A New Family of Preconditioners for Domain Decomposition

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Abstract. This paper presents a new approach to construct preconditioners for domain decomposition -based preconditioned conjugate gradient methods. The idea is to approximate the spectrum of the Schur complement by simple functions, such as rational approximations, which leads to solving an easy, lower dimension interface problem. The framework is easily extended to complicated applications. Examples are given for nonuniform grid on the domain interface which is a common situation for which no effective preconditioners now exist. Theory and experimental data are given to illustrate the effectiveness of our approach in this application.

Key words. domain decomposition, preconditioners, preconditioned conjugate gradient methods, iterative methods, partial differential equations, parallel computation

AMS(MOS) subject classifications. 65N55, 65F10, 65Y05

1. Introduction. Domain decomposition methods have undergone rapid development in recent years, especially due to their potential parallelism. A survey of these methods and their experimental performance can be found in [12]. A majority of them are basically preconditioned conjugate gradient *(PCG)* type methods. The key is to construct preconditioners for the *Schur complement* matrix on the interfaces of subdomains. A good preconditioner is characterized by (a) it is easily invertible, and (b) its spectrum well approximates that of the Schur complement matrix in the sense that the preconditioned system has small condition number or very clustered spectrum. Considerable theory has been established showing that under certain conditions, preconditioners can be chosen so that the number of *PCG* iterations is bounded by a constant independent of the system size. Among the most important preconditioner choices and related analysis is the work of Dryja [9], Golub and Mayers [10], Bjorstad and Widlund [2], Bramble, Pasciak and Schatz [3], Chan and Resasco [7], Xu [14], and Cai and Widlund [4]. Most of these preconditioners are derived from the model problem analysis. The effectiveness of these preconditioners, however, strongly depends on the model problem assumptions; its operator, geometry and discretization. These assumptions cause difficulty in using these preconditioners for general cases. For instance, many of them belong to the so-called $K^{1/2}$-family of preconditioners, where K can be viewed as the discrete operator corresponding to a second order elliptic differential operator on the interface. The efficiency of these preconditioners relies on the eigendecomposition of K. When the original PDE operator is separable and has constant coefficients, and when the grid points on the interface are equidistant, then K is usually a tridiagonal matrix with constant in each diagonal and therefore has an eigenvector system consisting of sine functions. In this case, the $K^{1/2}$ type pre-

conditioners can be easily inverted by the *FFT*. One can still extend these methods to an operator with nonconstant coefficients by considering an operator whose constant coefficients are certain averages of the original operator's coefficients. However, the lack of grid uniformity on the interface creates fundamental difficulties because the preconditioners can no longer be inverted using the *FFT*. In this case, solving the new problem is even more expensive than solving the original one because of the requirement of first computing the eigendecomposition and then computing a dense matrix-vector product at each iteration. Some preconditioners can still be applied for nonuniform grids, such as Bjorstad and Widlund's Neumann problem approach [2] and Chan's boundary probing approach [6]. However, the former requires solving a Neumann problem in one subdomain at each iteration which is more expensive than solving a lower dimension interface problem, and the latter requires solving $k + 1$ subdomain problems at the beginning to set up a symmetric matrix with semi-bandwidth k and then solving the band system at each iteration. It is also known [12] that Chan's probing approach approximates the Schur complement more poorly than the $K^{1/2}$-family for model problems.

This paper presents a new approach to construct preconditioners. The basic idea is to approximate the spectrum of the Schur complement by simple functions, which leads to solving an easy, lower dimension interface problem. Thus determining the preconditioner amounts to a function approximation; many theories can be applied to derive various new preconditioners. The framework is easily extended to more complicated applications. This paper focuses on the case of nonuniform grids on interfaces which is a very common situation, such as a general finite element mesh on a complicated geometric domain, an adaptive mesh for a solution with singularities, and so on. We are unaware of any previous *PCG* work in the literature for this important application.

The remainder of the paper is organized as follows. Section 2 gives some background on previous work, especially the $K^{1/2}$-family of preconditioners. Section 3 describes the fundamental framework for our new approach. Section 4 provides the theory for the nonuniform grid case. Section 5 illustrates the application of rational approximations to this approach. Section 6 reports on our experimental data to show the effectiveness of the approach. Finally, Section 7 concludes with some remarks.

2. Background. To illustrate the basic ideas, it suffices to consider the domain decomposition of two subdomains. In the case of more than two subdomains, it is shown by Bramble, Pasciak and Schatz [3] that preconditioning the Schur complement matrix on the interfaces can be further decoupled into preconditioning each Schur complement submatrix on each individual interface piece with two adjacent subdomains plus solving an easy and small system for the cross-points on the interfaces.

We start with stating the known theory for the model problem that is a Poisson equation with Dirichlet condition on a rectangle Ω. The problem is discretized using the *5-point-star* finite difference, or equivalently the linear finite element Galerkin approximation, on a uniform grid with spacing h in both directions. For simplicity, we assume that the x-region of Ω is $(0, 1)$. Ω is decomposed into two rectangular subdomains, denoted by Ω_1 and Ω_2, by the interface Γ which is a horizontal grid line with n the number of unknowns on the interface and $m1$ and $m2$ the number of interior horizontal grid lines in each subdomain, respectively. Ordering the subdomain interior unknowns first followed by those on Γ, we obtain a linear system with a symmetric

positive definite (*SPD*) coefficient matrix A of the form:

$$A = \begin{bmatrix} A_1 & & B_1 \\ & A_2 & B_2 \\ B_1^T & B_2^T & D \end{bmatrix} \tag{2.1}$$

where A_i is the stiffness matrix for Ω_i, D for Γ; and B_i represents the coupling between Ω_i and Γ.

The corresponding *Schur complement* or the *capacitance matrix* S on Γ is then defined by

$$S \doteq D - \sum_{i=1}^{2} B_i^T A_i^{-1} B_i \tag{2.2}$$

which is still *SPD*. The original problem can then be reduced to an interface system with the coefficient matrix S, which is a common practice in the *substructuring* or *capacitance matrix* approach. One can apply the *PCG* to either the original or the interface system. A preconditioner for S can also be used to construct an *incomplete LU* preconditioner for A as S is a component in the block *LU* factors. These two approaches are essentially equivalent for the model problem as shown by Eisenstat [12]. Therefore, the main task is to construct good preconditioners for S.

