A Coarse Space to Remove the Logarithmic Dependency in Neumann-Neumann Methods

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1 Introduction

Domain Decomposition Methods are widely used methods for solving large linear systems that arise from the discretization of partial differential equations in parallel. The one level versions of these method are in general not scalable[1], since communication is just between neighboring subdomains, as it was pointed out already in [15], and one must add an additional coarse correction in order to share global information between subdomains. Examples of early such coarse corrections are proposed in [5, 6] for the additive Schwarz method, and in [12, 13, 14, 12, 7] for Neumann-Neumann and FETI methods, for a comprehensive treatment, see [16].

We are interested here in Neumann-Neumann methods for Laplace's equation in two spatial dimensions, for which the one level condition number κ_1 and the two-level condition number κ_2 with a piecewise constant coarse space satisfy the estimates

$$\kappa_1 \leq \frac{C}{H^2}\left(1+\log^2(\frac{H}{h})\right), \quad \kappa_2 \leq C\left(1+\log^2(\frac{H}{h})\right), \tag{1}$$

where H is the typical size of a subdomain, h is the mesh size, and the constant C is independent of h and H, see [4, 12, 13]. These condition number estimates guarantee robust convergence when Neumann-Neumann is used as a preconditioner for a Krylov method, up to the logarithmic term.

We are interested here in understanding precisely where this logarithmic term is coming from, and how it can be removed using an appropriately chosen coarse space. To this end, we study the Neumann-Neumann method directly as an iterative method, not as a preconditioner, and consider two specific decompositions: a strip

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[1] Notable exceptions are the time dependent wave equation with finite speed of propagation [8], and the Laplace equation in certain molecular simulations with specific geometry [2, 3].

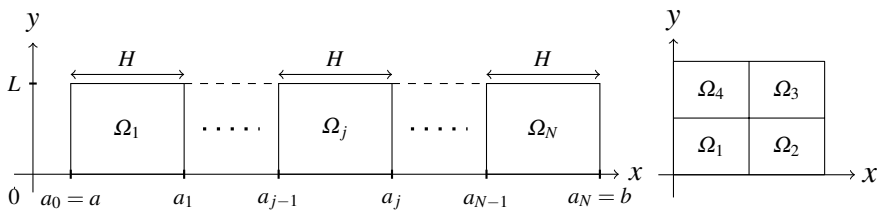

Fig. 1: Left: Strip decomposition. Right: Decomposition with a cross point

decomposition into a one dimensional sequence of subdomains, and a decomposition including a cross point, see Figure 1.

For the strip decomposition, we will show that in the case of Dirichlet boundary conditions, the one level iterative Neumann-Neumann algorithm is convergent and can be weakly scalable, even without coarse grid, for a specific setting, and there are no polylogarithmic terms in the convergence estimate. In the case of Neumann boundary conditions, a coarse space of constant functions is needed to make the Neumann-Neumann method weakly scalable, and again there are no polylogarithmic terms in the convergence estimate. For a decomposition with cross points, we show that the iterative Neumann-Neumann algorithm does not converge, due to logarithmically growing modes at the cross point, and following ideas in [9, 11, 10], we enrich the coarse space with the corresponding modes to obtain a convergent iterative Neumann-Neumann algorithm without polylogarithmic growth.

2 Neumann-Neumann algorithm for a strip decomposition

We start by studying the convergence and weak scalability of the Neumann-Neumann algorithm for the Laplace equation,

$$\begin{aligned} -\Delta u &= f, \quad \text{in } \Omega, \\ u(a,\cdot) &= 0, \quad u(b,\cdot) = 0, \\ u(\cdot,0) &= 0, \quad u(\cdot,L) = 0, \end{aligned} \tag{2}$$

