 \varepsilon_i^2 \quad \forall i \quad (44)$$

Equations (43) and (44) describe the quality of the smoother required to ensure the convergence of the two-level scheme for a given tentative prolongation operator.

## 4.5 Discussion

There are several factors affecting the convergence of the two-level process, namely:

(i) The smoother. The ability of the prolongation and the two-level smoothers to reduce the higher frequency modes of error is one of the key factors affecting convergence. From (43) and (44) it can be seen that  $G_i^1 < 1$  is a necessary condition for convergence. In the context of Richardson-based preconditioner this condition is satisfied if either the stiffness matrix is positive definite or both the prolongation and iteration smoothings are carried out with respect to normal equations, i.e.,  $\beta = 2$ . For stronger preconditioners, such as SSOR, there might be a weaker condition satisfying  $G_i^1 < 1$ .

(ii) The prolongation operator. The quality of the tentative prolongation operator,  $\tilde{Q}$ , is governed by the ratio  $\varepsilon_i = |\alpha_i^1 / \alpha_i^0|$ . In the case of the optimal prolongation operator, i.e.  $\varepsilon_i \rightarrow 0$ , the necessary condition  $G_i^1 < 1$  becomes the sufficient condition provided that the system is non-singular, i.e.,  $\Lambda_i \neq 0$ .

(iii) Spectral characteristics of the linear system of equations. For positive definite systems  $G_i^1(\beta, \rho)$  is minimal with respect to exponents  $\beta$  and  $\rho$  for  $\beta = \rho = 1$  and equation (43) represents the sufficient conditions for convergence. When the multilevel scheme is applied to normal equations, i.e.  $\rho = 2$ , (43) represents sufficient conditions as well. In the case of indefinite systems, i.e.  $\rho = 1$ , both equations (43) and (44) comprise the sufficiency conditions with (43) for  $\Lambda_i > 0$  and (44) for  $\Lambda_i < 0$ . By comparing equations (43) and (44) it can be seen that the existence of extreme eigenvalues with opposite signs slows down the converge of the two-level method or may require stronger smoother (or increase the value of  $p$ ) to prevent divergence.

(iv) The size of the coarse model. As the size (number of equations) of the coarse model approaches the size of the source grid, i.e.,  $\lambda_i^1 \rightarrow \hat{\lambda}$ ,  $G_i^1$  defined in (37) approaches zero provided that  $G_i^1 < 1$ .

## 5.0 Prolongation operator

The tentative prolongation operator can be constructed using either Geometric Multigrid (GM) method or the aggregation approach [5], [6], [8], [9] which falls into the category of Algebraic Multigrid (AMG) methods. While geometric multigrid approach constructs the prolongation operator from auxiliary coarser grids, the method of aggregation accomplishes the same goal on the basis of the information available in the source grid. In the present manuscript we focus on the aggregation approach.

In an aggregation scheme the coarse model is directly constructed from the source grid by grouping finite elements into either nonoverlapping or overlapping subdomains referred to as aggregates, and then for each aggregate assigning a reduced number of modes with an intent of effectively capturing the lower frequency response of the source system.

In an attempt to construct an efficient prolongation operator in terms of its spectral characteristics, the following key issues are discussed in the remainder of this section: (i) construction of the auxiliary aggregated model (Section 4.1), (ii) construction of the tentative prolongation operator (Section 4.2), and (iii) enhancement of the tentative prolongation operator (Section 4.3).

## 5.1 Aggregation algorithm

Prior to describing the technical details of the aggregation algorithm, we introduce the concept of “stiff” and “soft” elements which is utilized in the process of aggregation. The element is considered “stiff” if the spectral radius of its stiffness matrix is relatively large compared to other elements and vice versa. It has been shown in [8], [9] that it is advantageous to place the “soft” elements at the interface between the aggregates, and “stiff” elements within the aggregates. This approach is a counterpart of the idea of “weak” and “strong” nodal connectivity employed in [4].

The maximal eigenvalue of the element stiffness matrix,  $\lambda_{max}^e$ , estimated using the Gerschgorin theorem

$$\lambda_{max}^e \leq \beta^e \quad \beta^e = \max_i \left( \sum_j |k_{ij}^e| \right) \quad (45)$$

is used to quantify the element stiffness. We consider a finite element mesh consisting of  $N_E$  elements and  $N_N$  nodes. Let  $C_N(i)$  be the set of nodes belonging to the element  $E^i$

$$C_N(i) = \{N^j : N^j \in E^i\} \quad (46)$$

where subscripts  $E$  and  $N$  denote sets of elements and nodes, respectively.

### Step 1. Setup.

1.1. For each node  $N^j$ ,  $j = [1, N_N]$  select the elements containing this node:

$$B_E(j) = \{E^i : N^j \in E^i\} \quad (47)$$

1.2. For each element  $E^i$ ,  $i = [1, N_E]$  select the set of neighboring elements  $F_E(i)$ , i.e., elements containing common nodes:

$$F_E(i) = \{E^k: E^k \in B_E(j), j \in C_N(i)\} \setminus E^i \quad (48)$$

Step 2. Start-up aggregation.

2.1. Define the set of elements  $T_E$  available for aggregation. These are all the elements which do not contain nodes with essential boundary conditions or the ‘slave’ nodes:

$$T_E = [1, N_E] \setminus \{B_E(j), N^j \in S_N\} \quad (49)$$

where  $S_N$  is the set of ‘slave’ nodes, which depends on so called ‘master’ degree(s)-of-freedom, and nodes with essential boundary conditions. We denote  $T_E^0$  as the initial set.

**Remark 1:** We include the slave nodes in the set  $S_N$  so that we could deal with multi-point constraints in a conventional way. See [9] for details.

2.2. Find the “peripheral” element  $E^s$ , i.e., the element with minimal number of neighbors:

$$s = \underset{i \in T_E}{\operatorname{argmin}} |F_E(i)| \quad (50)$$

where  $|X|$  is a number of elements in the set  $X$ . Element  $E^s$  is a starting element for the aggregation algorithm.

2.3. Setup:

- the current aggregate counter  $i = 1$ ;
- the set of interface elements  $I_E = [1, N_E] \setminus T_E$ , i.e., elements between aggregates.

Step 3. Formation of the current nonoverlapping aggregate.