Using the Fourier analysis, Chan [5] gives an explicit eigendecomposition of S by

$$S = W \Lambda_C W^T \tag{2.3.1}$$

where

$$[W]_{ij} = \sqrt{2h}\ \sin\ ij\pi h, \tag{2.3.2}$$

and

$$\Lambda_C = diag(\lambda_j^C) \tag{2.3.3}$$

where

$$\lambda_j^C = \left(\frac{1 + \rho_j^{m_1+1}}{1 - \rho_j^{m_1+1}} + \frac{1 + \rho_j^{m_2+1}}{1 - \rho_j^{m_2+1}} \right) \sqrt{\sigma_j + \frac{\sigma_j^2}{4}} \tag{2.3.4}$$

with

$$\sigma_j = 4\sin^2 \frac{j\pi h}{2}, \tag{2.3.5}$$

and

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$$\rho_j = \frac{r_{j-}}{r_{j+}} \tag{2.3.6}$$

where

$$r_{j\pm} = 1 + \frac{\sigma_j}{2} \pm \sqrt{\sigma_j + \frac{\sigma_j^2}{4}}. \tag{2.3.7}$$

Denoting

$$\Lambda_K = diag(\sigma_j), \tag{2.4.1}$$

and

$$K = W\Lambda_K W^T, \tag{2.4.2}$$

then K is simply a tridiagonal matrix $[-1, 2, -1]$ which is the discrete one dimensional Laplace operator on Γ. Bank and Rose [1] also discover the same decomposition in terms of the Chebyshev polynomials. They show that

$$S = s_{m_1}^{-1}(T)s_{m_2}^{-1}(T)s_{m_1+m_2+1}(T) \tag{2.5.1}$$

where

$$T = 2I + K, \tag{2.5.2}$$

and $s_m(x)$ is the *modified Chebyshev polynomial* which can be explicitly expressed for $x > 2$ by

$$s_m(x) = \frac{\gamma^{(m+1)} - \gamma^{-(m+1)}}{\gamma - \gamma^{-1}}, \qquad \gamma = \frac{x}{2} + \sqrt{(\frac{x}{2})^2 - 1}, \quad x > 2. \tag{2.5.3}$$

Therefore, denoting

$$f(x) = \frac{s_{m_1+m_2+1}(x)}{s_{m_1}(x)s_{m_2}(x)}, \tag{2.6.1}$$

we have

$$\lambda_j^G = f(t_j) \tag{2.6.2}$$

with

$$t_j = 2 + \sigma_j. \tag{2.6.3}$$

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A number of well-known preconditioners can then be related to this eigendecomposition, and they are often referred to as the $K^{1/2}$-family in the literature. We follow the common notations and ignore a scalar factor that is not essential to a preconditioner. These preconditioners are denoted by M_D (Dryja), M_G (Golub and Mayers), M_B (Bjorstad and Widlund) and M_C (Chan) with $\Lambda_D = diag(\lambda_j^D)$, $\Lambda_G = diag(\lambda_j^G)$, and $\Lambda_B = diag(\lambda_j^B)$ denoting the corresponding eigenvalue diagonal matrices, respectively. They can be expressed by:

$$M_D \equiv K^{1/2} = W\Lambda_D W^T \qquad (2.7.1)$$

with

$$\lambda_j^D = \sqrt{\sigma_j}; \qquad (2.7.2)$$

$$M_G \equiv (K + \frac{1}{4}K^2)^{1/2} = W\Lambda_G W^T \qquad (2.8.1)$$

with

$$\lambda_j^G = \sqrt{\sigma_j + \frac{\sigma_j^2}{4}}; \qquad (2.8.2)$$

$$M_B = W\Lambda_B W^T \qquad (2.9.1)$$

with

$$\lambda_j^B = \left(\frac{1 + \rho_j^{m_1+1}}{1 - \rho_j^{m_1+1}} \right) \sqrt{\sigma_j + \frac{\sigma_j^2}{4}}; \qquad (2.9.2)$$

and

$$M_C = W\Lambda_C W^T. \qquad (2.10.1)$$

It is seen that these preconditioners can be viewed as the increasingly improved approximations towards the Schur complement in terms of the spectrum. When $\Omega_1 = \Omega_2$, M_C is reduced to M_B. Under the assumptions in this section, M_C is equal to S, and therefore, becomes an exact solver.

3. A new approach to construct preconditioners. As stated earlier, it is difficult to extend these preconditioners to complicated cases since they depend either on too much information of the eigensystem of S, or on solving a subdomain problem at each iteration for which the cost is of the same order as the total computation (or in other words, it increases the overall cost by a factor) assuming that the number of PCG iterations is independent of the system size. We present a new approach

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to construct preconditioners that are both efficient in computation and effective in convergence.

We first informally describe our fundamental idea that is simple. The model problem analysis (2.5)–(2.6) suggests that the Schur complement matrix is spectrally equivalent to a reference matrix T with a mapping $f(x)$ in the sense that

$$S = f(T) = Wf(\Lambda_T)W^T \tag{3.1.1}$$

where

$$T = W\Lambda_T W^T. \tag{3.1.2}$$

Let the matrix $F \equiv f(T)$ be the *function of the matrix* T [11], we see that $f(x)$ is essentially a mapping from the spectrum of T to that of S:

$$\sigma(S) = \sigma(F) = f(\sigma(T)) \tag{3.2}$$

where $\sigma(\cdot)$ denotes the spectrum. Thus $C(f,T) \equiv (f(\sigma(T)), \sigma(T))$ defines a curve that characterizes $\sigma(S)$. T is usually a very simple matrix corresponding to a discrete second order elliptic differential operator on the interface. In the model problem, T is a symmetric tridiagonal matrix. However, $f(x)$ is complicated, and may be defined implicitly without a closed form. The more complicated $f(x)$ is, the more difficult it is to invert the generated matrix F. Notice that a preconditioner M for S only needs to have $\sigma(M) \sim \sigma(S)$. Though obtaining the whole curve $C(f,T)$ might be difficult and expensive, it is, however, possible to recover its essential behavior from part of the information in $C(f,T)$. As seen later, $f(x)$ usually has some special properties that can be predicted from theoretical analysis; therefore, one can find a simple function $r(x)$ to approximate $f(x)$ such that the curve $C(r,T)$ well approximates $C(f,T)$.

From the above observations, we thus propose a new approach to construct preconditioners as follows. *Assuming $f(x)$ is a function characterizing the spectrum of S in terms of a simple matrix T, find a simple function $r(x)$ that approximates $f(x)$ and then use matrix $R \equiv r(T)$ as a preconditioner for S.* More specifically, suppose T, which may be nonsymmetric, has the eigendecomposition

$$T = W\Lambda_T W^{-1}, \tag{3.3.1}$$

we have for F and R:

$$F = Wf(\Lambda_T)W^{-1}, \tag{3.3.2}$$

and

$$R = Wr(\Lambda_T)W^{-1}. \tag{3.3.3}$$

Then the preconditioned matrix $R^{-1}F$ may be expressed as

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$$R^{-1}F = Wr^{-1}(\Lambda_T)f(\Lambda_T)W^{-1} = Wq(\Lambda_T)W^{-1} \qquad (3.4.1)$$

where

$$q(x) \equiv f(x)/r(x), \qquad (3.4.2)$$

i.e., $\sigma(R^{-1}F) = \{q(t_i)\}$ where $\{t_i\} = \sigma(T)$.