on the rectangular domain $\Omega := (a,b)\times(0,L)$ decomposed into strips, as shown in Figure 1 on the left, where $a_j = a + jH$ for $j = 0,\ldots,N$, and $\Omega_j := (a_{j-1},a_j)\times(0,L)$ for $j = 1,\ldots,N$. Given an initial guess g_j^0 at the interfaces, where we define $g_0^n = g_N^n = 0$ for convenience, the Neumann-Neumann algorithm computes for iteration index $n = 0,1,\ldots$ first solutions of the Dirichlet problems

$$\begin{aligned} -\Delta u_j^n &= f_j \quad \text{in } \Omega_j, \\ u_j^n(a_{j-1},\cdot) = g_{j-1}^n,\ u_j^n(a_j,\cdot) &= g_j^n, \end{aligned} \tag{3}$$

with outer boundary conditions $u_j^n(\cdot,0) = u_j^n(\cdot,L) = 0$, followed by solving Neumann problems on interior domains Ω_j, $j = 2,3,\ldots,N-1$, given by

$$\begin{aligned} -\Delta \psi_j^n &= 0 \quad \text{in } \Omega_j, \\ \partial_x \psi_j^n(a_{j-1},\cdot) &= (\partial_x u_j^n(a_{j-1},\cdot) - \partial_x u_{j-1}^n(a_{j-1},\cdot))/2, \\ \partial_x \psi_j^n(a_j,\cdot) &= (\partial_x u_j^n(a_j,\cdot) - \partial_x u_{j+1}^n(a_j,\cdot))/2, \end{aligned} \tag{4}$$

and on the left and right most subdomains the Neumann problems are

$$\begin{aligned} -\Delta \psi_1^n &= 0 \quad \text{in } \Omega_1, \\ \psi_1^n(a,\cdot) &= 0, \quad \partial_x \psi_1^n(a_1,\cdot) = (\partial_x u_1^n(a_1,\cdot) - \partial_x u_2^n(a_1,\cdot)/2, \\ -\Delta \psi_N^n &= 0 \quad \text{in } \Omega_N, \\ \psi_N^n(b,\cdot) &= 0, \quad \partial_x \psi_N^n(a_{N-1},\cdot) = (\partial_x u_N^n(a_{N-1},\cdot) - \partial_x u_{N-1}^n(a_{N-1},\cdot))/2, \end{aligned}$$

all with outer boundary conditions $\psi_j^n(\cdot,0) = 0$ and $\psi_j^n(\cdot,L) = 0$, $j = 1,\ldots,N$. The new interface traces are then obtained by the updating formula

$$g_j^{n+1} := g_j^n - (\psi_j^n(a_j,\cdot) + \psi_{j+1}^n(a_j,\cdot))/2, \quad j = 1,\ldots,N-1. \tag{5}$$

To study the convergence of this iterative Neumann-Neumann method, it suffices by linearity to apply the algorithm to Equation (2) with $f = 0$, and to study the convergence of the approximate solution u^n to the zero solution. Since the subdomains are rectangles, the iterates can be expanded in a sine series,

$$u_j^n(x,y) = \sum_{m=1}^{\infty} \widehat{u}_j^n(x,m)\sin(k_m y), \quad \psi_j^n(x,y) = \sum_{m=1}^{\infty} \widehat{\psi}_j^n(x,m)\sin(k_m y), \tag{6}$$

where $k_m := \frac{m\pi}{L}$, which allows us to study the convergence based on the Fourier coefficients.

Lemma 1. *Let* $\widehat{\boldsymbol{u}}^n(m) = \left[\widehat{u}_1^n(a_1,m), \widehat{u}_2^n(a_2,m), \ldots, \widehat{u}_{N-1}^n(a_{N-1},m)\right]^T \in \mathbb{R}^{N-1}$, *then for*[2] $N \geq 3$ *we have* $\widehat{\boldsymbol{u}}^n(m) = T(m,H)\widehat{\boldsymbol{u}}^{n-1}(m)$, *where* $T(m,H) \in \mathbb{R}^{(N-1)\times(N-1)}$ *is given by*

$$T(m,H) = -\frac{1}{4\sinh^2(k_m H)} \begin{bmatrix} 1 & \frac{1}{\cosh(k_m H)} & -1 & 0 & \cdots & \cdots & 0 \\ 0 & 2 & 0 & -1 & \ddots & & \vdots \\ -1 & 0 & 2 & 0 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 2 & 0 & -1 \\ \vdots & & \ddots & -1 & 0 & 2 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & \frac{1}{\cosh(k_m H)} & 1 \end{bmatrix}.$$

[2] For $N = 2$ the structure of $T(m,H)$ is not the same since there are no inner subdomains.