3.1 An aggregate with zero neighbors is defined as follows:

$$A_E^i(0) = E^s \quad (51)$$

3.2 An aggregate with one neighbor,  $A_E^i(1)$ , contains the element  $E^s$  and those of its available neighbors which satisfy the relative stiffness condition:

$$A_E^i(1) = E^s \cup \{E^j \in F_E(s) \cap T_E, \beta^j \geq \mu \beta^s\} \quad (52)$$

where  $\beta^j$  is a Gerschgorin upper bound on  $j$ -the element stiffness matrix maximal eigenvalue, and  $\mu$  is a coarsening parameter. If on the other hand the element stiffness informa-

tion is not available in the aggregation process, then the aggregate with one neighbor is defined as

$$A_E^i(1) = E^s \cup (F_E(s) \cap T_E) \quad (53)$$

Similarly we can define an aggregate  $i$  with arbitrary number neighbors, denoted as  $A_E^i$ .

**Remark 2.** Numerical experiments have shown that for higher order elements ( $p \geq 3$ ) the zero-neighbors version is typically more efficient, whereas for lower order elements the one- or two- neighbor aggregation scheme is more appropriate.

Step 4. Update the sets of the interface and available elements.

4.1. Update the set of the interface elements:

$$I_E = I_E \cup \{(E^k \in F_E(j), E^j \in A_E^i) \cap (E^k \notin A_E^i)\} \quad (54)$$

4.2. Update the set of the available elements:

$$T_E = T_E \setminus \{(E^k \in F_E(j), E^j \in A_E^i) \cup A_E^i\} \quad (55)$$

4.3 Update the set of aggregates:

$$A_E = A_E \cup \{(E^k \in F_E(j), E^j \in A_E^i) \cap A_E^i\} \quad (56)$$

Step 5. Find the new starting element.

Form the set of “frontal” elements  $R_E$ , i.e., available elements neighboring the interface elements

$$R_E = \{(E^k \in F_E(j), E^j \in I_E) \cap T_E\} \quad (57)$$

and select the stiffest new starting element from the set  $R_E$  defined as

$$s = \underset{j: E^j \in R_E}{\operatorname{argmax}}(\beta^j) \quad (58)$$

If on the other hand the stiffness information is not available in the aggregation process we simply select an arbitrary starting element belonging to  $R_E$ .

Step 6. Stopping criteria for nonoverlapping aggregation.

If  $R_E = \emptyset$  then stop; else  $i = i + 1$  and repeat steps 3-6.

Step 7. Define the element-free aggregates

7.1 Each node in  $S_N$  is classified as an element-free aggregate

$$A_N^j = N^j \quad \forall N^j \in S_N \quad (59)$$

7.2 Find the set of nodes which is not contained in one of the aggregates.

$$V_N = \{N^j: ([1, N_N] \setminus (N^j \in C_N(k), E^k \in A_E) \setminus S_N)\} \quad (60)$$

For higher order elements there will be a significant number of nodes belonging to  $V_N$  primarily in the interface region between the aggregates. For linear elements it is also possible that  $V_N \neq \emptyset$  as shown in Figure 2. There are two approaches to deal with the set  $V_N$ :

(i) collapse  $N^j \in V_N$  and the corresponding elements to one of the neighboring aggregates as shown in Figure 2. If such collapsing makes the aggregate invalid (attaching the node without elements) make  $N^j \in V_N$  a 'master' node in the coarse model and classify it as an element free-aggregate, or

(ii) consider  $N^j \in V_N$  as a 'slave' nodes in the coarse model and interpolate the solution in  $N^j$  from the adjacent nodes in  $A_E$ .

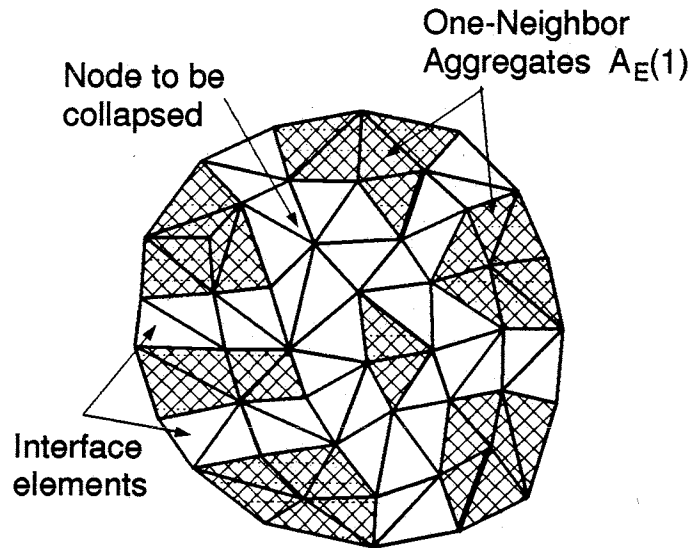


Figure 2: A typical nonoverlapping one-neighbor aggregation model

In the present manuscript the first approach is adopted.

Step 8. Formation of the overlapping aggregates (for overlapping version only)

For each nonoverlapping aggregate  $A_E^i$  define a corresponding overlapping aggregate  $\underline{A}_E^i(1)$  with one overlapping layer of elements:

$$\underline{A}_E^i(1) = \{(E^k \in F_E(j), E^j \in A_E^i) \cup A_E^i\} \cap T_E^0 \quad (61)$$

Similarly, an overlapping aggregate with  $k+1$  overlapping layers of elements is defined as

$$\underline{A}_E^i(k+1) = \{(E^k \in F_E(j), E^j \in \underline{A}_E^i(k)) \cup \underline{A}_E^i(k)\} \cap T_E^0 \quad (62)$$

## 5.2 Construction of the tentative prolongation

The goal of the aggregation method is to approximate the eigenmodes  $\Phi^0 \in \mathfrak{R}^{n \times m}$  corresponding to the lowest eigenvalues of the source stiffness matrix (in the absolute value) by a linear combination of  $C^0$  continuous local functions defined over the individual aggregates. The following four choices have been considered:

### 5.2.1 *A priori* selected functions on nonoverlapping aggregates

By this technique a finite element mesh is decomposed into nonoverlapping aggregates (steps one to seven in Section 4.1). On each aggregate  $A_E^i$ , a low order polynomial function (constant or linear field) is used to approximate the solution (typically for Poisson or elasticity equations with constant coefficients). For problems where eigenfunctions  $\Phi^0$  are oscillatory, such as in the case of elasticity with oscillatory coefficients or Helmholtz equation, an analytical solution with either periodic boundary conditions [11] or on unbounded domains is used instead. Figure 3(a) illustrates a linear approximation over nonoverlapping aggregates.