From the *PCG* theory [8], the convergence is determined by the spectrum of the preconditioned matrix in the sense that the number of iterations is bounded by the condition number according to

$$\frac{\|\mathbf{x}^k - \mathbf{x}\|_A}{\|\mathbf{x}^0 - \mathbf{x}\|_A} \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \qquad (3.5)$$

with $\| \cdot \|_A$ denoting the A-norm where A is the original matrix and κ denotes the condition number of the preconditioned matrix $M^{-1}A$ for the preconditioner M. The *PCG* algorithm produces exact convergence in a number of iterations which is at most the number of distinct eigenvalues of $M^{-1}A$. From (3.4),

$$\kappa(R^{-1}F) = \frac{\max_i |q(t_i)|}{\min_i |q(t_i)|}. \qquad (3.6)$$

Thus, if $\max_i |q(t_i)|/\min_i |q(t_i)|$ is small or $\{q(t_i)\}$ are clustered, then applying the preconditioner R to F produces good convergence. Since F is spectrally equivalent, or nearly equivalent, to S, so R is also a preconditioner for S. We now formalize our new approach as follows.

Preconditioner construction through function approximation. *Given the matrix T and the function $f(x)$, find an approximation $r(x)$ to $f(x)$, such that, with $q(x) \equiv f(x)/r(x)$,*

(a) $\qquad\qquad \dfrac{\max_i |q(t_i)|}{\min_i |q(t_i)|} \sim 1$, *or $\{q(t_i)\}$ are clustered;* $\qquad (3.7.1)$

where $\{t_i\} = \sigma(T)$, and

(b) $\qquad\qquad R \equiv r(T)$ *is easily invertible.* $\qquad (3.7.2)$

R is then taken as a preconditioner for $F \equiv f(T)$.

Various choices of $r(x)$ yield different preconditioners. One has large freedom in constructing $r(x)$ according to the properties of a given $f(x)$ to satisfy the conditions (a) and (b). As examples, all of the $K^{1/2}$-family of preconditioners can then be interpreted in terms of this approach by taking K as T, $s_{m_1+m_2+1}(2 + x)/(s_{m_1}(2 + x)s_{m_2}(2 + x))$ as $f(x)$. This function behaves like $x^{1/2}$ near $x = 0$, thus the corresponding $r(x)$ for each preconditioner also contains the *square-root* in its expression in order to satisfy condition (a). For condition (b), however, R is too complicated for general cases. R can be easily inverted when T has sine eigenvectors W, which is only true for the model problem with uniform grid. In that case,

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$$R^{-1} = W r^{-1}(\Lambda_T) W^T \qquad (3.8)$$

is evaluated using the *FFT*.

The advantage of the new approach is that the complicated preconditioning problem is replaced by a function approximation. Even when W is, in general, not available through the *FFT*, the approximation theory still provides ways to find other simple approximations $r(x)$ to $f(x)$, such that matrix R is easy enough to invert. We later illustrate the application of this general approach in examples.

4. Preconditioning for nonuniform grids. This section extends the theory of the Schur complement eigendecomposition to the nonuniform grid case. We assume that the grid on the interface (the x-direction grid) is nonuniform with the grid points $0 = x_0 < x_1 < x_2 < \ldots < x_n < x_{n+1} = 1$; and the y-direction grid is uniform. Let $h_x^i \equiv x_i - x_{i-1}$, $i = 1, \ldots, n + 1$, denote the spacing of each x-subinterval; and h_y denote the y-direction spacing. Let A_{FE}^2 denote the stiffness matrix generated from the linear finite element discretization of the model problem. The corresponding *5-point-star* stencil at position (i, j) is expressed by

$$\begin{bmatrix} 0 & a_N & 0 \\ a_W & a_P & a_E \\ 0 & a_S & 0 \end{bmatrix} \qquad (4.1.1)$$

with

$$a_P = \frac{h_x^i + h_x^{i+1}}{h_y} \left(1 + \frac{(h_y)^2}{h_x^i h_x^{i+1}} \right), \qquad (4.1.2)$$

$$a_N = a_S = -\frac{h_x^i + h_x^{i+1}}{2 h_y}, \qquad (4.1.3)$$

$$a_W = -\frac{h_y}{h_x^i}, \qquad (4.1.4)$$

$$a_E = -\frac{h_y}{h_x^{i+1}}. \qquad (4.1.5)$$

Introducing an $n \times n$ scaling operator Θ and an $n \times n$ tridiagonal matrix Σ:

$$\Theta = diag\left(\frac{h_x^i + h_x^{i+1}}{2} \right), \qquad (4.2.1)$$

$$\Sigma = \left[-\frac{h_y}{h_x^i}, \quad \frac{h_x^i + h_x^{i+1}}{h_y} \left(1 + \frac{(h_y)^2}{h_x^i h_x^{i+1}} \right), \quad -\frac{h_y}{h_x^{i+1}} \right], \qquad (4.2.2)$$

we have the expression of A_{FE}^2 given in Lemma 4.1.

LEMMA 4.1.

$$A_{FE}^2 = \left[-\frac{1}{h_y}\Theta, \Sigma, -\frac{1}{h_y}\Theta \right] \tag{4.3}$$

Similarly, for the one dimensional counterpart in the x-direction, let A_{FE}^1 denote the stiffness matrix corresponding to the 1-D Laplacian, and the corresponding stencil at $x = x_i$ is expressed by

$$\left[-\frac{1}{h_x^i}, \quad \frac{h_x^i + h_x^{i+1}}{h_x^i h_x^{i+1}}, \quad -\frac{1}{h_x^{i+1}} \right]. \tag{4.4}$$

Let A_{FD}^1 denote the standard finite difference operator, which is not symmetric, with the stencil

$$\left[-\frac{2}{h_x^i(h_x^i + h_x^{i+1})}, \quad \frac{2}{h_x^i h_x^{i+1}}, \quad -\frac{2}{h_x^{i+1}(h_x^i + h_x^{i+1})} \right]. \tag{4.5}$$

Then the following two lemmas state the relationship among the four operators Σ, Θ, A_{FE}^1, and A_{FD}^1.

LEMMA 4.2.

$$\Sigma = \frac{2}{h_y}\Theta + h_y A_{FE}^1 \tag{4.6}$$

LEMMA 4.3.

$$A_{FE}^1 = \Theta A_{FD}^1 \tag{4.7}$$

It is easy to verify Lemma 4.1 through Lemma 4.3. In terms of these notations, we are able to give an explicit expression for the Schur complement matrix S, which is an extension of the theory of Chan (2.3) or Bank and Rose (2.5).

THEOREM 4.4. *With $f(x)$ as defined by (2.5.3) and (2.6.1), then the Schur complement matrix S for the nonuniform grid can be expressed by either*

(i) $$S = \frac{1}{h_y}\Theta^{1/2} f(T)\Theta^{1/2} \tag{4.8.1}$$

where

$$T = h_y \Theta^{-1/2}\Sigma\Theta^{-1/2}; \tag{4.8.2}$$

or

(ii) $$S = \frac{1}{h_y}\Theta f(\Pi) \tag{4.9.1}$$

where

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$$\Pi = h_y \Theta^{-1} \Sigma. \qquad (4.9.2)$$

In addition, we have:

(iii)
$$\Pi = \Theta^{-1/2} T \Theta^{1/2}; \qquad (4.10)$$

(iv)
$$\sigma(T) = \sigma(\Pi) \subset (2, \mu) \qquad (4.11.1)$$
where
$$\mu = 2 + 4(\tfrac{h_y}{\tilde{h}_x})^2, \tilde{h}_x = \min_i\{h_x^i\}. \qquad (4.11.2)$$

To prove Theorem 4.4, we need a lemma from [1].