Proof. For each $m \geq 1$ and $j = 2, \ldots, N-1$, $u_j^n(x,m)$ and $\psi_j^n(x,m)$ satisfy

$$\begin{array}{rlrl} k_m^2 \widehat{u}_j^n - \partial_{xx} \widehat{u}_j^n = 0, & & k_m^2 \widehat{\psi}_j^n - \partial_{yy} \widehat{\psi}_j^n = 0, & \\ \widehat{u}_j^n(a_{j-1},m) = \widehat{g}_{j-1}^n(m), & & \widehat{\psi}_j^n(a_{j-1},m) = (\partial_x u_j^n(a_{j-1},m) - \partial_x u_{j-1}^n(a_{j-1},m))/2, & \\ \widehat{u}_j^n(a_j,m) = \widehat{g}_j^n(m), & & \widehat{\psi}_j^n(a_j,m) = (\partial_x u_j^n(a_j,m) - \partial_x u_{j+1}^n(a_j,m))/2. & \end{array}$$

The solution of the Dirichlet problems on interior subdomains are thus

$$\widehat{u}_j^n(x,m) = \widehat{g}_j^n(m) \frac{\sinh(k_m(x-a_{j-1}))}{\sinh(k_m H)} + \widehat{g}_{j-1}^n(m) \frac{\sinh(k_m(a_j - x))}{\sinh(k_m H)}, \ j = 2, \ldots, N-1,$$

and on the subdomains on the left and right we get

$$\widehat{u}_1^n(x,m) = \widehat{g}_1^n(m) \frac{\sinh(k_m(x-a_0))}{\sinh(k_m H)}, \quad \widehat{u}_N^n(x,m) = \widehat{g}_{N-1}^n(m) \frac{\sinh(k_m(a_N - x))}{\sinh(k_m H)}.$$

Similarly for the Neumann problems on the interior subdomains, we obtain

$$\begin{aligned} \widehat{\psi}_j^n(x,m) = & \left(2\,\widehat{g}_j^n(m) \frac{\cosh(k_m H)}{\sinh(k_m H)} - \frac{\widehat{g}_{j-1}^n(m)}{\sinh(k_m H)} - \frac{\widehat{g}_{j+1}^n(m)}{\sinh(k_m H)} \right) \frac{\cosh(k_m(x-a_{j-1}))}{2\sinh(k_m H)} \\ & + \left(2\,\widehat{g}_{j-1}^n(m) \frac{\cosh(k_m H)}{\sinh(k_m H)} - \frac{\widehat{g}_{j-2}^n(m)}{\sinh(k_m H)} - \frac{\widehat{g}_j^n(m)}{\sinh(k_m H)} \right) \frac{\cosh(k_m(a_j - x))}{2\sinh(k_m H)}, \end{aligned}$$

and for the first and last subdomains we find

$$\begin{aligned} \widehat{\psi}_1^n(x,m) &= \left(2\,\widehat{g}_1^n(m) \frac{\cosh(k_m H)}{\sinh(k_m H)} - \frac{\widehat{g}_2^n(m)}{\sinh(k_m H)} \right) \frac{\sinh(k_m(x-a_0))}{2\cosh(k_m H)}, \\ \widehat{\psi}_N^n(x,m) &= \left(2\,\widehat{g}_{N-1}^n(m) \frac{\cosh(k_m H)}{\sinh(k_m H)} - \frac{\widehat{g}_{N-2}^n(m)}{\sinh(k_m H)} \right) \frac{\sinh(k_m(a_N - x))}{2\cosh(k_m H)}. \end{aligned}$$

Using now (5) and the fact that $\widehat{u}_j^n(a_j,m) = \widehat{g}_j^n(m)$ for each $m \geq 1$, we get the stated recurrence relation.