### 5.2.2 Eigenmodes on nonoverlapping aggregates with Neumann boundary conditions

An alternative to selecting analytical functions on  $A_E^i$  is to conduct a local eigenvalue analysis on each aggregate

$$K^i \phi^i = \lambda^i \text{diag}(K^i) \phi^i \quad (63)$$

with zero Neumann boundary conditions on  $A_E^i$  and to select the eigenmodes for which  $\lambda^i \leq \gamma$ . In (63)  $\text{diag}(K^i)$  denotes the diagonal of the aggregate stiffness matrix  $K^i$ .

The value of  $\gamma$  controls the effectiveness of the aggregated model. In the limit as  $\gamma \rightarrow \max_i(\lambda^i)$ , the auxiliary coarse model captures the response of the source system for



all frequencies and therefore the two-level procedure converges in a single iteration even without smoothing. On the negative side, for large values of  $\gamma$ , the eigenvalue analysis on each aggregate becomes prohibitively expensive and the auxiliary matrix becomes both large and dense. At the other extreme in the limit as  $\gamma \rightarrow 0$ , the prolongation operator contains rigid body modes only, and thus the auxiliary coarse model becomes inefficient for ill-posed problems. For best performance of the iterative process the value of parameter  $\gamma$  should be in the range of  $10^{-1}$  to  $10^{-3}$  [8], [9]. The optimal value depends on the problem type (3D elasticity, shells, Helmholtz). Typically 6-50 modes satisfying  $\lambda^i \leq \gamma$  are selected. The Lanczos algorithm with partial orthogonalization [13] is utilized for local eigenvalue analysis.

The aforementioned approach [8], [9] does not require *a priori* knowledge of the solution characteristics nor does it utilize any information regarding the choice of coordinate functions or the nature of the discrete approximation (i.e., rotations, displacements, pressures, etc.). As such it falls into the category of ‘black-box’ solvers.

### 5.2.3 Eigenmodes on overlapping aggregates with Dirichlet boundary conditions

For normal equations,  $K^p x = f$ ,  $\rho = 2$ , it is not trivial to construct a local Neumann problem due to coupling resulting from the product of two global matrices. Instead, a local eigenvalue problem with Dirichlet boundary conditions can be constructed by extracting appropriate information from the global matrix  $K^2$ . This approach can be also applied to the source system.

For each overlapping aggregate  $A_E^i$  we conduct a local eigenvalue analysis

$$\underline{K}^i \underline{\phi}^i = \underline{\lambda}^i \text{diag}(\underline{K}^i) \underline{\phi}^i \quad (64)$$

and select eigenmodes  $\underline{\phi}^i$  for which  $\underline{\lambda}^i \leq \underline{\gamma}$ ;  $\underline{K}^i$  is a block within the global stiffness matrix corresponding to the aggregate  $A_E^i$ . Typically  $\underline{\gamma} < \underline{\gamma}$  since the Dirichlet problem is stiffer than the corresponding Neumann problem. Figure 3(b) shows a typical approximation for the 1D problem on overlapping aggregates.

### 5.2.4 Mixed prolongation

In [8] we have shown that the coarse model approximation space should satisfy the homogenous differential equation. For elasticity problems this means that each aggregate should be able to represent rigid body modes, whereas for Helmholtz equations it should contain functions of the form  $e^{ikx}$ , where  $k$  is the wavenumber.

The eigenvalue problem with Dirichlet boundary conditions (64) is usually overconstrained, and thus in general the eigenfunction  $\phi^i$  does not satisfy homogeneous problem. For this reason we define a mixed approximation scheme by which the coarse model approximation space consists of: (i) functions satisfying homogeneous solution or eigenfunctions  $\phi^i$  computed from the eigenvalue problem with Neumann boundary conditions on nonoverlapping aggregates, and (ii) eigenfunctions  $\phi^i$  computed from the eigenvalue problem with Dirichlet boundary condition on overlapping aggregates.

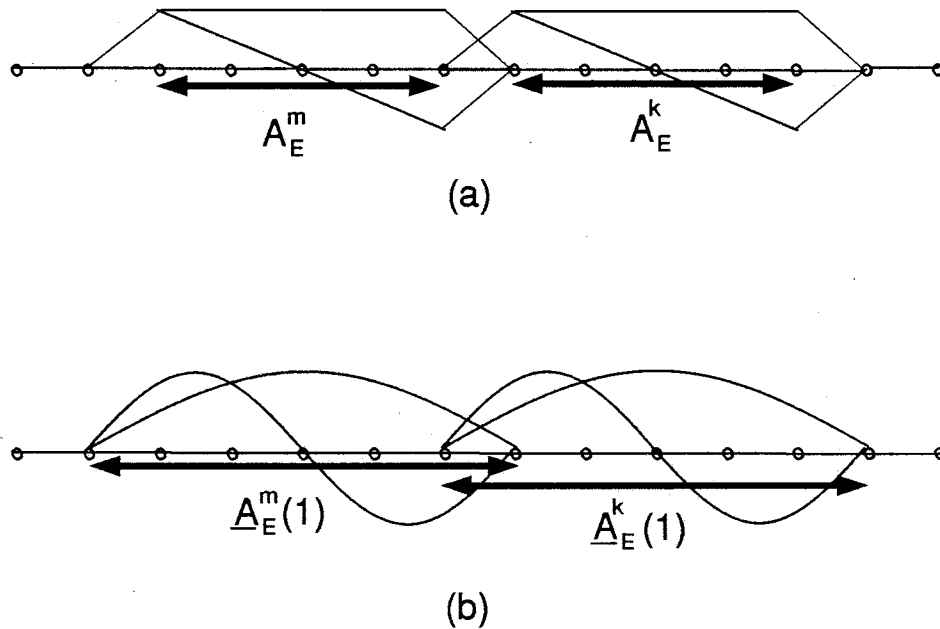


Figure 3: (a) Linear interpolation on non-overlapping aggregates, (b) Eigenfunctions on overlapping aggregates with Dirichlet boundary conditions

### 5.3 Enhanced prolongation

The quality of the initial prolongation operator  $\tilde{Q}$  can be improved by smoothing:

$$Q = (I_n - P^{-1}K^\beta)^p \tilde{Q} \quad (65)$$

where  $\beta$  is equal to one if smoothing is carried out with respect to the source system, or two if it is applied to normal equations. The goal is to construct an efficient prolongation smoothing process (65) with minor or no additional memory requirements that will result in a sparse prolongation  $Q$  and will significantly reduce the iteration count. In practice, however, it is not trivial to bridge between these contradicting requirements. For example, an efficient prolongation smoother, which may significantly reduce the iteration count, might increase the total computational cost since smoothing has to be carried out for as many vectors as the number of equations. Furthermore, the prolongation smoothing may result in a non-sparse prolongation making the stiffness restriction process a dominant part of the solution cost.