LEMMA 4.5 (BANK AND ROSE). *Denote*

$$M_p = [-I, T, -I], \qquad \text{of block dimension } p \times p,$$

$$v_p^T = [0 \ 0 \ \dots \ 0 \ -I], \quad \text{of block dimension } 1 \times p,$$

$$w_p^T = [-I \ 0 \ 0 \ \dots \ 0], \quad \text{of block dimension } 1 \times p,$$

where T is a square matrix. Then we have

$$T - v_{m_1}^T M_{m_1}^{-1} v_{m_1} - w_{m_2}^T M_{m_2}^{-1} w_{m_2} = s_{m_1}^{-1}(T) s_{m_2}^{-1}(T) s_{m_1+m_2+1}(T). \qquad (4.12)$$

The proof of Lemma 4.5 is implied in (4.3) of [1] by taking $m_1 = i - 1$, $m_2 = n - i$, and $n = m_1 + m_2 + 1$. Note that the matrix in this lemma is the Schur complement for the model problem, see (2.5.1). We now give the proof of Theorem 4.4.

Proof of (i). We extend the idea of Lemma 4.5 and introduce

$$\tilde{M}_p = [-\tfrac{1}{h_y}\Theta, \Sigma, -\tfrac{1}{h_y}\Theta],$$

$$\tilde{v}_p^T = [0 \ 0 \dots 0 \ -\tfrac{1}{h_y}\Theta],$$

$$\tilde{w}_p^T = [-\tfrac{1}{h_y}\Theta \ 0 \ 0 \dots 0].$$

Similar to the matrix (4.12) (which is the Schur complement in the uniform grid case), we now have for S:

$$S = \Sigma - \tilde{v}_{m_1}^T \tilde{M}_{m_1}^{-1} \tilde{v}_m - \tilde{w}_{m_2}^T \tilde{M}_{m_2}^{-1} \tilde{w}_{m_2} \qquad (4.13)$$

Recall the relations between M_p and $\tilde{M}_p$, v_p and $\tilde{v}_p$, and w_p and $\tilde{w}_p$, respectively, and also recall (4.8.2), then

$$
\begin{aligned}
S &= \Sigma - \tilde{v}_{m_1}^T \left(diag((\tfrac{1}{h_y}\Theta)^{1/2})M_{m_1}diag\left((\tfrac{1}{h_y}\Theta)^{1/2}\right)\right)^{-1}\tilde{v}_{m_1} \\
&\quad - \tilde{w}_{m_2}^T \left[diag\left((\tfrac{1}{h_y}\Theta)^{1/2}\right) M_{m_2}diag\left((\tfrac{1}{h_y}\Theta)^{1/2}\right)\right]^{-1}\tilde{w}_{m_2} \\
&= \Sigma - \left(\tfrac{1}{h_y}\Theta\right)^{1/2}v_{m_1}^T M_{m_1}^{-1}v_{m_1}\left(\tfrac{1}{h_y}\Theta\right)^{1/2} - \left(\tfrac{1}{h_y}\Theta\right)^{1/2}w_{m_2}^T M_{m_2}^{-1}w_{m_2}\left(\tfrac{1}{h_y}\Theta\right)^{1/2} \\
&= \tfrac{1}{h_y}\Theta^{1/2}s_{m_1}^{-1}(T)s_{m_2}^{-1}(T)s_{m_1+m_2+1}(T)\Theta^{1/2}.
\end{aligned}
$$
(4.14)

This yields (i) from (4.12) and the definition of $f(x)$.

Proof of (iii). (4.10) is trivial from the definitions of (4.9.2) and (4.9.4).

Proof of (ii). From (i) and (iii) we have

$$
\begin{aligned}
S &= \tfrac{1}{h_y}\Theta^{1/2}f(T)\Theta^{1/2} \\
&= \tfrac{1}{h_y}\Theta^{1/2}f(\Theta^{1/2}\Pi\Theta^{-1/2})\Theta^{1/2}.
\end{aligned}
$$
(4.15)

Since $f(x)$ is a rational function, we have

$$
f(\Theta^{1/2}\Pi\Theta^{-1/2}) = \Theta^{1/2}f(\Pi)\Theta^{-1/2}, \tag{4.16}
$$

and (ii) then immediately follows.

Proof of (iv). From (4.8.2) and Lemma 4.2, we have

$$
\begin{aligned}
T &= h_y\Theta^{-1/2}(\tfrac{2}{h_y}\Theta + h_y A_{FE}^1)\Theta^{-1/2} \\
&= 2I + (h_y)^2\Theta^{1/2}A_{FE}^1\Theta^{-1/2}.
\end{aligned}
$$
(4.17)

Since A_{FE}^1 is SPD, we have

$$
\lambda_{min}(T) > 2 \tag{4.18}
$$

where $\lambda_{min}(T)$ is the minimum eigenvalue of T.

On the other hand, for any real vector $\mathbf{x}$, denoting $\mathbf{y} = \Theta^{-1/2}\mathbf{x}$, from (4.17) and the finite element analysis we have

$$
\begin{aligned}
\mathbf{x}^T T\mathbf{x} &= 2\mathbf{x}^T\mathbf{x} + (h_y)^2\mathbf{y}^T A_{FE}^1\mathbf{y} \\
&= 2\mathbf{x}^T\mathbf{x} + (h_y)^2\sum_i \int_0^{h_x^i}(\tfrac{y_i - y_{i-1}}{h_x^i})^2 dx \\
&= 2\mathbf{x}^T\mathbf{x} + (h_y)^2\sum_i \tfrac{1}{h_x^i}\int_0^1(y_i - y_{i-1})^2 dx
\end{aligned}
$$
(4.19)

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with $y_0 = y_{n+1} = 0$. Therefore, it follows that

$$
\begin{aligned}
\mathbf{x}^T T \mathbf{x} &\le 2\mathbf{x}^T\mathbf{x} + \frac{(h_y)^2}{h_x}\mathbf{y}^T K\mathbf{y} \\
&\le 2\mathbf{x}^T\mathbf{x} + 4\frac{(h_y)^2}{h_x}\mathbf{y}^T\mathbf{y} \\
&= 2\mathbf{x}^T\mathbf{x} + 4\frac{(h_y)^2}{h_x}\sum_i \left(\frac{h_x^i + h_x^{i+1}}{2}\right)^{-1} x_i^2 \\
&\le 2\mathbf{x}^T\mathbf{x} + 4\left(\frac{h_y}{h_x}\right)^2 \mathbf{x}^T\mathbf{x}.
\end{aligned}
\tag{4.20}
$$

where (2.3.5) is used. By the Rayleigh principle, we have

$$
\lambda_{max}(T) < \mu
\tag{4.21}
$$

where $\lambda_{max}(T)$ is the maximum eigenvalue of T. Combining (4.18) and (4.21), we obtain (iv). This completes the proof of Theorem 4.4.