Lemma 2. *If $H/L > \ln(1+\sqrt{2})/\pi$ then for any $m \geq 1$ we have $\|T(m,H)\|_\infty < 1$.*

Proof. It is straightforward to see that $\|T(m,H)\|_\infty \leq \frac{1}{\sinh^2(k_m H)}$ for each m and since $m \mapsto \frac{1}{\sinh^2(k_m H)}$ is strictly decreasing for $m \geq 1$, we have that $\frac{1}{\sinh^2(k_m H)} < \frac{1}{\sinh^2(k_1 H)}$ which is strictly smaller than 1 if $H/L > \ln(1+\sqrt{2})/\pi$, which concludes the proof.

Theorem 1. *For $N \geq 3$, the Neumann-Neumann method satisfies the L^2 error bound*

$$\left(\sum_{j=1}^{N-1} \|u_j^n(a_j,\cdot)\|_2^2 \right)^{1/2} \leq \frac{1}{\sinh^{2n}(k_1 H)} \left(\sum_{j=1}^{N-1} \|u_j^0(a_j,\cdot)\|_2^2 \right)^{1/2}.$$

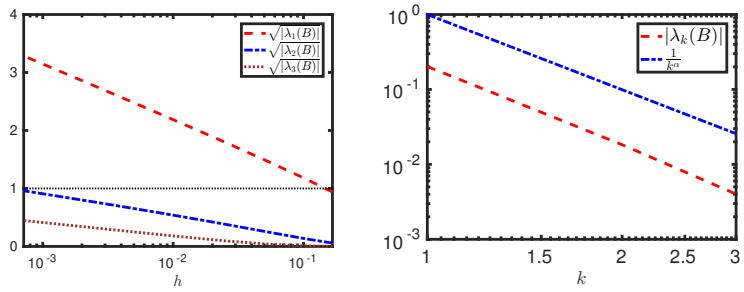

Fig. 2: Left: dependence of $\sqrt{|\lambda_k(B)|}$, $k = 1,\ldots,3$ on the mesh size h in semi-log scale. Right: dependence of the semi-log scale slope of $|\lambda_k(B)|$, $k = 1,\ldots,3$ on k, with $\alpha := \frac{10}{3}$.

Proof. Since for $N \geq 3$ we have that $\|T(m,H)\|_2 \leq \sqrt{\|T(m,H)\|_\infty \|T(m,H)\|_1} \leq \frac{1}{\sinh^2(k_1 H)}$, and using the Parseval identity $\|u_j^n(a_j,\cdot)\|_2^2 = \frac{L}{2}\sum_{m=1}^{\infty} \widehat{u}_i^n(a_j,m)^2$, we get the result stated.

Theorem 1 shows that under a minimal assumption, the one level Neumann-Neumann algorithm for the strip decomposition is weakly scalable, provided H remains fixed, i.e. more and more subdomains of the same size are added, see also [2, 3] for the corresponding Schwarz scaling. If the original Laplace problem (2) has however Neumann conditions at $y = 0$ and $y = L$, then the interior subdomains become floating in the Neumann-Neumann algorithm, and a minimal coarse space consisting of piecewise constant functions is required in order to remove the kernel, and this is sufficient to make the algorithm weakly scalable as in the previous case with an L^2 bound as in Theorem 1, see [1].