The key to constructing an efficient smoothing process is to exploit the sparsity structure of the tentative prolongation  $\tilde{Q}$  and the locality of pollution effects. These two guiding principles are employed within the framework of the incomplete SSOR.

### 5.3.1 The incomplete SSOR prolongation smoother for the source system

Consider the decomposition  $K = D + L + L^T$ , where  $D$  and  $L$  are the diagonal and strict lower part of  $K$ , respectively. Let  $\mathcal{N}^s$  be a set of degrees-of-freedom corresponding to a nonoverlapping aggregate  $A_E^s$ , and  $\underline{\mathcal{N}}^s$  be the corresponding set on  $\underline{A}_E^s(\omega)$ , where  $\omega$  is the user-defined number of overlapping layers of elements. Let  $\tilde{Q}^s \in \mathcal{R}^{n \times m_s}$  be the prolongation operator corresponding to the set  $\mathcal{N}^s$ , and  $m_s$  be the number of degrees-of-freedom in the aggregates  $A_E^s$ . For each  $\tilde{Q}^s$  we define an incomplete SSOR preconditioner,  $P^s$ , as follows:

$$P^s = (D + L^s)D^{-1}(D + L^{sT}) \quad (66)$$

where

$$L_{kl}^s = \begin{cases} L_{kl} & k, l \in \underline{\mathcal{N}}^s \\ 0 & \text{otherwise} \end{cases} \quad (67)$$

It can be seen that even if aggregates are nonoverlapping the enhanced prolongation is overlapping with  $\omega$  controlling the size of the overlap. Increasing the value of  $\omega$  reduces the number of iterations but increases the cost of prolongation smoothing and stiffness restriction. Numerical experiments indicate that for optimal performance  $\omega$  should be in the range of one to three.

The incomplete SSOR preconditioner (66), (67) is based on the topological information only. An incomplete SSOR preconditioner based on the concept of strong and weak connections in the stiffness matrix has been developed in [14].

### 5.3.2 The incomplete SSOR prolongation smoother for normal equations

An efficient implementation of the SSOR preconditioner for normal equations,  $K^2 x = f$ , which does not require explicit formation of  $K^2$  has been developed in [3]. Here we focus on the incomplete version of this algorithm.

Starting from the initial approximation of the prolongation  $Q^s$ ,  $Q^s = \tilde{Q}^s$ , the forward Gauss-Seidel sweep is based on succession of relaxation steps of the form

$$Q_{new}^s = Q_{old}^s + e_k(\delta_k)^T \quad (68)$$

where  $e_k \in \mathfrak{R}^n$  is the  $k$ -th column of the identity matrix  $I_n$  and  $\delta^k \in \mathfrak{R}^{m_s}$  is a column vector of unknowns. For  $k \in \underline{\mathcal{N}}^s$  the vector  $\delta_k$  is chosen so that the  $k$ -th component of the residual,  $(f 1^T - K^2 Q_{new}^s)^T e_k$ , becomes zero, where  $1 \in \mathfrak{R}^{m_s}$  is a vector of ones. Otherwise  $\delta_k = 0$ , which yields:

$$\delta_k = \begin{cases} \frac{1f^T e_k - (KQ_{old}^s)^T K e_k}{(K e_k)^T (K e_k)} & k \in \underline{\mathcal{N}}^s \\ 0 & otherwise \end{cases} \quad (69)$$

Relaxation steps (68), (69) are carried out for all  $s$  and  $k$  for which  $k \in \underline{\mathcal{N}}^s$ .

## 6.0 Numerical Examples and Discussion

Various aggregation schemes described in Section 5 have been applied to a sequence of examples involving Helmholtz equation on bounded domains and linearized shear banding problems with strain softening.

### 6.1 Helmholtz equation on bounded domains

Consider Helmholtz's equation in the region enclosed between two concentric cubes of length 2 ( $\Gamma_0$ ) and 6 ( $\Gamma_1$ ). The strong form of the governing equations is given as

$$\nabla^2 u(x) + k^2 u(x) = 0, \quad x \in \Omega \quad (70)$$

$$\frac{\partial u}{\partial n} = \frac{\partial}{\partial r}(e^{ikr}/r) \Big|_{\Gamma_0} \quad x \in \Gamma_0 \subset \partial\Omega \quad (71)$$

$$\frac{\partial u}{\partial n} = \frac{\partial}{\partial r}(e^{ikr}/r) \Big|_{\Gamma_1} \quad x \in \Gamma_1 \subset \partial\Omega \quad (72)$$

where  $n$  is a coordinate in a direction normal to  $\Gamma_0$  and  $\Gamma_1$ ;  $\Gamma_0 \cup \Gamma_1 = \partial\Omega$  and  $\Gamma_0 \cap \Gamma_1 = \emptyset$ ;  $r$  is distance from the center of the cube. Equations (70)-(72) describe the acoustic pressure  $u$  of a wave in a transmitting media.

Because of symmetry, one-eighth of the domain is discretized. Three meshes consisting of 3072, 23,925 and 156,009 4-node linear tetrahedral elements have been considered. The coarsest discretization is shown in Figure 4.

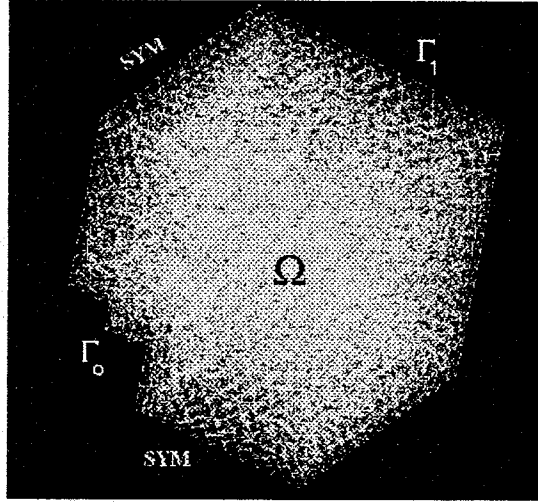


Figure 4: Typical finite element mesh and boundary conditions

The resulting discrete linear system of equations,  $Kx = F$ , is symmetric, complex and indefinite. It is convenient to transform the complex symmetric linear system into a real symmetric system by replacing each term in the stiffness,  $K_{AB}$ , force vector,  $F_A$ ; and

the solution vector,  $x_A$ , by  $\begin{bmatrix} K_{AB}^R & K_{AB}^I \\ K_{AB}^I & -K_{AB}^R \end{bmatrix}$ ,  $\begin{bmatrix} F_A^R \\ F_A^I \end{bmatrix}$  and  $\begin{bmatrix} x_A^R \\ -x_A^I \end{bmatrix}$ , respectively. The superscripts

$R$  and  $I$  denote the real and imaginary parts, which can be interpreted as two degrees-of-freedom per node.