Remark 4.1. Although S itself no longer has the same eigenvector system as a simple interface operator, a modified matrix by a scaling still has. That is, for the symmetric case, the symmetrically scaled Schur complement $h_y \Theta^{-1/2} S \Theta^{-1/2}$ is similar to T; and for the nonsymmetric case, the simply scaled Schur complement $h_y \Theta^{-1} S$ is similar to Π.

Remark 4.2. The *SPD* matrix T is symmetrically scaled from Σ that is actually the finite element discrete operator on the interface grid, ignoring a factor, of the interface differential operator L^1:

$$
L^1 u \equiv -(h_y)^2 \frac{d^2 u}{dx^2} + 2u.
\tag{4.22}
$$

Correspondingly, the nonsymmetric matrix Π is simply the finite difference approximation of L^1. In addition, T and Π are similar matrices, and both of them are tridiagonal. Their eigenvectors no longer consist of sine functions, however, they can be easily inverted directly.

Remark 4.3. The spectrum of T, or Π, is contained in an interval $(2, \mu)$. So, $f(x)$ still has a closed expression in terms of (2.5.3) and (2.6.1). We know $\mu = 6$ for a uniform grid with $h_x = h_y$. In general, however, μ may be a lot larger.

5. Applying rational approximation to construct preconditioners. From the theory in Section 4, preconditioning S can be done by preconditioning $f(T)$, or $f(\Pi)$, plus a scaling. The approach presented in Section 3 then requires to find a simple function $r(x)$ that approximates $f(x)$ in the interval $(2, \mu)$. To do this, it is important to first study the behavior of $f(x)$ for $x > 2$. From (2.5.3) and (2.6.1), $f(x)$ can be written as

$$
\begin{aligned}
f(x) &= \frac{\delta^{(m_1+m_2+2)}-1}{(\delta^{(m_1+1)}-1)(\delta^{(m_2+1)}-1)}\frac{(\delta-1)}{\sqrt{\delta}} \\
&= \frac{1}{2}\left(\frac{\delta^{(m_1+1)}+1}{\delta^{(m_1+1)}-1} + \frac{\delta^{(m_2+1)}+1}{\delta^{(m_2+1)}-1}\right)\frac{(\delta-1)}{\sqrt{\delta}}
\end{aligned}
\tag{5.1.1}
$$

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where

$$\delta = \left(\frac{x}{2} + \sqrt{(\frac{x}{2})^2 - 1}\right)^2 .$$ (5.1.2)

$f(x)$ can be characterized by two parts. When x moves left a little bit away from 2,

$$f(x) \approx \sqrt{\delta} \approx x,$$ (5.2)

so $f(x)$ behaves like a linear function. We call this the *easy part* which corresponds to most of the eigenvalues (higher frequencies) of S.

When x is near 2, however, $f(x)$ is less smooth. For fixed m_1 and m_2, we have

$$\lim_{x \to 2} f(x) = \frac{1}{m_1 + 1} + \frac{1}{m_2 + 1}$$ (5.3)

If m_1 and m_2 are large enough or x is in the transition area between $x = 2$ and the linear part, the coefficient factor

$$\frac{\delta^{(m_1+1)} + 1}{\delta^{(m_1+1)} - 1} + \frac{\delta^{(m_2+1)} + 1}{\delta^{(m_2+1)} - 1}$$

is around a constant depending on the aspect ratios of subdomains [5], so $f(x)$ behaves like a *square-root* function:

$$f(x) \approx \frac{\delta - 1}{\sqrt{\delta}} = \sqrt{x^2 - 4}.$$ (5.4)

We call this the *hard part* which corresponds only to a few smallest eigenvalues (low frequencies) of S.

From the above discussion, we see that $f(x)$ has a *two-part* property. In Fig.1 the curves of $f(x)$ are plotted for three sets of (m_1, m_2) that are of practical interest. It is very hard to distinguish these curves for different (m_1, m_2) in a large region. The difference can only be seen in the *hard part* that is very close to $x = 2$.

To make the condition number in (3.6) small we must approximate $f(x)$ in the whole interval $(2, \mu)$. Therefore, both the *easy* and *hard* parts need to be taken care of. The simplest choice is, of course, the polynomial approximation. However, it is not appropriate for a square-root like function. A good candidate for approximating less smooth functions is rational approximation, for which $r(x)$ is a rational function

$$r(x) \equiv \frac{p_l(x)}{q_m(x)}$$ (5.5)

where $p_l(x)$ and $q_m(x)$ are l-th and m-th order polynomials, respectively. To solve a linear system with coefficient matrix $R \equiv r(T)$, $Rx = b$, then amounts to solving $Px = Qb$ where $P \equiv p_l(T)$ and $Q \equiv q_m(T)$. In practice, one can either first expand the tridiagonal matrix T explicitly to band matrices P and Q from $p_l(x)$ and $q_m(x)$
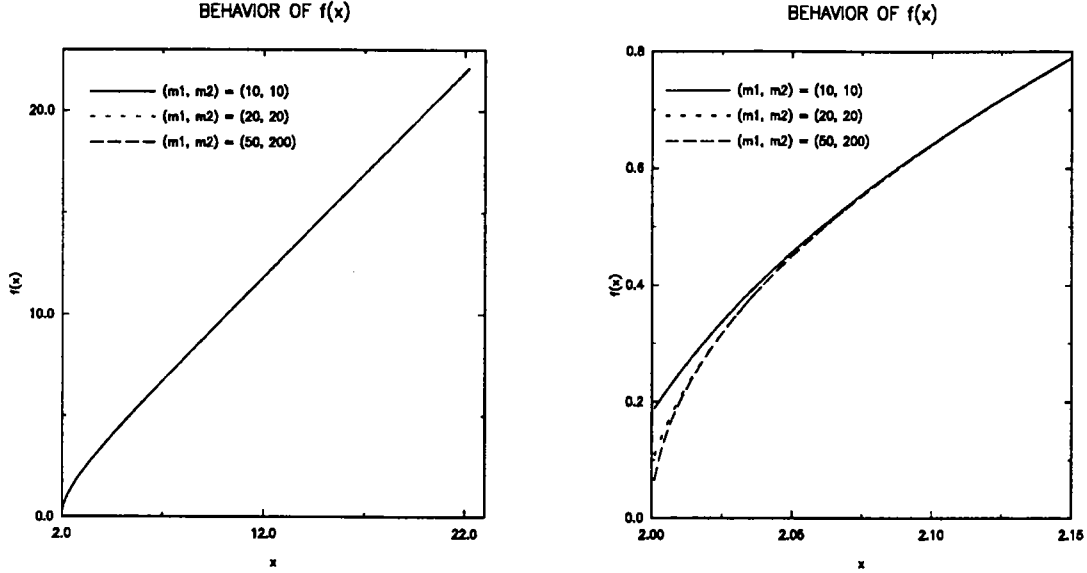
Figure 1. *Behavior of $f(x)$ in a large region (left figure) and near $x = 2$ (right figure).*

and then solve $Px = Qb$; or first factor $p_l(x)$ and $q_m(x)$ into linear factors and then perform a series of tridiagonal matrix computations. That depends, for example, on the requirements of parallelism, time and storage saving, and so on.