3 Neumann-Neumann algorithm with cross points

We now study the convergence properties of the iterative Neumann-Neumann algorithm for decompositions with cross points, like the one shown in Figure 1 on the right. Since in this case the algorithm might not be well defined at the continuous level due to discontinuities at the cross point, we study numerically the convergence of the fixed point iteration

$$\mathbf{u}_{n+1} = B\mathbf{u}_n + \mathbf{f}, \tag{7}$$

where $B \in \mathbb{R}^{d\times d}$ and $\mathbf{f} \in \mathbb{R}^d$ are obtained by discretizing the Neumann-Neumann algorithm using a standard five-point finite difference discretization. We first show in Figure 2 on the left the three largest (double) eigenvalues in modulus of B when the mesh is refined. We clearly see logarithmic growth, and the iterative Neumann-Neumann method will diverge as soon as the mesh size h is small enough, in our example $h = 0.12$. Hence, in contrast to the classical alternating and parallel Schwarz

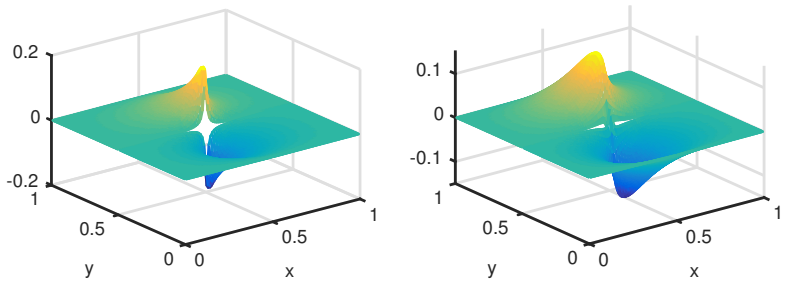

Fig. 3: Left: dominant eigenmode of B. Right: second eigenmode of B.

methods, the Neumann-Neumann method can then not be used as an iterative solver. We note however also that the logarithmic growth of the first dominant eigenvalue is faster than the second and the third one. On the right in Figure 2, we show how the growth rate (the slope) of these diverging modes depends on the eigenvalue index k. We see that the growth decays very rapidly, like $1/k^{\alpha}$ with $\alpha = 10/3$, so when h goes to zero, there are only $O(k)$ divergent modes (those with corresponding eigenvalues greater than 1 in modulus), where $1/k^{\alpha}\log^2(h) \lesssim 1$, i.e $k \sim (\log^2(h))^{1/\alpha}$.

We next show in Figure 3 the two corresponding dominant eigenmodes of B for the mesh size $h = 0.01$. Since their eigenvalues are double eigenvalues, we chose from the two dimensional subspace of eigenmodes the one vanishing at the interface aligned with the x axis; the other eigenmode has the same shape, just rotated by 90 degrees. We see that the cross point causes the iterative Neumann-Neumann method to generate eigenmodes with a singular behavior at the cross point, and these modes lead to divergence of the iterative Neumann-Neumann method.

To avoid such logarithmic growth, and obtain a convergent iterative Neumann-Neumann method, one can remove the few divergent modes using an enriched coarse space. Let F be a subspace of $\mathbb{R}^d$ and $F^{\perp}$ be its orthogonal complement with respect to the standard inner product. Then we can use the reordering

$$B = \begin{matrix} \\ F \\ F^{\perp} \end{matrix} \begin{matrix} \begin{matrix} F & F^{\perp} \end{matrix} \\ \begin{bmatrix} \widetilde{B} & C \\ G & \widehat{B} \end{bmatrix} \end{matrix}, \quad \mathbf{u} = \begin{matrix} F \\ F^{\perp} \end{matrix} \begin{bmatrix} \widetilde{\mathbf{u}} \\ \widehat{\mathbf{u}} \end{bmatrix}, \quad \mathbf{f} = \begin{matrix} F \\ F^{\perp} \end{matrix} \begin{bmatrix} \widetilde{\mathbf{f}} \\ \widehat{\mathbf{f}} \end{bmatrix}, \tag{8}$$

and the iterative Neumann-Neumann algorithm (7) becomes

$$\begin{bmatrix} \widetilde{\mathbf{u}}_{n+1} \\ \widehat{\mathbf{u}}_{n+1} \end{bmatrix} = \begin{bmatrix} \widetilde{B} & C \\ G & \widehat{B} \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{u}}_{n} \\ \widehat{\mathbf{u}}_{n} \end{bmatrix} + \begin{bmatrix} \widetilde{\mathbf{f}} \\ \widehat{\mathbf{f}} \end{bmatrix}. \tag{9}$$