We consider two approaches of constructing aggregation-based prolongation operator: (i) eigenfunctions defined on nonoverlapping aggregates with Neumann boundary conditions, (ii) eigenfunctions defined on overlapping aggregates with Dirichlet boundary con-

ditions. The two schemes have been applied to both the source system and the normal equations. We denote the resulting four methods as: Source-N(eumann), Source-D(irichlet), Normal-N(eumann), Normal-D(irichlet).

For normal equations we employ a dedicated conjugate gradient acceleration for normal systems [3] and Incomplete Cholesky preconditioner for normal equations [3] as a two-level smoother. For the source system a combination of QMR [2] accelerator and SSOR smoother is adopted.

Preliminary numerical investigation revealed that for all problems and methods considered a nearly optimal performance has been obtained with the following combination of algorithmic parameters: (i) the limiting eigenvalue parameter,  $\gamma = 0.1$ , for both Neumann and Dirichlet problems, (ii) one-neighbor approach,  $A_E(1)$ , for nonoverlapping aggregates, and two layers of element overlaps,  $A_E(2)$ , for overlapping aggregates.

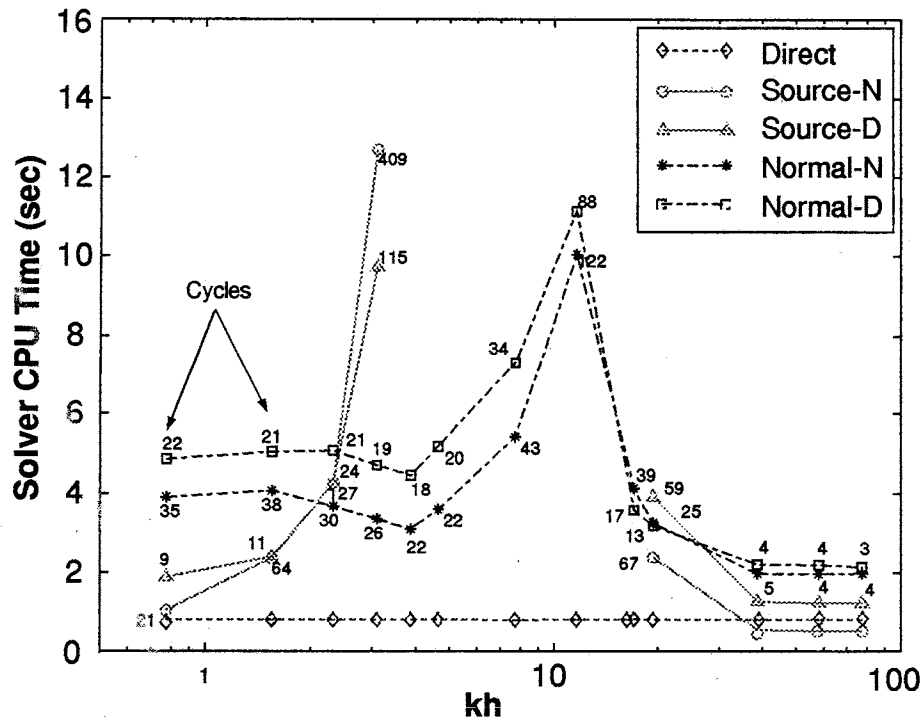


Figure 5: CPU/Cycles versus  $kh$  for discrete Helmholtz linear system with 1478 equations

Figures 5-7 show the CPU time and iteration count versus the product of the average element size and the wavenumber,  $kh$ , for the three meshes considered. The product  $kh$  has been selected since it represents a measure of solution accuracy [16]. No smoothing was carried out for prolongation operator. Results of the four iterative methods are compared to the state-of-the-art multifrontal solver [15].

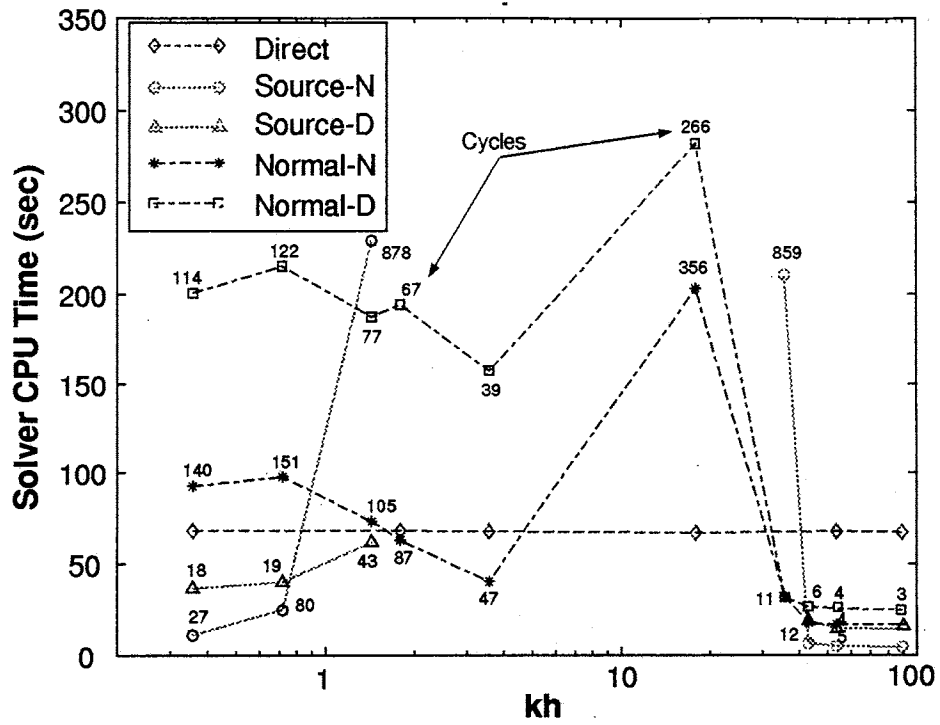


Figure 6: CPU/Cycles versus  $kh$  for discrete Helmholtz linear system with 9648 equations