The approximation behavior is determined by the polynomial degrees l and m. Usually, the larger l and m are, the better the approximation is. At the extreme, one can take $p_l(x) = s_{m_1+m_2+1}(x)$ and $q_m(x) = s_{m_1}(x)s_{m_2}(x)$, which makes $r(x)$ exactly equal to $f(x)$. However, for the purpose of efficiency, it is necessary to keep l and m as small as possible. The most interesting choice is then for $l = m = 1$, where we can easily determine an $r(x)$ using three interpolation points. It is easily seen that given interpolation points $P_i \equiv (f_i, z_i)$, $i = 0, 1, 2$, the rational approximation

$$r(x) \equiv \frac{ax + b}{cx + d} \tag{5.8}$$

that interpolates $\{P_i\}$ is determined by

$$a = f_{02}f_1 - f_{01}f_{12}; \quad b = -az_0 - f_{12}f_0; \quad c = f_{02}; \quad d = -f_{02}z_0 - f_{12} \tag{5.9.1}$$

where

$$f_{ij} = f[z_i, z_{i+1}, \ldots, z_j], \qquad i < j \tag{5.9.2}$$

denote the divided differences. In practice, since a scalar factor does not affect the condition number, $r(x)$ can be scaled to

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$$\frac{x + e_1}{x + e_2} \qquad (5.10.1)$$

where

$$e_1 = \frac{b}{a}; \qquad e_2 = \frac{d}{c}. \qquad (5.10.2)$$

Therefore, the preconditioner is simply

$$(T + e_1 I)\mathbf{x} = (T + e_2 I)\mathbf{b} \qquad (5.11)$$

which can be viewed as solving an interface *ODE* problem

$$Lu = \tilde{L}v \qquad (5.12.1)$$

with

$$Lu \equiv -(h_y)^2 \frac{d^2 u}{dx^2} + (2 + e_1)u; \qquad (5.12.2)$$

$$\tilde{L}v \equiv -(h_y)^2 \frac{d^2 v}{dx^2} + (2 + e_2)v. \qquad (5.12.3)$$

The remaining problem is to choose the interpolation points. Experiments show that for a nearly uniform grid, the condition number in (3.6) can be reduced to a range from 1.2 to 1.8, depending on m_1, m_2 and n, by fixing $z_0 = \lambda_{min}(T)$ and adjusting z_1 and z_2 in the interval (z_0, μ). The optimal selection of interpolation points to minimize the condition number is of further theoretical interest. In fact, it can be shown in a forthcoming paper that this optimal approximation problem can be solved by using some standard *weighted rational approximation* algorithms. In this paper, to illustrate the effectiveness of the new preconditioner construction approach, we simply use another more intuitive strategy described as follows.

Recall that $f(x)$ consists of an *easy* part and a *hard* part. We can thus approximate $f(x)$ in two phases correspondingly. First, the *hard part* near $x = 2$ is approximated by a rational approximation of (5.8) denoted by $r_1(x)$. It is natural to select the interpolation points corresponding to the first three smallest eigenvalues in $\sigma(T)$. Then, $f(x)/r_1(x)$ is almost like a linear function in the whole range $(2, \mu)$, so we apply another rational approximation, denoted by $r_2(x)$, to $f(x)/r_1(x)$. This time, the interpolation points for $r_2(x)$ are chosen corresponding to the smallest and the two largest eigenvalues in $\sigma(T)$. Therefore, $r(x)$ is defined as

$$r(x) = r_1(x)r_2(x). \qquad (5.13)$$

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The procedure is called the *two-phase rational approximation*. Experiments show that this intuitive strategy is very effective even for very nonuniform grids for which interval $(2, \mu)$ is very big.

Another important property of this *two-phase* procedure is its stability in the sense that the condition number in (3.6) is not sensitive to the interpolation points for $r_1(x)$ and $r_2(x)$. Therefore, although the computation for those smallest and largest eigenvalues of the tridiagonal *SPD* matrix T is not very expensive, one still only needs to roughly estimate those values. For this, consider the matrix T^* which is the counterpart of T corresponding to the uniform grid with the same number of grid points. $\sigma(T^*)$ is given by the formula

$$\lambda_i(T^*) = 2 + 4(\frac{h_y}{h_x})^2 \sin^2 \frac{i\pi h_x}{2}, \quad h_x = \frac{1}{n+1}. \tag{5.14}$$

Thus, we can simply use $\lambda_i(T^*)$, $i = 1, 2, 3, n-1, and \ n$, for the corresponding values $\lambda_i(T)$. Usually, they approximate well for small i, and poorly for large i, which, however, is not important because of the linearity of $f(x)$ when i is large. We will show in the next section that this approach is very stable and produces very satisfactory preconditioners. The condition number is usually around 1.1.

Besides making the condition number small, another way to choose $r(x)$ is to make $\{q(t_i)\}$ clustered as required in (3.7.1). From (5.2), $f(x) \approx x$ for most part of $\sigma(T)$, it is therefore natural to choose

$$r(x) \equiv x \tag{5.15}$$

which simply leads to T as a preconditioner for F. We call this the *linear approximation*. We will see that the corresponding condition number can be significantly large, though the number of iterations is not as big.

Once $r(x)$ is determined, one can then use either

$$M = \Theta^{1/2} r(T) \Theta^{1/2}, \tag{5.16.1}$$

or

$$M = \Theta r(\Pi) \tag{5.16.2}$$

as a preconditioner for the Schur complement matrix S.

6. Numerical experiments. This section reports on experimental data to illustrate the effectiveness of our approach. There are no existing preconditioners available that are designed for nonuniform grids, so we use for comparison the four $K^{1/2}$-family of preconditioners that we can think of as extensions from the uniform grid case. To make them still solvable by the *FFT*, we simply take them as the preconditioner matrices from the corresponding uniform grid. It is trivial for M_D and M_G. For M_B and M_C, when $h_y \neq h_x$, the formulas in (2.3) and (2.9) are modified according to the theory developed in Section 4. The preconditioners constructed from the two-phase rational approximation and linear approximation in Section 5 are denoted by M_R and

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M_L, respectively. We also introduce a modified M_R, denoted by $M_{R'}$, by changing the rightmost interpolation point from $\lambda_{\max}(T^*)$ to $\lambda_{\max}(T)$. In addition, we also compare with the standard CG without preconditioner, denoted by I.

The six grids as plotted in Fig.2 are used in the experiments. They vary from coarse to fine, from nearly uniform (by adding one or two lines to a uniform grid) to very nonuniform (by making some lines very close, or using an adaptive finite element grid), and from uniform to nonuniform in the y-direction. Grid 6 is a grid adapted to the x^α-distribution for $\{h_x^i\}$ which is often used for solutions with the $x^{\alpha-l}$-type singularity at $x = 0$, where l is an integer. Grid 6 is generated by taking $\alpha = 1.5$ and $\max_i\{h_x^i\} = 0.1$, and starting from $x = 1$ towards $x = 0$ until the specified number of grid points is reached. The sizes of six grids are $9 \times 5, 31 \times 31, 31 \times 31, 61 \times 31, 61 \times 33$, and 61×33, respectively. The aspect ratios of subdomains also vary when m_1 and m_2 change. We believe these examples reflect most of practical situations in domain decomposition.