To correct the problem of the divergent modes, we propose to use the iteration

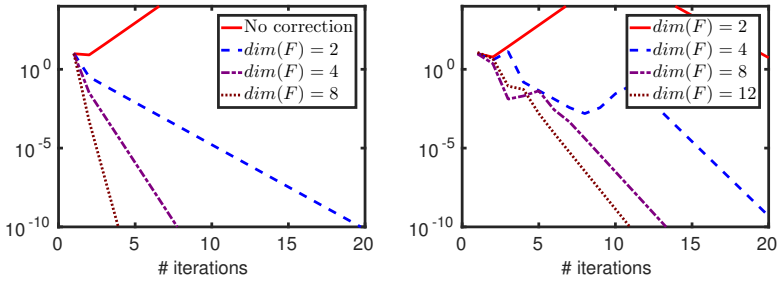

Fig. 4: Left: error of iteration (10) for different dimensions of F. Right: same, but using orthogonal iteration to approximate F.

$$\widehat{\mathbf{u}}_{n+1} = \widehat{B}\widehat{\mathbf{u}}_n + \widehat{\mathbf{f}} + G\widetilde{\mathbf{u}}_n, \tag{10a}$$

$$(I - \widetilde{B})\widetilde{\mathbf{u}}_{n+1} = C\widehat{\mathbf{u}}_{n+1} + \widetilde{\mathbf{f}}, \tag{10b}$$

where (10b) is solved exactly.

Theorem 2. *If F is spanned by all eigenmodes of B corresponding to eigenvalues greater or equal to 1 in modulus, then iteration (10) converges for any $\mathbf{u}_0 \in \mathbb{R}^d$.*

Proof. From (10), we obtain

$$\widehat{\mathbf{u}}_{n+1} = (\widehat{B} + G(I - \widetilde{B})^{-1}C)\widehat{\mathbf{u}}_n + \widehat{\mathbf{f}} + G(I - \widetilde{B})^{-1}\widetilde{\mathbf{f}},$$
$$\widetilde{\mathbf{u}}_{n+1} = (I - \widetilde{B})^{-1}(C\widehat{\mathbf{u}}_{n+1} + \widetilde{\mathbf{f}}),$$

and hence the method is convergent iff $\rho(\widehat{B} + G(I - \widetilde{B})^{-1}C) < 1$. Since F is spanned by the divergent eigenmodes of B we have that G is zero and the condition for convergence becomes $\rho(\widehat{B}) < 1$, which is satisfied since $\widehat{B}$ does not contain the divergent eigenmodes of B.

We show in Figure 4 on the left the error of iteration (10) as a function of the iteration number n for different choices of the dimension of F, using the same mesh size $h = 0.01$ in a semi-log scale. We see that with $\dim(F) = 2$, the iterations start already to converge while without correction the iteration diverges. Increasing the dimension of F improves convergence further. Using just orthogonal iterations to approximate F gives already satisfactory results, as shown on the right in Figure 4.

4 Conclusion

We showed that the logarithmic growth in the condition number estimate of the Neumann-Neumann method comes from modes which are generated at cross points

in the decomposition. Without cross points, the iterative Neumann-Neumann method is convergent and can be made scalable just using a constant per subdomain in the coarse space. With cross points, one can add the logarithmically divergent modes to the coarse space to obtain a convergent iterative Neumann-Neumann method, without logarithmic term in the convergence estimate. We also showed that orthogonal iteration permits already to include such modes numerically, and we are currently trying to determine appropriate coarse functions analytically.

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