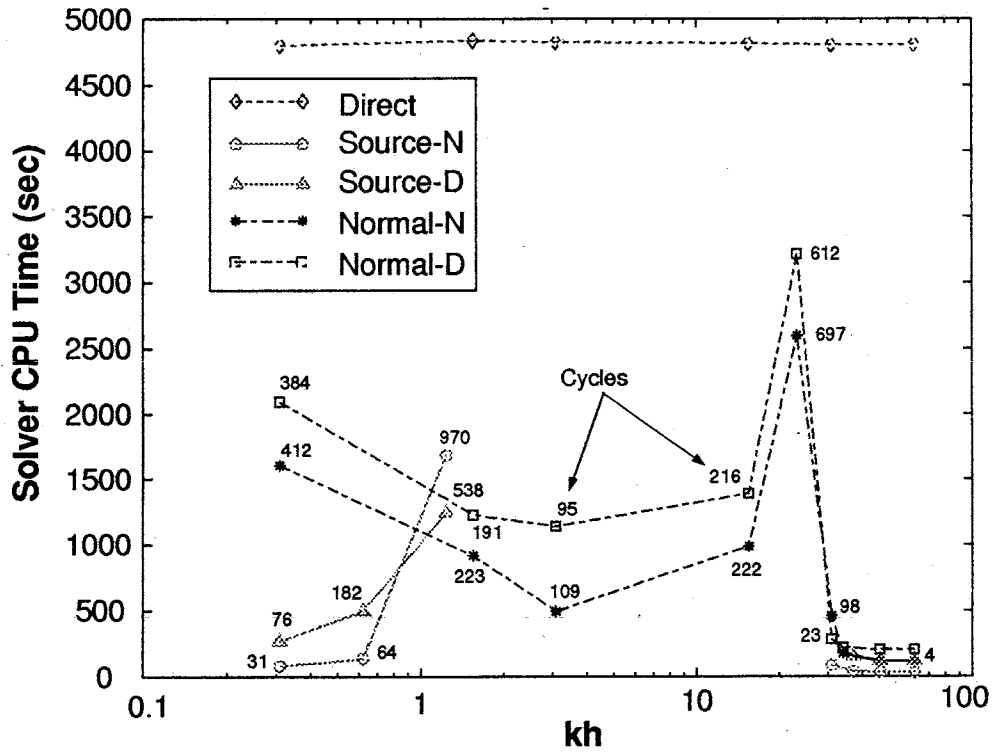


Figure 7: CPU/Cycles vs  $kh$  for discrete Helmholtz linear system with 57586 equations

Even though practitioners dealing with wave propagation problems are primarily interested in the range,  $kh < 1$ , required for solution accuracy [17], we conduct numerical experiments outside the range of the usual interest. Our interest in a much wider spectrum of  $kh$  values stems from the fact that not only the analyst may frequently encounter highly nonuniform meshes, where the precise definition of  $h$  is questionable, but primarily, because our ultimate goal is to develop a generic black-box equation solver for positive definite and indefinite systems.

It can be seen from Figures 5-7 that for  $kh < 1$  the two-level method rapidly converges for the source system. In the case of  $kh < 1$  the break even point between the one [15] and two-level methods considered is approximately 5000 equations. For  $kh < 0.5$  the aggregation scheme based on nonoverlapping aggregates [8], [9] is more efficient in terms of CPU time, whereas for  $0.5 < kh < 2$  the aggregation scheme based overlapping aggregates works better. For  $kh > (2 - 4)$  the use of normal equations cannot be avoided. Figure 6 shows that the two-level method with nonoverlapping aggregates is competitive to the direct method at approximately 10,000 equations, and is faster than the direct method by a factor of 2-10 in the case of 50,000 unknowns. It is not surprising that for  $kh > (20 - 40)$  the iterative methods converge in 3-5 iterations, since the eigenvalues of the stiffness matrix are all negative.

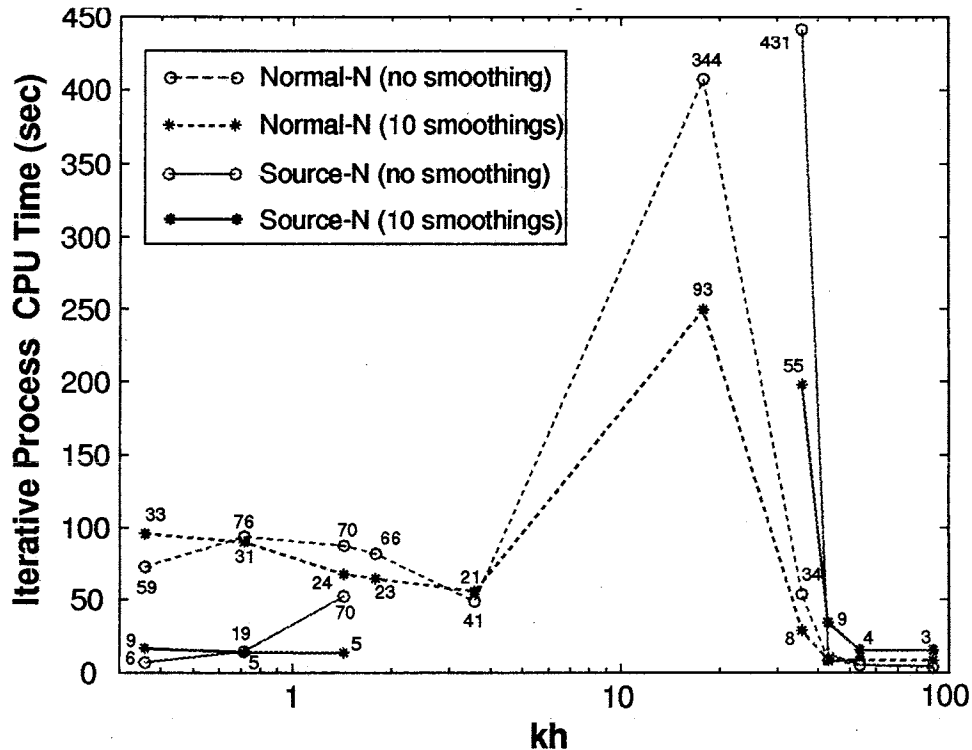


Figure 8: Influence of prolongation smoothing on the iterative process

Figure 8 compares the CPU time of the iterative process and the iteration count obtained with the enhanced (10 smoothings) and the tentative (no smoothing) prolongation operators on nonoverlapping aggregates. It can be seen that the prolongation smooth-



ing considerably reduces the iteration count (factor of up to 14 for the problems considered), and at a lesser extent the CPU time of the iterative process. This is because the enhanced prolongation is denser, resulting in increased cost of restriction and prolongation. The overall CPU time obtained with the enhanced prolongation is increased primarily due to the computational cost associated with prolongation smoothing. Nevertheless, for problems with multiple right hand sides, the overhead generated from prolongation smoothing and coarse model factorization, might be negligible, and thus the use of enhanced prolongation could be advantageous.