Fig.3 through Fig.6 show example function curves involved in the two-phase rational approximation preconditioners. Fig.3 and Fig.4 are for M_R and $M_{R'}$, respectively, on grid 2 with two equal subdomains. Fig.5 is for M_R on grid 2 with $m_1 = 4$ and $m_2 = 24$. Fig.6 is for M_R on grid 4 with two equal subdomains. We see in these figures that $q(x)$ is always very clustered and near 1 as required by (3.7.1). Also seen from Fig.6 is that, due to the grid nonuniformity, $\lambda_{\max}(T)$ is about 10 times larger than 6 that is the upper bound of eigenvalues in the case of uniform grids with $h_x = h_y$.

The convergence performance of these preconditioners is listed in Table 1, where k denotes the number of iterations and κ denotes the corresponding condition number of the preconditioned system. We use the Lanczos method to estimate κ as a by-product of the PCG iterations, this technique is implemented in [13] and is shown to be effective in [12]. The tolerance for convergence is 10^{-5} and we call the iteration 'failed' if it does not converge in 100 steps. The computation is performed in single precision on the $SPARC/2$ workstation.

From the experiments, we see that $M_{R'}$ is always a very good preconditioner. Its convergence rate is independent of problem size, grid uniformity, and subdomain aspect ratio; and is also insensitive to the rational approximation used, i.e., the interpolation point estimation. In contrast, the extensions of the $K^{1/2}$-family of preconditioners also speed up the convergence, but they are much poorer than $M_{R'}$. Unlike in the uniform grid case, their convergence rates now also depend on problem size. M_L has roughly the same convergence rate as the $K^{1/2}$-family. As far as M_R is concerned, unless grids are extremely nonuniform such as grid 6, M_R is as good as $M_{R'}$, although it usually increases the condition number slightly.

Grid 6 is an example of extremely nonuniform grids, for which $\lambda_{min}(T) = 2.0096$ and $\lambda_{max}(T) = 1.87 \times 10^6$, while $\lambda_{max}(T^*) = 16.05$. So it is easy to see why M_R is not good in this case. In fact, as soon as the rightmost interpolation point in M_R is changed to a fairly good estimate for $\lambda_{max}(T)$, say roughly of the same order of magnitude, one then gets a very good preconditioner. Note also that M_L is not affected by grid 6. However, all the $K^{1/2}$-family of preconditioner as well as the standard CG method are failed in this case. So, they are sensitive to the grid uniformity.
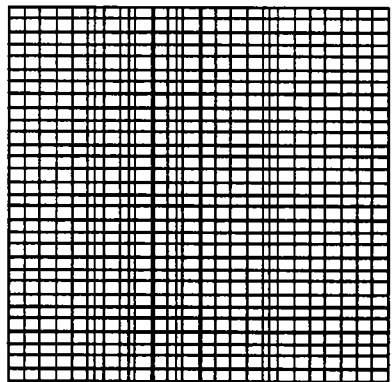
It is also important to notice the experiments with grid 5 and grid 6, where we use nonuniform grids in both the x and y directions. We see that the new preconditioners do not rely on the y- direction uniformity very much, although the theory in Section 4 assumes that the y-direction grid is uniform. This supports the view that our new
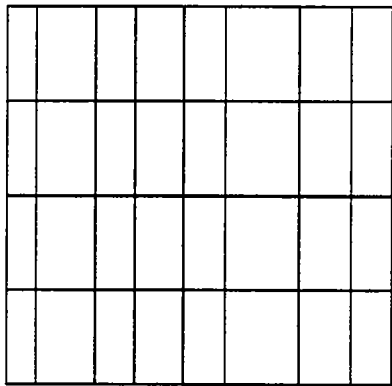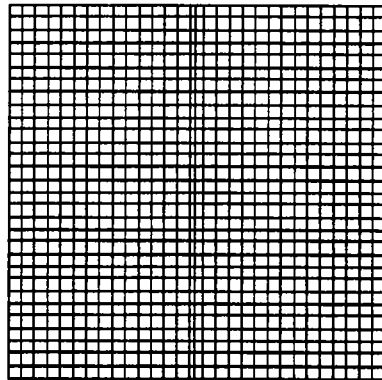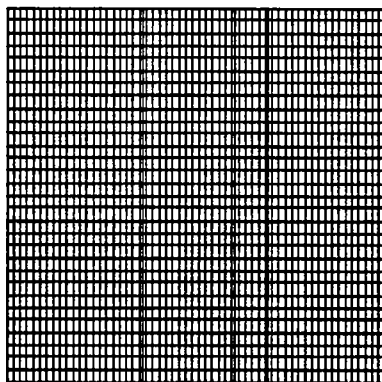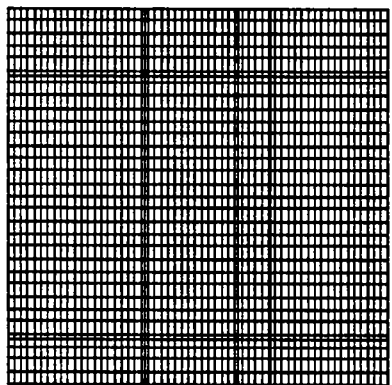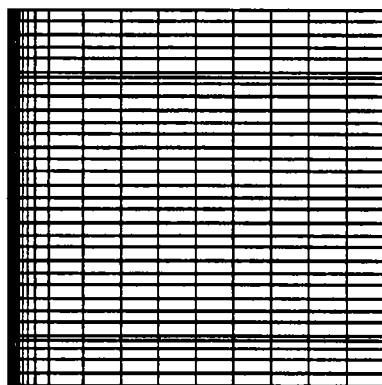
Figure 2. *Six grids used in the experiments*

FUNCTION CURVES IN THE TWO—PHASE RATIONAL APPROXIMATION

Figure 3. *Function curves in the two-phase rational approximation for* M_R, *grid 2 with* $m_1 = m_2 = 14$

FUNCTION CURVES IN THE TWO—PHASE RATIONAL APPROXIMATION

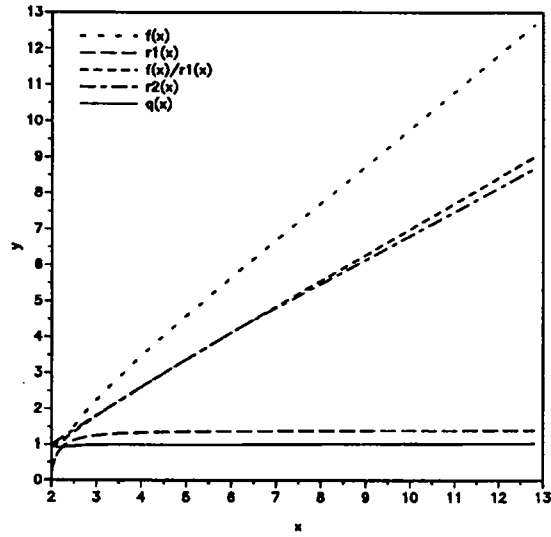**Figure 4.** *Function curves in the two-phase rational approximation for* $M_{R'}$, *grid 2 with* $m_1 = m_2 = 14$