Other variants of multilevel methods for Helmholtz equation have been described in [10] and [12].

## 6.2 Shear banding problem

We consider a linearized shear banding problem, illustrated in Figure 1. The cube is discretized with  $16 \times 16 \times 16$ ,  $24 \times 24 \times 24$  and  $32 \times 32 \times 32$  8-node hexahedral elements totaling to 14739, 46875 and 107811 degrees-of-freedom. We assume that a shear band (softening zone) develops on the diagonal plane of two layers of elements [18]. We consider the spectrum of ratios between the stiffness inside and outside the shear band,  $E_{band}/E$ , in the range of 0.3 and -0.7.

Three approaches of constructing aggregation-based prolongation have been tested: (i) eigenfunctions defined on nonoverlapping aggregates with Neumann boundary conditions, (ii) linear fields defined on nonoverlapping aggregates, (iii) eigenfunctions defined on overlapping aggregates combined with rigid body modes defined on nonoverlapping aggregates. The three schemes have been applied to both the source system and normal equations. We denote the resulting six methods as: Source-N(eumann), Source-L(inear), Source-D(irichlet)/R(igid)B(ody), Normal-N(eumann), Normal-L(inear), Normal-D(irichlet)/R(igid)B(ody).

The following combination of algorithmic parameters have been considered: the limiting eigenvalue parameter,  $\gamma$ , equal to 0.0001, 0.01, 0.1, 0.3 for Normal-D/RB, Source-D/RB, Source-N, and Normal-N aggregation schemes, respectively. The topology of aggregated model, the acceleration schemes and two-level smoothers employed are the same as in Section 6.1.

Figures 9, 10 and 11 show the CPU time and iteration count versus  $E_{band}/E$  for the three meshes considered. It can be seen that for positive definite systems with oscillatory coefficients and for weakly indefinite system,  $E_{band}/E > -0.1$ , the behavior of the two-level methods as applied to the source system is similar to that of Helmholtz equations with  $kh < 1$ . For  $E_{band}/E = -0.1$  the break even point between one [15] and two level methods is approximately 10,000 equations. The linear interpolation over nonoverlapping aggregates performs well for positive definite systems, but is less efficient than methods based on selection of eigenfunctions for  $E_{band}/E = -0.1$ .

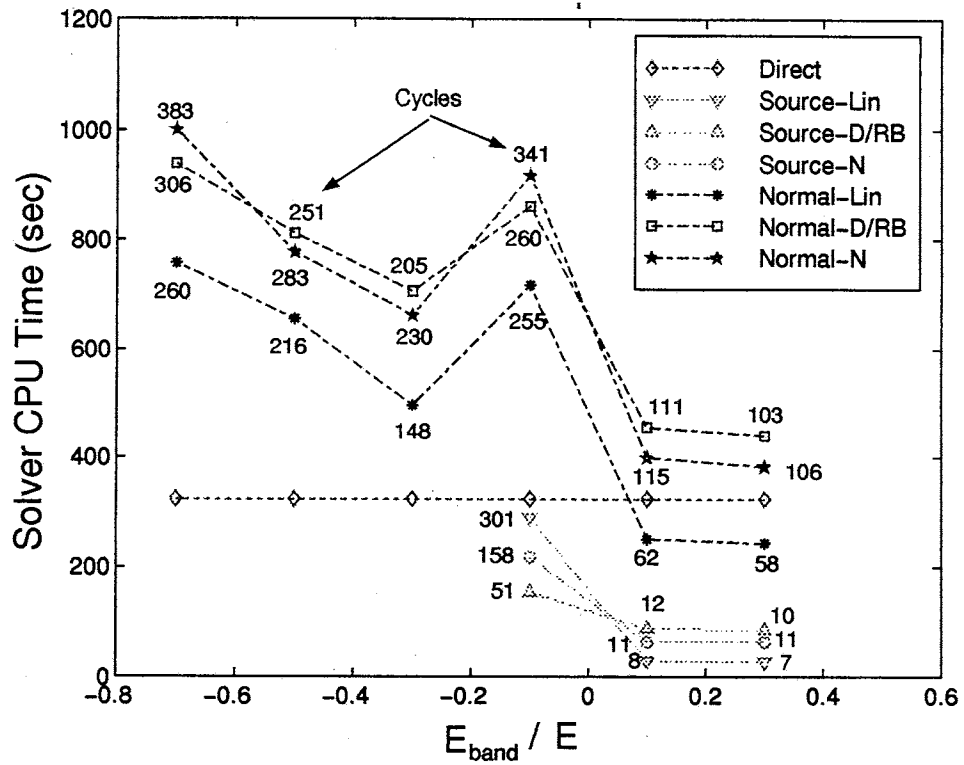


Figure 9: CPU/Cycles vs  $E_{band} / E$  for shear banding problem with 14739 equations

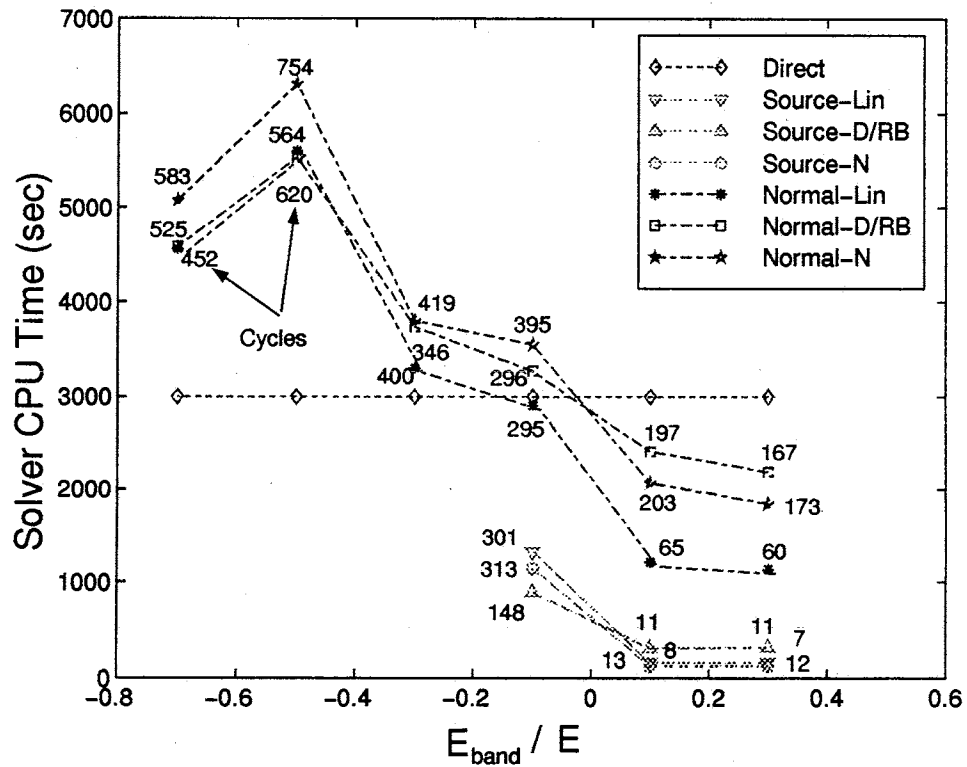


Figure 10: CPU/Cycles vs  $E_{band} / E$  for shear banding problem with 46875 equations

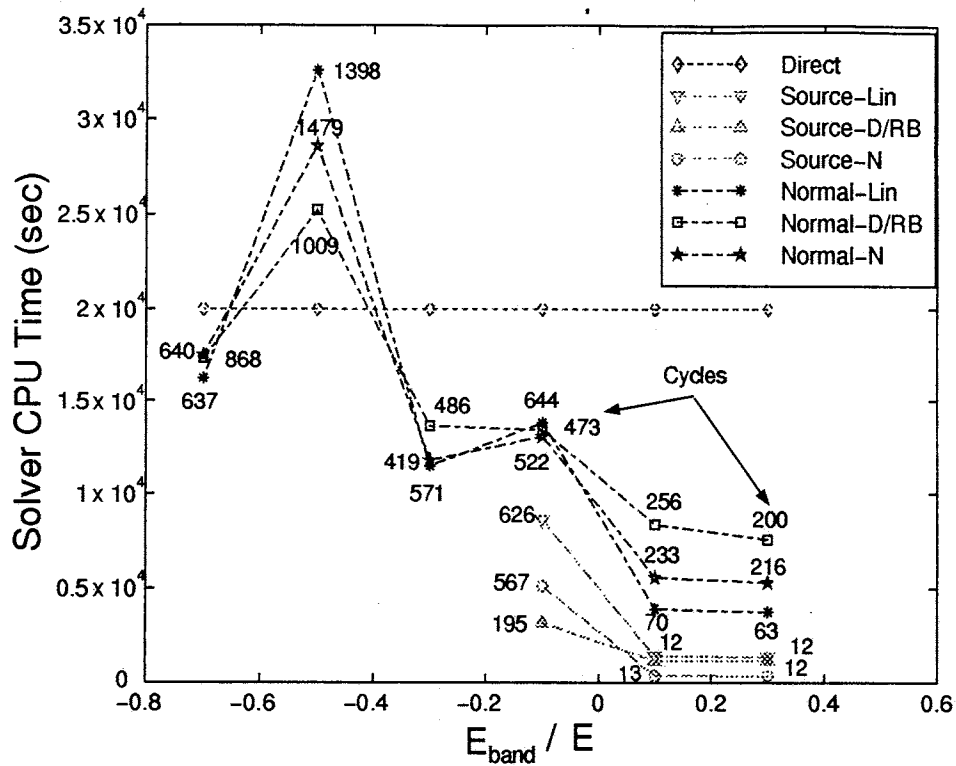


Figure 11: CPU/Cycles vs  $E_{band}/E$  for shear banding problem with 107811 equations

For highly indefinite systems the direct solver is more efficient in terms of CPU time than the iterative schemes applied to normal equations for problems below 100000 unknowns. Among the three two-level schemes considered the prolongator based on the linear interpolation on nonoverlapping aggregates, had in general the best performance with few exceptions ( $E_{band}/E = -0.5$  in Figure 11). This can be explained by the fact that linear fields represent the Kernel of normal equations with constant coefficients, and the prolongator based on linear interpolation does not involve overhead associated with local eigenvalue analysis.

The influence of prolongation smoothing on the solver performance was similar to that illustrated in Figure 8, i.e., significant reduction in iteration count, minor gains in CPU time of the iterative process and increased total computational cost for problems with a single right hand side vector.

For utilization of geometric multigrid methods in plasticity with strain hardening we refer to [19], [20].

## 7.0 Future work

The manuscript represents the first step towards developing an automated general purpose multilevel solver for indefinite systems. It is critical that such a solver should be robust. It may use different strategies, such as utilizing normal equations for highly indefinite problems or the source system for weakly indefinite problems, but it should not fail.

This goal have been partially accomplished. We have demonstrated that such a hybrid solver exist, but we have not addressed the issue of how to select an optimal solution strategy. In particular, what is an optimal number of levels, how to construct an optimal prolongation operator, will the method converge for the source system or should the normal equations be used instead and what is an optimal accelerator and smoother for a problem at hand? Clearly, the answer to these questions depends on the problem data, including the sparsity, the spectrum of eigenvalues, the problem size, and the number of right hand sides. For positive definite systems a decision graph-based methodology has been developed in [9] and we indent to generalize this or a similar framework to indefinite systems.

Even though a family of efficient two-level solvers, which does not require an explicit formation of normal system of equations, has been developed for normal equations it is evident that these normal solvers are below par with two-level methods directly applied to the source system (provided that they converge). Therefore, further improvement of prolongators, smoothers and accelerators is critical if we are to extend the range of applicability of the two- and multi- level methods for indefinite (source) system of equations.

## ACKNOWLEDGMENT

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