FUNCTION CURVES IN THE TWO-PHASE RATIONAL APPROXIMATION

Figure 5. *Function curves in the two-phase rational approximation for M_R, grid 2 with $m_1 = 2, m_2 = 24$*
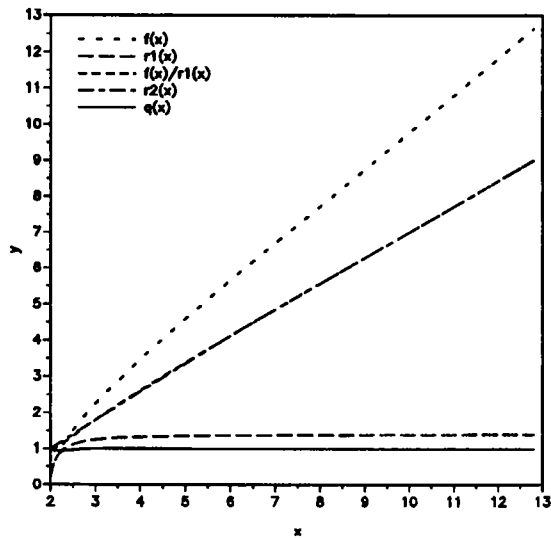
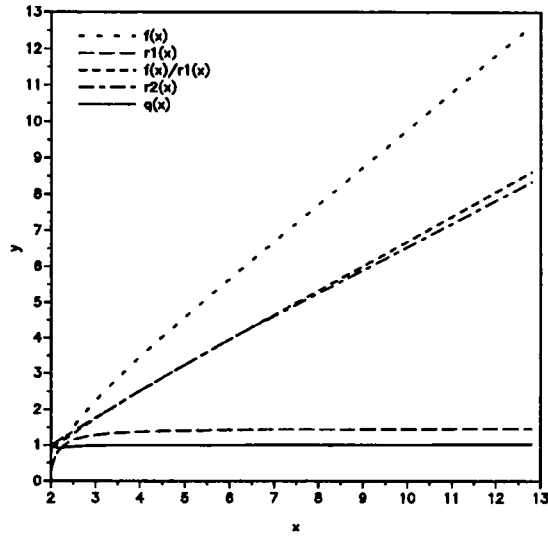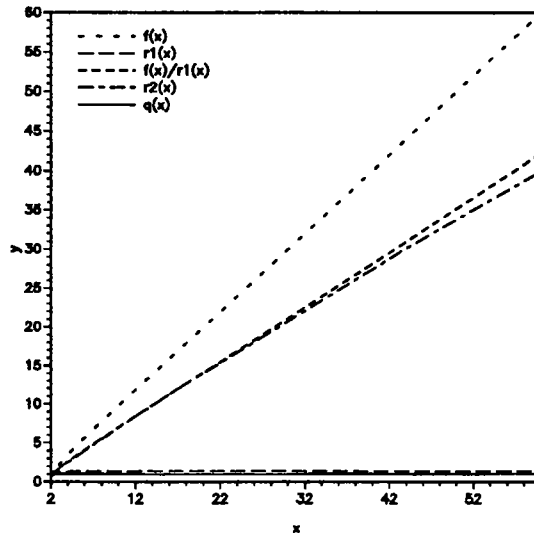FUNCTION CURVES IN THE TWO-PHASE RATIONAL APPROXIMATION

Figure 6. *Function curves in the two-phase rational approximation for M_R, grid 4 with $m_1 = m_2 = 14$*

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Table 1

Convergence performance of preconditioners, k is the number of iterations, κ is the condition number of the preconditioned system.

	M_R	M_D	M_G	M_B	M_C	M_L	$M_{R'}$	I
Grid 1, $m_1 = 1$, $m_2 = 1$								
k	3	8	7	7	7	4	3	7
κ	1.023	2.271	1.941	2.018	2.018	1.404	1.049	9.286
Grid 2, $m_1 = 14$, $m_2 = 14$								
k	4	7	6	6	6	11	3	19
κ	1.113	2.323	1.866	1.882	1.882	8.688	1.076	34.78
Grid 2, $m_1 = 4$, $m_2 = 24$								
k	4	7	6	8	6	10	4	18
κ	1.107	2.267	1.854	2.275	1.905	6.125	1.070	24.62
Grid 3, $m_1 = 14$, $m_2 = 14$								
k	4	11	10	12	12	12	4	24
κ	1.208	5.322	4.309	6.461	6.461	8.722	1.091	70.24
Grid 4, $m_1 = 14$, $m_2 = 14$								
k	4	15	13	13	13	12	4	44
κ	1.111	6.850	5.419	5.555	5.555	8.750	1.124	188.5
Grid 5, $m_1 = 14$, $m_2 = 16$								
k	5	14	12	11	11	13	5	38
κ	1.201	5.916	4.576	4.678	4.520	9.903	1.156	158.1
Grid 6, $m_1 = 14$, $m_2 = 16$								
k	failed	failed	failed	failed	failed	14	5	failed
κ	*	*	*	*	*	9.982	1.164	*

approach can also be extended to more general cases.

As far as the computation complexity is concerned for each preconditioning step, $M_{R'}$, M_R and M_L are all of the order of $O(n)$, while all the $K^{1/2}$-family of preconditioners are of $O(n \log n)$. Therefore, the three new preconditioners $M_{R'}$, M_R and M_L constructed from our new approach are in general superior to the $K^{1/2}$-family of preconditioners in both efficiency and effectiveness.

7. Conclusions. This paper presents a new approach for the domain decomposition -based *PCG* methods. A new family of preconditioners is constructed through variants of function approximation. The eigendecomposition theory for the Schur complement is extended to the nonuniform grid case. By applying the rational approximation to this theory, we show that the new approach is very simple, effective, and stable.

This approach can be further extended to more general cases, such as, complicated operators, geometries, decompositions, discretizations and so on. In general, one can expect that S is spectrally equivalent, or nearly equivalent, to a simple interface matrix that corresponds to a second order elliptic operator on the interface Γ. One can see this from the experiments on grid 5 and grid 6, where the rigorous theory in Section 4 does not apply. This is also supported by the observation of Bramble, Pasciak and Schatz [3] that the Schur complement corresponds to a norm in the trace space $H^{1/2}(\Gamma)$. We outline this reasoning and, for simplicity, we do not distinguish a continuous operator

with its discrete counterpart. From the Sobolev space interpolation theory, $H^{1/2}(\Gamma)$ is the interpolation of two spaces $H^0(\Gamma)$ and $H^1(\Gamma)$, and correspondingly, the same is true for their norms; on the other hand, the *1-D* Laplacian is a norm in $H^1(\Gamma)$. That explains why people use $K^{1/2}$-type matrices to approximate the Schur complement. But, this observation also suggests that one may use other combinations of the norms in $H^0(\Gamma)$ and $H^1(\Gamma)$, i.e., some second order elliptic operators, to approximate the Schur complement. The application of this new approach to more general cases is under investigation.

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